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Curvature and the Petrov Canonical Forms*

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The Petrov classification for the curvature tensor of an Einstein space M^4 is related to the critical-point theory of the sectional-curvature function σ, regarded as a function on the manifold of nondegenerate tangent 2-planes at each point of the space. It is shown that the Petrov type is determined by the number of critical points. Furthermore, all the invariants in the canonical form can be computed from a knowledge of the critical value and the Hessian quadratic form of σ at any single critical point.

I. INTRODUCTION

The Petrov classification[1] of spaces supporting gravitational fields is a local classification of the curvature tensor at each point m of the space–time manifold. It proceeds by an algebraic reduction of the matrix of components of the curvature tensor at m to a canonical form. The purpose of this paper is to exhibit some of the geometric content of Petrov's classification and in particular to obtain a geometric interpretation of the invariants in the canonical forms.

The geometric concept which we shall use is that of the sectional curvature σ regarded as a function on the manifold of nondegenerate tangent 2-planes at m. We shall show that the Petrov classification reflects the critical-point behavior of the function σ. More precisely, the Petrov type is determined by the number of critical points of σ. Furthermore, half of the invariants which appear in the canonical forms are critical values of σ, and all the invariants can be computed from a knowledge of the critical value and the Hessian quadratic form of σ at any single critical point.

We include, in Sec. III, a derivation of the canonical forms. This derivation is essentially a variation on Petrov's,[2] but its use of the Hodge star operator to make the space of bivectors at m into a complex vector space considerably simplifies the computations. We also include as a postscript a proof that the sectional curvature cannot in general be extended to be a continuous function on the manifold of all tangent 2-planes at m.

II. GEOMETRIC PRELIMINARIES

Let M^4 be a 4-dimensional Lorentz manifold and let V denote the tangent space to M^4 at some point $m \in M^4$. Thus V is a 4-dimensional vector space provided with an inner product $\langle\ ,\ \rangle$ of signature $(+++-)$. Let Λ^2 denote the (6-dimensional) space of 2-vectors[3] of V. The space Λ^2 is equipped with its standard inner product whose value on decomposable elements is given by

$$\langle v_1 \wedge v_2, w_1 \wedge w_2 \rangle = \det [\langle v_i, w_j \rangle], \quad v_i, w_j \in V.$$

Note that, if $\{e_1, e_2, e_3, e_4\}$ is a Lorentz orthonormal basis for V, then

$$\{e_1 \wedge e_2, e_1 \wedge e_3, e_2 \wedge e_3, e_3 \wedge e_4, e_4 \wedge e_2, e_1 \wedge e_4\} \quad (1)$$

is an orthonormal basis for Λ^2. In particular, the inner product on Λ^2 has signature $(+++---)$. We shall refer to a basis of type (1) as a *Lorentz basis* for Λ^2.

Let $G_\pm$ denote the submanifolds of Λ^2 consisting of all decomposable 2-vectors of length ± 1. Then G_+ (respectively, G_-) can be identified with the set of all spacelike (respectively, timelike) oriented 2-dimensional linear subspaces of V by $v \wedge w \leftrightarrow P$ where P is the oriented subspace of V generated by $\{v, w\}$. If, under this identification, we set $P_1 = e_1 \wedge e_2$, $P_2 = e_1 \wedge e_3$, and $P_3 = e_2 \wedge e_3$, then the Lorentz basis (1) for Λ^2 is of the form

$$\{P_1, P_2, P_3, P_1^\perp, P_2^\perp, P_3^\perp\}, \quad (1')$$

where, for $P \in G_+ \cup G_-$, $P^\perp$ is the oriented orthogonal complement of P in V. Here we are assuming that V is given a definite orientation and that the basis $\{e_1, \cdots, e_4\}$ for V is compatible with that orientation. Note that $G_+ \cup G_-$ consists of all nondegenerate 2-dimensional oriented subspaces of V; that is, those 2-dimensional oriented subspaces P of V such that the restriction to P of the inner product of V is a nonsingular inner product on P.

Given an orientation on V, there is defined on Λ^2 another element of structure, the star operator $*\ .\ *$ is the self-adjoint linear operator on Λ^2 defined by the

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[1] A. Z. Petrov, Sci. Trans. Kazan State Univ. **114**, 55 (1954). An English translation of this article, by M. Karweit of the Jet Propulsion Laboratory, is available from the OTS Clearinghouse, Springfield, Va. 22151. See also A. S. Petrow (Petrov), *Einstein-Räume* (Akademie-Verlag, Berlin, 1964).

[2] See also M. Cahen, R. Debever, and L. Defrise, J. Math. & Mech. **16**, 761 (1967).

[3] For definitions and basic properties, see, e.g., A. I. Mal'cev, *Foundations of Linear Algebra* (W. H. Freeman and Co., San Francisco, 1963), Chap. 8.

formula $\xi \wedge \eta = \langle \xi, *\eta \rangle \omega$ ($\xi, \eta \in \Lambda^2$), where ω is the generator for the 1-dimensional space Λ^4 of 4-vectors of V given by $\omega = e_1 \wedge \cdots \wedge e_4$, $\{e_1, \cdots, e_4\}$ being any Lorentz-orthonormal basis for V compatible with the orientation of V. Geometrically, $*$ is the operator on Λ^2 such that, for $P \in \mathbf{G}_+ \cup G_-$, $*P = -\epsilon(P)P^\perp = \epsilon(P^\perp)P^\perp$ where ϵ is the function defined on $G_+ \cup G_-$ by $\epsilon(P) = \langle P, P \rangle = \pm 1$. In particular, note that $*: G_\pm \to G_\mp$ and that $*^2 = -$identity. The matrix for $*$ relative to a Lorentz basis (1) for Λ^2 is given by

$$[*] = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \tag{2}$$

where I denotes the 3×3 identity matrix.

Using the operator $*$, the vector space Λ^2 may be regarded as a complex 3-dimensional vector space as follows: for $\xi \in \Lambda^2$ and $a + ib$ a complex number, we set $(a + ib)\xi = a\xi + b*\xi$. Moreover, the complex-valued symmetric bilinear form g, defined on Λ^2 by

$$g(\xi, \eta) = \langle \xi, \eta \rangle - i\langle \xi, *\eta \rangle, \tag{3}$$

makes Λ^2 into a complex Euclidean space. Given a Lorentz basis (1′) for Λ^2, the set $\{P_1, P_2, P_3\}$ is then a basis for the complex space Λ^2 which is g orthonormal.

This complex Euclidean structure on Λ^2 enables us to give a simple description of the submanifolds $G_\pm$. The condition $\xi \wedge \xi = 0$, or equivalently $\langle \xi, *\xi \rangle = 0$, is well known[4] to be a necessary and sufficient condition that $\xi \in \Lambda^2$ be decomposable. It follows that $\xi \in \Lambda^2$ is decomposable if and only if $g(\xi, \xi)$ is real, and $\xi \in G_\pm$ if and only if $g(\xi, \xi) = \pm 1$.

One important consequence of this description of G_+ is the following:

Lemma: Suppose $\{\xi_1, \xi_2, \xi_3\}$ is a g-orthonormal set in Λ^2. Then $\xi_j \in G_+$ for each j and, moreover, a Lorentz basis (1′) for Λ^2 is obtained by setting $P_j = \pm \xi_j$ ($j = 1, 2, 3$) where any two (and perhaps all three) of the signs $\pm$ may be taken to be $+$.

Proof: Let $P_j = \xi_j$ ($j = 1, 2, 3$). By the above remarks, $P_j \in G_+$ for each j. Since $P_j^\perp = -*P_j$, the Lorentz orthonormality in Λ^2 of the set (1′) so obtained is immediate from the definition (3) of g. Now we would like to construct a Lorentz orthonormal basis $\{e_1, \cdots, e_4\}$ for V such that $P_1 = e_1 \wedge e_2$, $P_2 = e_1 \wedge e_3$, and $P_3 = e_2 \wedge e_3$. Since $\langle P_1, *P_2 \rangle = 0$, we have $P_1 \wedge P_2 = 0$ and hence there exists a nonzero vector e_1 in $P_1 \cap P_2$, which we may take to be a unit vector. Let e_2 and e_3 be unit vectors such that $\langle e_1, e_2 \rangle = \langle e_1, e_3 \rangle = 0$ and $e_1 \wedge e_2 = P_1, e_1 \wedge e_3 = P_2$. Then $\langle e_2, e_3 \rangle = \langle P_1, P_2 \rangle = 0$ also. Completing a Lorentz orthonormal basis $\{e_1, \cdots, e_4\}$ for V, we have $P_3 = \sum a_{jk} e_j \wedge e_k$ for real a_{jk} with $a_{kj} = -a_{jk}$, and the orthogonality relations on the $\xi_j = P_j$ imply that in fact $P_3 = \pm e_2 \wedge e_3$.

If $P_3 = +e_2 \wedge e_3$, we are done. If $P_3 = -e_2 \wedge e_3$, then clearly setting $P_3 = -\xi_3$ at the beginning would have corrected the situation. However we could as well have set $P_1 = -\xi_1$ and followed the above procedures thereby negating the vector e_2 obtained, or we could have set $P_2 = -\xi_2$ thereby negating the vector e_3 obtained. In any case, an appropriate basis for V is obtained and the proof is complete.

Remark: The action of the Lorentz group of V on V induces an action of this group on Λ^2 as a group of complex rotations; that is, the natural induced action of the Lorentz group of V on Λ^2 defines a representation of the Lorentz group $O(3, 1)$ in the complex rotation group $SO(3, \mathbb{C})$. Upon restriction, this representation gives an isomorphism of the proper Lorentz group onto $SO(3, \mathbb{C})$. The reason that the one possible negative sign in the above lemma cannot be avoided is that negating a basis element is not a complex rotation and so this operation on Λ^2 cannot be induced by a change of Lorentz basis in V.

III. THE PETROV TYPES

Let R denote the curvature tensor at the point m of the Lorentz manifold M^4. We shall regard R as a self-adjoint linear operator on Λ^2. Explicitly, R is the linear operator such that

$$\langle e_i \wedge e_j, R(e_k \wedge e_l) \rangle = R_{ijkl},$$

where R_{ijkl} are the components of the curvature tensor relative to the basis $\{e_1, \cdots, e_4\}$ for V. In the usual discussions of Petrov types, the curvature tensor is regarded as a quadratic (i.e., symmetric bilinear) form on Λ^2; we shall denote this quadratic form by Q. Q and R are related by the formula

$$\langle \xi, R(\eta) \rangle = Q(\xi, \eta), \quad \xi, \eta \in \Lambda^2.$$

Note that, although the matrix $[Q]$ for Q relative to a Lorentz basis (1′) is symmetric, the matrix $[R]$ for R relative to this basis is not. Since the (i, j) entry of $[R]$ is $\epsilon(P_i)$ times the (i, j) entry of $[Q]$, these matrices are related as follows:

$$[Q] = \begin{bmatrix} A & B \\ B^{\mathrm{T}} & C \end{bmatrix} \Leftrightarrow [R] = \begin{bmatrix} A & B \\ -B^{\mathrm{T}} & -C \end{bmatrix}. \tag{4}$$

Here A, B, and C are 3×3 matrices with A and C symmetric.

[4] See Ref. 3, p. 281, problem 3.

The first step in Petrov's derivation of his canonical forms is the observation that, if M^4 is an Einstein space, i.e., if the Einstein field equations (expressing the condition that the Ricci tensor of M^4 be a scalar multiple of the metric tensor) are satisfied, then the matrix for the quadratic form Q relative to a Lorentz basis for Λ^2 is of the form

$$[Q] = \begin{bmatrix} A & B \\ B & -A \end{bmatrix}, \tag{5}$$

where A and B are symmetric. Conversely, it is easy to check that if $[Q]$ is of the form (5) at each point then M^4 is an Einstein space. By (4), condition (5) on $[Q]$ is the same as the following condition on $[R]$:

$$[R] = \begin{bmatrix} A & B \\ -B & A \end{bmatrix}, \tag{6}$$

where A and B are symmetric. But a matrix $[R]$ of the form (4) is of the form (6) if and only if it commutes with the matrix $[*]$ of Eq. (2). Thus *M^4 is an Einstein space if and only if the linear operators $*$ and R commute*; that is, if and only if $*R = R*$. Equivalently, since $*^2 = -$identity, M^4 is Einstein if and only if

$$*R* = -R. \tag{7}$$

(Note that, although the star operator is defined in terms of an orientation on V, a change of orientation merely replaces $*$ by its negative so this condition is independent of any orientation on V.) In terms of the complex Euclidean structure on Λ^2 described in the previous section, this characterization takes the following form: *M^4 is Einstein if and only if $R: \Lambda^2 \to \Lambda^2$ is complex linear.*

The standard classification of symmetric transformations of complex Euclidean spaces now leads to Petrov's classification.

Theorem (Petrov): The curvature tensor at a point m of an Einstein space is of one of three possible types: there exists a Lorentz basis (1) for the space Λ^2 of 2-vectors at m such that the matrix for R relative to this basis is of the form

$$[R] = \begin{bmatrix} A & B \\ -B & A \end{bmatrix},$$

where, according to the type of R, the matrices A and B are of the form

Type I:

$$A = \begin{bmatrix} \alpha_1 & & \\ & \alpha_2 & \\ & & \alpha_3 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_1 & & \\ & \beta_2 & \\ & & \beta_3 \end{bmatrix},$$

$$\sum \beta_j = 0.$$

Type II:

$$A = \begin{bmatrix} \alpha_1 & & \\ & \alpha_2 + 1 & \\ & & \alpha_2 - 1 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_1 & 0 & 0 \\ 0 & \beta_2 & 1 \\ 0 & 1 & \beta_2 \end{bmatrix},$$

$$\beta_1 + 2\beta_2 = 0.$$

Type III:

$$A = \begin{bmatrix} \alpha & 1 & 0 \\ 1 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}.$$

Proof: According to standard normal-form theory, there exists a basis $\{\xi_1, \xi_2, \xi_3\}$ for Λ^2 (as a complex vector space) such that the matrices $[g]$ for g and $[R]$ for R relative to this basis are simultaneously cast into one of the following forms:

Type I:

$$[g] = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}, \quad [R] = \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{bmatrix},$$

Type II:

$$[g] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad [R] = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & \gamma \\ 0 & 0 & \lambda_2 \end{bmatrix},$$

Type III:

$$[g] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad [R] = \begin{bmatrix} \lambda & \gamma & 0 \\ 0 & \lambda & \gamma \\ 0 & 0 & \lambda \end{bmatrix},$$

where γ may be taken to be any nonzero complex member.[5] For our purposes, γ will be taken to be real.

For each type, an appropriate Lorentz basis for Λ^2 is obtained from $\{\xi_1, \xi_2, \xi_3\}$ as follows:

Type I: $\{\xi_1, \xi_2, \xi_3\}$ is a g-orthonormal set in Λ^2. By the lemma of the previous section we obtain a Lorentz basis for Λ^2 by setting $P_1 = \xi_1$, $P_2 = \xi_2$, and $P_3 = \pm\xi_3$ for some appropriate choice of sign. Defining the real numbers α_j and β_j by $\lambda_j = \alpha_j + i\beta_j$ we find

$$RP_j = (\alpha_j + i\beta_j)P_j = \alpha_j P_j + \beta_j * P_j$$
$$= \alpha_j P_j - \beta_j P_j^{\perp}, \quad j = 1, 2, 3,$$

and hence the matrix for R relative to this Lorentz basis is of the required form. The condition $\sum \beta_j = 0$ is just the algebraic Bianchi identity.

[5] See Ref. 3, pp. 228–230. Although, in Mal'cev's book, the superdiagonal elements in the Jordan blocks are taken to be 1's they may, by an elementary change of basis, be taken to be any preassigned nonzero complex number.

Type II: A g-orthonormal set $\{P_1, P_2, P_3\}$, defining a Lorentz basis for Λ^2, is obtained by setting

$$P_1 = \pm\xi_1, \quad P_2 = i(\xi_2 - \xi_3)/\sqrt{2}, \quad P_3 = (\xi_2 + \xi_3)/\sqrt{2}.$$

Elementary computations then show that

$$\begin{aligned} RP_1 &= \alpha_1 P_1 - \beta_1 P_1^{\perp}, \\ RP_2 &= (\alpha_2 - \gamma/2)P_2 - \beta_2 P_2^{\perp} + (\gamma/2)P_3^{\perp}, \\ RP_3 &= (\alpha_2 + \gamma/2)P_3 + (\gamma/2)P_2^{\perp} - \beta_2 P_3^{\perp}, \end{aligned} \tag{8}$$

where $\lambda_j = \alpha_j + i\beta_j$. For example,

$$\begin{aligned} RP_2 &= iR(\xi_2 - \xi_3)/\sqrt{2} = i[\lambda_2\xi_2 - (\lambda_2\xi_3 + \gamma\xi_2)]/\sqrt{2} \\ &= \lambda_2 P_2 - (i\gamma/2)(P_3 - iP_2) \\ &= (\alpha_2 - \gamma/2)P_2 + i(\beta_2 P_2 - (\gamma/2)P_3) \\ &= (\alpha_2 - \gamma/2)P_2 - \beta_2 P_2^{\perp} + (\gamma/2)P_3^{\perp}. \end{aligned}$$

Now by taking $\gamma = -2$, Eqs. (8) show that $[R]$ is of the form required for Type II. The condition $\beta_1 + 2\beta_2 = 0$ is again just the Bianchi identity.

Type III: A g-orthonormal set $\{P_1, P_2, P_3\}$, defining a Lorentz basis Λ^2, is obtained by setting

$$P_1 = (\xi_1 + \xi_3)/\sqrt{2}, \quad P_2 = \pm\xi_2, \quad P_3 = -i(\xi_1 - \xi_3)/\sqrt{2},$$

and we find

$$\begin{aligned} RP_1 &= \alpha P_1 \pm (\gamma/\sqrt{2})P_2 - \beta P_1^{\perp}, \\ RP_2 &= \pm(\gamma/\sqrt{2})P_1 + \alpha P_2 - \beta P_2^{\perp} - (\pm\gamma/\sqrt{2})P_3^{\perp}, \\ RP_3 &= \alpha P_3 - (\pm\gamma/2)P_2^{\perp} - \beta P_3^{\perp}, \end{aligned}$$

where $\lambda = \alpha + i\beta$. By the Bianchi identity, $\beta = 0$. Taking $\gamma = \pm\sqrt{2}$ (the sign being the same as that in the equation $P_2 = \pm\xi_2$), we see that $[R]$ is of the form required for Type III.

Remarks: From the above proof, the following facts are clear:

(i) The Petrov classification of a curvature tensor R depends only on the fact that it commutes with the star operator. Given any curvature tensor (not necessarily of an Einstein space), it has an invariant splitting (invariant under the action of the Lorentz group) into a sum of two "curvature tensors" (i.e., self-adjoint linear operators on Λ^2) S and A with the properties that $S* = *S$ and $A* = -*A$. Explicitly, $S = \frac{1}{2}(R - *R*)$ and $A = \frac{1}{2}(R + *R*)$. The tensor S is equal to $C + \frac{1}{6}(\mathrm{Tr}\, R)I$, where C is the Weyl conformal curvature tensor and I is the identity operator on Λ^2. It follows that, as is well known, the Petrov classification extends to arbitrary Lorentz manifolds M^4 by considering, in general, S (or equivalently C) instead of R.

(ii) The Petrov type of a curvature tensor depends only on the Jordan canonical form of the tensor (or in a non-Einstein space, of its conformal curvature tensor) regarded as a complex linear transformation on Λ^2. In particular, R is of Type I, II, or III depending on whether R has 3, 2, or 1 independent eigenvectors. In terms of the complex Euclidean structure on Λ^2, Type I is characterized by the existence of a (complex) basis of nonnull eigenvectors, Type II is characterized by the existence of exactly one independent nonnull eigenvector, and Type III by the existence of no nonnull eigenvectors.

Remark: Another concept which has proven useful[6] in the study of Petrov types is that of the "principal null directions." These directions are obtained as follows: Except when R is a scalar multiple of the identity (the constant curvature or "Type O" case), the common zeros of the complex quadratic forms $g(\xi, \xi)$ and $g(R\xi, \xi)$ form a collection of at most four complex 1-dimensional subspaces of Λ^2. Given a 2-vector ξ in one of these subspaces, the condition $g(\xi, \xi) = 0$ says that ξ is decomposable and of length zero and so represents a 2-dimensional subspace of V tangent to the light cone in V. The directions in V determined by the intersections of these 2-planes with the light cone are the principal null directions. There are at most four such directions since complex linearly dependent null 2-vectors represent planes in V intersecting the light cone in the same line.

IV. SECTIONAL CURVATURE

Henceforth we denote the tangent space to M^4 at m by $V(m)$ and the corresponding associated spaces discussed previously by $\Lambda^2(m)$, $G_+(m)$, and $G_-(m)$. The *sectional curvature* of M^4 is the real-valued function σ defined on the manifold

$$G(M) = \bigcup_{m \in M} G_+(m) \cup G_-(m)$$

of all oriented nondegenerate tangent 2-planes of M by $\sigma(P) = \epsilon(P)\langle RP, P\rangle$. Since $\sigma(-P) = \sigma(P)$ for each $P \in G(M)$, the function σ may be regarded as a function on the manifold

$$\bar{G}(M) = \bigcup_{m \in M} \bar{G}_+(m) \cup \bar{G}_-(m)$$

of unoriented planes, obtained by identifying each $P \in G(M)$ with its negative. The characterization of Einstein spaces given in the previous section can be interpreted geometrically in terms of σ.

[6] See, e.g., R. K. Sachs, *Relativity, Groups, and Topology*, C. DeWitt and B. DeWitt, Eds. (Gordon & Breach Science Publishers, Inc., New York, 1964), Lecture VIII. See also Ref. 2.

Theorem: A 4-dimensional Lorentz manifold is an Einstein space if and only if its sectional curvature σ satisfies $\sigma(P^\perp) = \sigma(P)$ for all nondegenerate tangent 2-planes P.

Proof:

$$\sigma(P^\perp) = \epsilon(P^\perp)\langle RP^\perp, P^\perp\rangle = -\epsilon(P)\langle R * P, *P\rangle$$
$$= -\epsilon(P)\langle *R * P, P\rangle$$
$$\sigma(P) = \epsilon(P)\langle RP, P\rangle = -\epsilon(P)\langle -RP, P\rangle.$$

If M^4 is Einstein, then the characterization (7) shows that $\sigma(P^\perp) = \sigma(P)$ for all $P \in G(M)$. Conversely, if $\sigma(P^\perp) = \sigma(P)$ for all $P \in G(M)$, then the above computation shows that

$$\langle *R * P, P\rangle = \langle -RP, P\rangle, \tag{9}$$

for all $P \in G(M)$; that is, the "curvature tensors" $*R*$ and $-R$ have the same sectional-curvature functions. Since both satisfy the algebraic Bianchi identity,[7] they must be the same[8] so M^4 is Einstein.

Let σ_m denote the restriction of σ to $G_+(m) \cup G_-(m)$. The following lemma will allow us to tie the sectional curvature of M^4 in with the Petrov canonical forms.

Lemma: $P \in G_+(m) \cup G_-(m)$ is a critical point of σ_m if and only if

$$RP = \alpha P - \beta P^\perp, \tag{10}$$

for some real numbers α and β. The number α is the (critical) value of σ_m at P.

Proof[9]*:* Suppose first that $P \in G_+(m)$. Let $\{e_1, \cdots, e_4\}$ be a Lorentz orthonormal basis for $V(m)$ such that $P = e_1 \wedge e_2$. Then a coordinate system of $G_+(m) \cup G_-(m)$ in a neighborhood of P is provided by the map

$$\phi: (x_1, \cdots, x_4) \to (e_1 + x_1e_3 + x_2e_4) \wedge (e_2 + x_3e_3 + x_4e_4)/\| \ \|, \tag{11}$$

where

$$\| \ \| = [(1 + x_1^2 - x_2^2)(1 + x_3^2 - x_4^2) - (x_1x_3 - x_2x_4)^2]^{\frac{1}{2}}.$$

Computing partial derivatives of $\sigma \circ \phi$ then shows that P is a critical point of σ_m if and only if $R_{kl12} = 0$ for $(k, l) \neq (1, 2)$ or $(3, 4)$; that is, if and only if

$$R(e_1 \wedge e_2) = R_{1212}e_1 \wedge e_2 - R_{3412}e_3 \wedge e_4.$$

Setting $\alpha = R_{1212}$ and $\beta = R_{3412}$ completes the proof for $P \in G_+(m)$. Clearly, $\alpha = \langle RP, P\rangle = \sigma(P)$. The proof for $P \in G_-(m)$ is similar.

For Einstein spaces, one consequence of this lemma is that if $P \in G_+(m) \cup G_-(m)$ is a critical point of σ_m then so is $P^\perp$. For, indeed,

$$RP^\perp = \epsilon(P^\perp)R*P = \epsilon(P^\perp)*RP$$
$$= \epsilon(P^\perp) * [\alpha P - \beta P^\perp] = \alpha P^\perp + \beta(P^\perp)^\perp.$$

Hence, through the operation of orthogonal complementation, spacelike and timelike critical points are paired off with one another. Thus in considering critical points of σ_m it suffices to consider only spacelike ones; that is, it suffices to consider the restriction of σ_m to $G_+(m)$. Further, for purposes of counting critical points it is convenient to regard σ_m as a function on the manifold $\bar{G}_+(m)$ of unoriented spacelike tangent 2-planes at m, since consideration of oriented planes would lead to counting each critical plane twice, once with each orientation.

Theorem: Let R be the curvature tensor at some point m in an Einstein space M^4. Let σ_m denote the sectional-curvature function regarded as a function on the manifold of unoriented nondegenerate tangent 2-planes at m. Then the Petrov type of R is determined by the number n of spacelike critical points of σ_m at m: for Type I, $n = 3$ or ∞; for Type II, $n = 1$; and for Type III, $n = 0$.

Proof: Since, in terms of the complex structure on $\Lambda^2(m)$,

$$\alpha P - \beta P^\perp = (\alpha + i\beta)P,$$

the lemma says that each critical point of σ_m in $G_+(m)$ is an eigenvector of R. Conversely, since

$$G_+(m) = \{\xi \in \Lambda^2(m) \mid g(\xi, \xi) = 1\},$$

each nonnull eigenvector of R suitably normalized is a critical point of σ_m. By Remark (ii) at the end of the previous section it then follows that R is of Type III if and only if $n = 0$ and R is of Type II if and only if $n = 1$. The only remaining possibility is for R of

[7] This Bianchi identity for a curvature tensor $R: \Lambda^2(m) \to \Lambda^2(m)$ is just $\operatorname{Tr} B = 0$ where $\begin{bmatrix} A & B \\ -B^T & C \end{bmatrix}$ is the matrix for R relative to any Lorentz basis for $\Lambda^2(m)$.

[8] The validity of Eq. (9) on nondegenerate 2-planes implies its validity on nonnull decomposable 2-vectors. Since the set of nonnull decomposable 2-vectors is dense in the set of all 2-vectors, continuity then implies the validity of (9) on all decomposable 2-vectors. The proof that these two tensors are equal then proceeds as in S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Interscience Publishers, Inc., New York, 1963), Vol. I, p. 198.

[9] For an alternate proof, using the Lagrange-multiplier techniques, see I. M. Singer and J. A. Thorpe, "The curvature of 4-dimensional Einstein spaces" (to be published).

Type I when the number of nonnull eigendirections (hence of critical points of σ_m) is 3 (or possibly infinite in the case of equal eigenvalues).

The invariants α_j and β_j which appear in the Petrov canonical forms are the real and imaginary parts of the eigenvalues of the curvature tensor. But, by the lemma, the invariants α_j may also be interpreted geometrically as the critical values of the sectional-curvature function σ_m. In order to obtain a geometric interpretation of the remaining invariants, we must consider the Hessian quadratic form of σ_m at its critical points.[10]

Suppose that R is the curvature tensor at $m \in M^4$ and that $\{e_1, \cdots, e_4\}$ is a Lorentz orthonormal basis for $V(m)$ such that $e_1 \wedge e_2$ is a critical point of σ_m. Using the coordinates given by Eq. (11), an elementary computation shows that the Hessian matrix

$$[H] = \left[\frac{\partial^2(\sigma \circ \phi)}{\partial x_i \partial x_j}\right]$$

is given by

$$[H] = 2\begin{bmatrix} (R_{2323} - R_{1212}) & -R_{2342} & -R_{2313} & (R_{3412} - R_{2314}) \\ -R_{2342} & (R_{1212} + R_{4242}) & (R_{4213} - R_{3412}) & R_{4214} \\ -R_{2313} & (R_{4213} - R_{3412}) & (R_{1313} - R_{1212}) & R_{1314} \\ (R_{3412} - R_{2314}) & R_{4214} & R_{1314} & (R_{1212} + R_{1414}) \end{bmatrix}.$$

If R is of Type I and $\{e_1, \cdots, e_4\}$ is chosen to cast

$$[R] = \begin{bmatrix} A & B \\ -B & A \end{bmatrix}$$

into canonical form

$$A = \begin{bmatrix} \alpha_1 & & \\ & \alpha_2 & \\ & & \alpha_3 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_1 & & \\ & \beta_2 & \\ & & \beta_3 \end{bmatrix},$$

this Hessian matrix becomes

$$[H] = 2\begin{bmatrix} \alpha_3 - \alpha_1 & 0 & 0 & \beta_1 - \beta_3 \\ 0 & \alpha_1 - \alpha_2 & \beta_2 - \beta_1 & 0 \\ 0 & \beta_2 - \beta_1 & \alpha_2 - \alpha_1 & 0 \\ \beta_1 - \beta_3 & 0 & 0 & \alpha_1 - \alpha_3 \end{bmatrix}.$$

Since $\sum \beta_j = 0$, all the α_j's and β_j's are determined by H and $\alpha_1 = \sigma_m(e_1 \wedge e_2)$. Curvature tensors of Type II are handled similarly and we obtain the following:

Theorem: Let R be the curvature tensor at some point of an Einstein space. Suppose R is of Type I or II. Let $P \in G_+(m)$ be a critical point of the sectional curvature σ_m. Then all the invariants in the Petrov canonical form for R can be determined from the critical value $\sigma_m(P)$ and the Hessian of σ_m at P.

For curvature tensors of Type III, the only invariant is of course the scalar curvature.

V. POSTSCRIPT

While discussing the sectional curvature of Lorentz manifolds it seems appropriate to point out that, in spite of what is said occasionally in the literature,[11] the function σ_m cannot in general be extended by continuity to the manifold of *all* tangent 2-planes at m. To the contrary, this can be done only in spaces of constant curvature.

Theorem: Suppose the sectional-curvature function σ_m of the Lorentz manifold M^4 can be extended to a continuous function on the manifold of all tangent 2-planes at $m \in M^4$. Then σ_m is constant.

Proof: Suppose $\{u, v, w\}$ is a Lorentz-orthonormal set in $V(m)$ with u and v spacelike and w timelike. For each real number t, let P_t denote the plane spanned by u and $v + tw$. Then for $t \neq \pm 1$, P_t is nondegenerate and

$$\begin{aligned}\sigma(P_t) &= \langle R(u \wedge (v + tw)), u \wedge (v + tw)\rangle/(1 - t^2) \\ &= [\langle R(u \wedge v), u \wedge v\rangle + 2t\langle R(u \wedge v), u \wedge w\rangle \\ &\qquad + t^2\langle R(u \wedge w), u \wedge w\rangle]/(1 - t^2).\end{aligned}$$

In order for this to be defined and continuous as $t \to \pm 1$, $+1$ and -1 must be roots of the numerator, and hence we must have

$$\langle R(u \wedge v), u \wedge v\rangle = -\langle R(u \wedge w), u \wedge w\rangle,$$
$$\langle R(u \wedge v), u \wedge w\rangle = 0.$$

Applying this first condition as u, v, and w run through various subsets of a Lorentz orthonormal basis $\{e_1, \cdots, e_4\}$ yields

$$R_{1212} = -R_{1414} = R_{1313} = -R_{3434} = R_{3232} = -R_{2424}.$$

[10] This is in marked contrast to the case of positive-definite metrics where there are more critical points and in fact all the invariants are determined by the critical values of σ_m. See Ref. 9.

[11] See, e.g., Ref. 1, pp. 88–90.

This implies that the sectional curvature σ_m has the same value on each of the coordinate planes $e_k \wedge e_l$; this value must then be equal to one-twelfth the scalar curvature at m. Since every nondegenerate plane is a coordinate plane in some Lorentz basis, σ_m must be constant.

Remark: Although this proof is presented in the setting of 4-dimensional Lorentz manifolds, it requires only slight modifications in order to be valid for manifolds of arbitrary dimension carrying nondefinite metrics of arbitrary signature.

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Translational Invariance Properties of a Finite One-Dimensional Hard-Core Fluid Using the Grand Canonical Ensemble*

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(Received 12 February 1968)

Translational invariance properties of the single-particle distribution function $D_1(x, L, z)$ of the grand canonical ensemble are investigated for a one-dimensional hard-core fluid. For a fluid of finite length L it is shown that $D_1(x, L, z)$ is nowhere constant. It is shown that, in the thermodynamic limit and for x far from either wall, $D_1(x, L, z)$ is a constant equal to the grand canonical density ρ.

I. INTRODUCTION

Translational invariance properties of particle distribution functions of finite one-dimensional systems have been discussed by Leff and Coopersmith.[1,2] Their work was carried out using the formalism of the canonical ensemble. In particular, Ref. 1 was devoted to a discussion of a pure hard-core fluid of N particles, with a hard-core length d. The fluid may be considered to be contained within a length L by two additional particles fixed at $-\frac{1}{2}d$ and $L + \frac{1}{2}d$.[3] The single-particle canonical distribution function at position x is denoted by $D_1^{(N)}(x, L)$. Leff and Coopersmith have shown that for a finite system there exists a central region in which $D_1^{(N)}(x, L)$ is rigorously a constant provided only that $L \geq (2N - 1)d$. No central region exists if this inequality is violated.

The single-particle distribution function in the formalism of the grand canonical ensemble is defined by

$$D_1(x, L, z) = \sum_{N=1}^{\infty} \frac{z^N Z_N(L)}{N!\, \Xi(L, z)} D_1^{(N)}(x, L). \quad (1a)$$

The fugacity z is defined by

$$z = e^{\beta\mu}/\lambda,$$

where β^{-1} is Boltzmann's constant multiplied by the absolute temperature, μ is the chemical potential, and λ is the thermal wavelength. The canonical configurational partition function is the unordered integral

$$Z_N(L) = \int_0^L dx_N \cdots \int_0^L dx_1 \exp\left[-\beta \sum_{i<j}^{N} \phi(x_j - x_i)\right] \times \exp\left[-\beta \sum_{i=1}^{N} \phi\left(x_i + \frac{d}{2}\right)\right] \times \exp\left[-\beta \sum_{i=1}^{N} \phi\left(L + \frac{d}{2} - x_i\right)\right],$$

where $\phi(x)$ is the interaction between particles. The grand canonical partition function $\Xi(L, z)$ is given by the sum

$$\Xi(L, z) = \sum_{N=0}^{\infty} \frac{z^N}{N!} Z_N(L). \quad (1b)$$

It is of interest to ask whether $D_1(x, L, z)$ has translational invariance properties similar to those of $D_1^{(N)}(x, L)$. Intuitively, one expects the answer to be no. This is based on the fact that, according to Eq. (1a), $D_1(x, L, z)$ is a linear combination of its canonical counterparts $D_1^{(N)}(x, L)$ *for all values of N but fixed L*. Thus, it is clear that some of the terms in the

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[3] With this specification of the container walls, the particle *centers* are confined to the interval $[\frac{1}{2}d, L - \frac{1}{2}d]$, or a length $L - d$. This is in contrast with the work of Refs. 1 and 2, where the particle centers were confined to an interval of length L.

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summation violate the inequality $L \geq (2N-1)d$. The $D_1^{(N)}(x, L)$'s associated with such terms are non-constant functions of x, and it is considered unlikely that their sum is a constant for certain ranges of x, z, and L. Also, while the central region encountered in the canonical ensemble has a firm physical interpretation (see the discussion in Ref. 2), it is difficult to envision a corresponding statement in terms of the grand ensemble variables.

In this paper it is shown that, in fact, the above intuitive argument is correct. In Sec. II it is proved that, for a system of finite length, $D_1(x, L, z)$ is nowhere constant. In Sec. III, a useful identity, relating $D_1(x, L, z)$ to a product of grand partition functions, is established and is used to investigate $D_1(x, L, z)$ in the thermodynamic limit. When x is "far" from both walls, it is shown that $D_1(x, L, z)$ approaches ρ, the grand canonical density. A novel calculation of the grand partition function is contained in the Appendix.

II. PROOF THAT $D_1(x, L, z)$ IS NOWHERE CONSTANT FOR A ONE-DIMENSIONAL HARD-CORE FLUID OF FINITE LENGTH

Leff and Coopersmith have shown that $D_1^{(N)}(x, L)$ can be written as[4]

$$D_1^{(N)}(x, L) = \frac{N}{Z_N(L)} \sum_{n=0}^{N-1} \binom{N-1}{n} Z_n\left(x - \frac{d}{2}\right) \times Z_{N-1-n}\left(L - x - \frac{d}{2}\right), \quad (2)$$

where the two-particle potential consists of a hard-core repulsion plus a general nearest-neighbor interaction. Now, for a hard-core fluid,

$$Z_m(\tau) = (\tau - md)^m \theta(\tau - md), \quad (3)$$

where

$$\theta(s) = \begin{cases} 1, & \text{for } s \geq 0, \\ 0, & \text{for } s < 0. \end{cases} \quad (4)$$

Using (3), Eq. (2) takes the form

$$D_1^{(N)}(x, L) = \frac{N}{Z_N(L)} \sum_{n=0}^{N-1} \binom{N-1}{n} \left[x - \left(n + \frac{1}{2}\right)d\right]^n \times \left[L - x - \left(N - 1 - n + \frac{1}{2}\right)d\right]^{N-1-n} \times \theta\left[x - \left(n + \frac{1}{2}\right)d\right] \times \theta\left[L - x - \left(N - 1 - n + \frac{1}{2}\right)d\right]^{N-1-n}, \quad (5)$$

provided $L > Nd$.

[4] Because of the present definition of container walls, the present functions $Z_n(x - \frac{1}{2}d)$ correspond to the functions $\tilde{Z}_n(x)$ of Ref. 1.

Equation (5) can be rewritten in terms of a polynomial in x, of degree $N-1$, by making two binomial expansions:

$$D_1^{(N)}(x, L) = \frac{N}{Z_N(L)} \sum_{n=0}^{N-1} \binom{N-1}{n} \left[x - \left(n + \frac{1}{2}\right)d\right]^n \times \theta\left[x - \left(n + \frac{1}{2}\right)d\right] \theta\left[L - Nd - x + \left(n + \frac{1}{2}\right)d\right] \times \sum_{j=0}^{N-1-n} (-1)^j \left[x - \left(n + \frac{1}{2}\right)d\right]^j \times (L - Nd)^{N-1-n-j} \binom{N-1-n}{j}.$$

Substituting $n + j = l$ and changing summation variables to n and l, we have

$$\sum_{n=0}^{N-1} \sum_{j=0}^{N-1-n} = \sum_{l=0}^{N-1} \sum_{n=0}^{l}.$$

Then, expanding $[x - (n + \frac{1}{2})d]^l$, we find that

$$\frac{z^N Z_N(L)}{N!\, \Xi(L, z)} D_1^{(N)}(x, L) = \sum_{m=0}^{N-1} \alpha_m^{(N)} x^m, \quad (6)$$

where

$$\alpha_m^{(N)} = \frac{z^N}{(N-1)!\, \Xi(L, z)} \sum_{l=m}^{N-1} \sum_{n=0}^{l} \binom{N-1}{l} \binom{l}{n} \times \binom{l}{m} (-1)^{m+n} \left[\left(n + \frac{1}{2}\right)d\right]^{l-m} \times (L - Nd)^{N-1-l} \theta\left[x - \left(n + \frac{1}{2}\right)d\right] \times \theta\left[L - Nd - x + \left(n + \frac{1}{2}\right)d\right]. \quad (7)$$

Thus, $D_1^{(N)}(x, L)$ is a polynomial whose coefficients are not constant and which, in general, are complicated.

It is observed, however, that the $\alpha_m^{(N)}$'s have one simplifying property: the interval $[\frac{1}{2}d, L - \frac{1}{2}d]$ can be divided into segments within which all of the $\alpha_m^{(N)}$'s are constant. To see this, suppose M is the maximum number of particles that can be placed in the container, i.e.,

$$L - d < Md < L \quad (8)$$

or

$$L = Md + \delta, \quad \text{where} \quad 0 < \delta < d. \quad (9)$$

Now divide the interval $[\frac{1}{2}d, L - \frac{1}{2}d]$ into $2M - 1$ segments, as in Fig. 1. There are M segments of

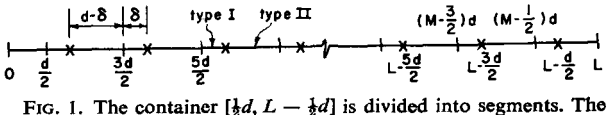

FIG. 1. The container $[\frac{1}{2}d, L - \frac{1}{2}d]$ is divided into segments. The boundaries of a segment are a vertical bar and an adjacent X. The bars are located at integral values of d from $\frac{1}{2}d$, and the X's at integral values of d from $L - \frac{1}{2}d$. Within any interval the $\alpha_m^{(N)}$'s and β_m's are constant.

length δ (Type I) and $M-1$ segments of length $d-\delta$ (Type II). From Eq. (7) it is seen that the x dependence of the $\alpha_m^{(N)}$'s enters only through the step functions. The step functions change values only at the boundaries of the above segments. Therefore, within any one of these segments the step functions are constant, and thus, the $\alpha_m^{(N)}$'s are constant.

The distribution function in the grand canonical ensemble (1) is obtained by summing Eq. (6):

$$D_1(x, L, z) = \sum_{N=1}^{M} \sum_{m=0}^{N-1} \alpha_m^{(N)} x^m.$$

Interchanging the orders of summation, we obtain

$$D_1(x, L, z) = \sum_{m=0}^{M-1} \sum_{N=m+1}^{M} \alpha_m^{(N)} x^m$$

or

$$D_1(x, L, z) = \sum_{m=0}^{M-1} \beta_m x^m, \tag{10}$$

where

$$\beta_m = \sum_{N=m+1}^{M} \alpha_m^{(N)}. \tag{11}$$

The $\alpha_m^{(N)}$'s are constant within any one of the segments discussed above and, hence, the β_m's must also be constant within any single segment. Therefore, $D_1(x, L, z)$ *is a polynomial with constant coefficients within any single segment.*

Since $D_1(x, L, z)$ is a polynomial with constant coefficients within each segment, $D_1(x, L, z)$ can equal a constant if and only if $\beta_m \equiv 0$ for all m $(m > 0)$. We now show that in each segment there is at least one β_m $(m > 0)$ not equal to zero. We start by looking at β_{M-1}. From Eqs. (11) and (7), we obtain

$$\begin{aligned}\beta_{M-1} &= \alpha_{M-1}^{(M)} \\ &= \frac{z^M}{(M-1)!\,\Xi(L, z)} \sum_{n=0}^{M-1} \binom{M-1}{n} (-1)^{M-1+n} \\ &\quad \times \theta\left[x - \left(n + \frac{1}{2}\right)d\right] \\ &\quad \times \theta\left[L - Md - x + \left(n + \frac{1}{2}\right)d\right].\end{aligned} \tag{12}$$

Using Eq. (9), we find

$$\begin{aligned}\beta_{M-1} = \frac{z^M}{(M-1)!\,\Xi(L, z)} &\sum_{n=0}^{M-1} \binom{M-1}{n} (-1)^{M-1+n} \\ &\times \theta\left[x - \left(n + \frac{1}{2}\right)d\right]\theta\left[\left(n + \frac{1}{2}\right)d + \delta - x\right].\end{aligned} \tag{13}$$

Due to the step functions, β_{M-1} is zero when x is within any of the segments of Type II. However, when x is within a segment of Type I, β_{M-1} is not zero and is equal to

$$\beta_{M-1} = \frac{z^M(-1)^{M-1+n}}{(M-1)!\,\Xi(L, z)} \binom{M-1}{n},$$
$$n = 0, 1, 2, \cdots, M-1.$$

In this expression, n denotes the Type I segment within which x lies. From this we conclude that $D_1(x, L, z)$ is not a constant if x lies within a segment of Type I.

We now turn our attention to β_{M-2}. From Eq. (11), we obtain

$$\beta_{M-2} = \alpha_{M-2}^{(M-1)} + \alpha_{M-2}^{(M)}. \tag{14}$$

From Eq. (7) we see that $\alpha_{M-2}^{(M)}$, just as $\alpha_{M-1}^{(M)}$, is zero in all regions of Type II. Therefore, for all regions of Type II,

$$\begin{aligned}\beta_{M-2} &= \alpha_{M-2}^{(M-1)} \\ &= \frac{z^{M-1}}{(M-2)!\,\Xi(L, z)} \sum_{n=0}^{M-2} \binom{M-2}{n} (-1)^{M-2+n} \\ &\quad \times \theta\left[x - \left(n + \frac{1}{2}\right)d\right] \\ &\quad \times \theta\left[L - (M-1)d - x + \left(n + \frac{1}{2}\right)d\right].\end{aligned}$$

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From the behavior of the step functions, β_{M-2} is a constant within each segment of Type II:

$$\beta_{M-2} = \frac{z^{M-1}}{(M-2)!\,\Xi(L, z)} \binom{M-2}{n} (-1)^{M-2+n},$$
$$n = 0, 1, \cdots, M-2.$$

In this expression, n denotes the Type II segment within which x lies.

We have shown that within any segment (Type I or II) there is at least one β_m $(m > 0)$ not equal to zero. Therefore, $D_1(x, L, z)$ is nowhere a constant. This proof is based on the property that the container can be divided into segments such that within any segment $D_1(x, L, z)$, for a pure hard-core fluid, is a polynomial with constant coefficients. This property, in general, does not exist if an attractive interaction is added to the hard core. For this reason a proof by a similar method does not seem possible for a more general one-dimensional fluid. However, if translational invariance properties do not exist for this simple

fluid, it seems unlikely that they would exist if an attractive interaction were added to the hard core. This reasoning is supported by the fact that, in the canonical ensemble formalism, if there are forces of range $R \geq d$, the length of the region of translational invariance is a *decreasing* function of R.

III. BEHAVIOR OF $D_1(x, L, z)$ IN THE THERMODYNAMIC LIMIT

We start by deriving an identity relating $D_1(x, L, z)$ to a product of grand partition functions. The identity is valid for a potential consisting of a hard-core repulsion plus nearest-neighbor interaction. Combining Eqs. (1) and (2), we obtain

$$D_1(x, L, z) = \sum_{N=1}^{\infty} \frac{z^N}{(N-1)!\,\Xi(L, z)} \sum_{n=0}^{N-1} \binom{N-1}{n} \times Z_n\left(x - \frac{d}{2}\right) Z_{N-1-n}\left(L - x - \frac{d}{2}\right). \quad (16)$$

Suppose

$$\gamma d < x - \frac{d}{2} < (\gamma + 1)d, \quad (17)$$

where γ (an integer) is the maximum number of particles which can be placed on a length $x - \frac{1}{2}d$. We note that, due to the hard-core potential, $Z_{n>\gamma}(x - \frac{1}{2}d) = 0$, or the sum on n must be such that $n \leq \gamma$. A similar constraint enters due to the $Z_{N-1-n}(L - x - \frac{1}{2}d)$ term. Since $M - \gamma - 1$ is the maximum number of particles placed within the length $L - x - \frac{1}{2}d$, we must add the additional constraint $N - 1 - n \leq M - \gamma - 1$. Equation (16) can now be written in the form

$$D_1\left[\left(\gamma + \frac{1}{2}\right)d < x < \left(\gamma + \frac{3}{2}\right)d, L, z\right] = \sum_{N=1}^{\infty} {\sum_{n=0}^{N-1}}' \frac{z^N}{(N-1)!\,\Xi(L, z)} \binom{N-1}{n} \times Z_n\left(x - \frac{d}{2}\right) Z_{N-1-n}\left(L - x - \frac{d}{2}\right), \quad (18)$$

where the $\sum'$ implies the constraints

$$n \leq \gamma, \qquad N - n \leq M - \gamma. \quad (19)$$

Looking at a plot of the summation points of Eqs. (18) and (19) on a N–n diagram (Fig. 2), we find that the summation includes all points on the shaded area. Interchanging the order of summation in Eq. (18),

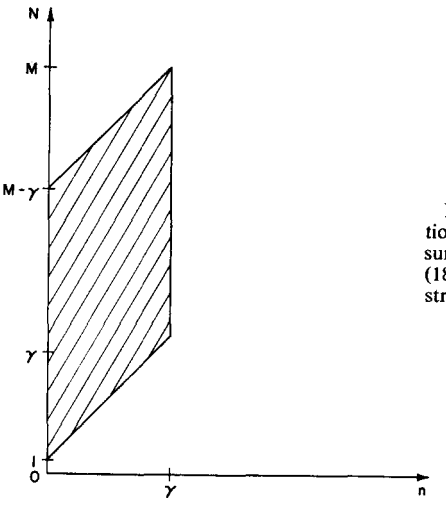

FIG. 2. An illustration of the domain of summation in Eq. (18), with the constraints (19).

we find

$$D_1\left[\left(\gamma + \frac{1}{2}\right)d < x < \left(\gamma + \frac{3}{2}\right)d, L, z\right] = \sum_{n=0}^{\gamma} \sum_{N=n+1}^{M-\gamma+n} \frac{z^N}{\Xi(L, z) n!} \frac{1}{(N-1-n)!} \times Z_n\left(x - \frac{d}{2}\right) Z_{N-1-n}\left(L - x - \frac{d}{2}\right).$$

Changing the summation variable N to $k = N - 1 - n$, we obtain

$$D_1\left[\left(\gamma + \frac{1}{2}\right)d < x < \left(\gamma + \frac{3}{2}\right)d, L, z\right] = \frac{z}{\Xi(L, z)} \sum_{n=0}^{\gamma} \sum_{k=0}^{M-\gamma-1} \frac{z^n}{n!} Z_n\left(x - \frac{d}{2}\right) \frac{z^k}{k!} Z_k\left(L - x - \frac{d}{2}\right).$$

Using Eq. (1b), we find

$$D_1\left[\left(\gamma + \frac{1}{2}\right)d < x < \left(\gamma + \frac{3}{2}\right)d, L, z\right] = \frac{z}{\Xi(L, z)} \Xi\left(x - \frac{d}{2}, z\right) \Xi\left(L - x - \frac{d}{2}, z\right) = D_1(x, L, z). \quad (20)$$

The last line follows because there are automatic cutoffs in the grand partition function for all configurations greater than closest packing.

For the case of a pure hard-core fluid, the behavior of $\Xi(L, z)$ in the thermodynamic limit is given by Eq. (A11) in the Appendix. Using this in Eq. (20), we obtain an expression valid in the limit of L, x, and $L - x$ approaching infinity:

$$D_1(x, L, z) \xrightarrow[L, x, L-x \to \infty]{} \frac{s_0}{1 + s_0 d} = \rho, \quad (21)$$

where Eq. (A13) has been used for the density ρ. We

have found that, in the thermodynamic limit and for x far from either wall, $D_1(x, L, z)$ approaches a constant which is just the grand canonical density ρ.

It is also possible to look at $D_1(x, L, z)$ at a wall, in the thermodynamic limit. Due to the definition of the walls, the smallest possible value of x is $\frac{1}{2}d$. Using Eqs. (20), (A11), and (A12) we find an expression for $D_1(x, L, z)$ at a wall, in the thermodynamic limit.

$$D_1(\tfrac{1}{2}d, L, z) \xrightarrow[L\to\infty]{} s_0 = \beta P. \tag{22}$$

This is a grand canonical wall theorem for a one-dimensional hard-core fluid. It should be noted that this expression is valid only in the thermodynamic limit. The wall theorem in the grand canonical ensemble is usually stated in terms of a grand canonical average of the canonical pressure, as in Eq. (24), rather than the grand canonical pressure, as in Eq. (22). The grand canonical wall theorem for a one-dimensional fluid follows from Eq. (8.5) of Ref. (5), which in our notation is given by

$$\begin{aligned}(\partial/\partial L) D_n(x_1, \cdots, x_n, z, L) \\ + \langle \beta P(N, L)\rangle_z D_n(x_1, \cdots, x_n, z, L) \\ = D_{n+1}(x_1, x_n, x_{n+1}, z, L)\big|_{x_{n+1}=L-\frac{1}{2}d},\end{aligned} \tag{23}$$

where $D_n(x_1, \cdots, x_n, z, L)$ is the grand canonical n-particle distribution function, $P(N, L)$ is the canonical pressure, and $\langle f\rangle_z$ is the grand canonical average of the quantity f. Taking the special case of $n = 0$, where $D_0(z, L) = 1$, Eq. (23) becomes

$$\begin{aligned}\langle \beta P(N, L)\rangle_z &= D_1\left(L - \frac{d}{2}, z, L\right) \\ &= D_1\left(\frac{d}{2}, z, L\right).\end{aligned} \tag{24}$$

The last step follows from the symmetry of $D_1(x, z, L)$ about $\frac{1}{2}L$. The correspondence between Eqs. (22) and (24) is not surprising since Eq. (22) is valid only in the thermodynamic limit. One expects that in the thermodynamic limit

$$\langle \beta P(N, L)\rangle_z = \beta P.$$

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APPENDIX: EVALUATION OF $\Xi(L, z)$ IN THE THERMODYNAMIC LIMIT FOR A HARD-CORE FLUID

The following calculation of the grand canonical partition function is carried out formally for a one-dimensional fluid with hard-core plus nearest-neighbor interaction. The resulting equation (A5) is applied specifically to the pure hard-core fluid. The calculation resembles in many respects that carried out by Gürsey,[6] who uses the convolution theorem repeatedly to obtain an expression for the Laplace transform of the canonical partition function. We show first that $\Xi(z, L)$ satisfies a renewal equation (A4). This equation is solved formally by taking its Laplace transform. Gürsey's calculation is carried out in the canonical ensemble. In his calculation, Gürsey uses a generating function $s(z, l)$ which is similar to the grand partition function but differs in that it is a function of l, the length per particle, instead of the container length L. A function of l has no clear interpretation in the grand canonical ensemble.

We consider a fluid of N particles with two-particle interaction $\phi(x)$ consisting of a hard-core of length d plus a possible nearest-neighbor interaction, i.e.,

$$\phi(x) = \begin{cases}\infty, & x < d, \\ w(x), & d < x < \eta d, \quad 1 < \eta < 2, \\ 0, & x > \eta d.\end{cases} \tag{A1}$$

The particles are confined to a length L by two additional particles located at $-\frac{1}{2}d$ and $L + \frac{1}{2}d$. The canonical configurational partition function is given by

$$\begin{aligned}Z_N(L) = N!\int_{-\infty}^{\infty} dx_N \cdots \int_{-\infty}^{\infty} dx_1 \\ \times \exp\left[-\beta \sum_{i=1}^{N-1} \phi(x_{i+1} - x_i)\right] \\ \times \exp\left[-\beta\phi\left(x_1 + \frac{d}{2}\right)\right] \\ \times \exp\left[-\beta\phi\left(L + \frac{d}{2} - x_N\right)\right] \\ = N\int_{-\infty}^{\infty} dx_N \exp\left[-\beta\phi\left(L + \frac{d}{2} - x_N\right)\right] \\ \times (N-1)!\int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1 \\ \times \exp\left[-\beta \sum_{i=1}^{N-2} \phi(x_{i+1} - x_i)\right] \\ \times \exp\left[-\beta\phi\left(x_1 + \frac{d}{2}\right)\right] \\ \times \exp\left\{-\beta\phi\left[\left(x_N - \frac{d}{2}\right) + \frac{d}{2} - x_{N-1}\right]\right\}\end{aligned}$$

$$\begin{aligned}Z_N(L) = N\int_{-\infty}^{\infty} dx_N \exp\left[-\beta\phi\left(L + \frac{d}{2} - x_N\right)\right] \\ \times Z_{N-1}\left(x_N - \frac{d}{2}\right).\end{aligned} \tag{A2}$$

[5] A. J. F. Siegert and E. Meeron, J. Math. Phys. 7, 741 (1966).

[6] F. Gürsey, Proc. Cambridge Phil. Soc. 46, 182 (1950).

The $N!$ is due to the integrals being ordered through the potential. Making the substitution $x_N - \frac{1}{2}d = L - \sigma$ we obtain

$$Z_N(L) = N\int_{-\infty}^{\infty} d\sigma\, e^{-\beta\phi(\sigma)} Z_{N-1}(L-\sigma). \quad \text{(A3)}$$

Multiply both sides of (A3) by $z^N/N!$, and sum on N from 1 to M, the number of particles for closest packing. Interchanging the order of summation and integration in Eq. (A3) and using Eq. (1b), we obtain

$$\Xi(L, z) - 1 = z\int_{-\infty}^{\infty} e^{-\beta\phi(\sigma)}\Xi(L-\sigma, z)\, d\sigma,$$

where the definition $Z_0(L) = 1$ has been used. Due to the fact that the integrand vanishes for $\sigma < d$ and $\sigma > L$, we may formally take the integral over the interval $[0, L]$:

$$\Xi(L, z) = 1 + z\int_0^L e^{-\beta\phi(\sigma)}\Xi(L-\sigma, z)\, d\sigma. \quad \text{(A4)}$$

Equation (A4) is of the type classified as a renewal equation.[7] An equation of this type can be solved formally by taking its Laplace transform:

$$\psi(s, z) = \int_0^{\infty} e^{-sL}\Xi(L, z)\, dL$$
$$= \frac{1}{s} + z\int_0^{\infty} e^{-sL}\, dL \int_0^L e^{-\beta\phi(\sigma)}\Xi(L-\sigma, z)\, d\sigma.$$

Using the convolution theorem, we have

$$\psi(s, z) = \frac{1}{s} + z\psi(s, z)\left[\int_0^{\infty} e^{-s\sigma}e^{-\beta\phi(\sigma)}\, d\sigma\right].$$

Solving for $\psi(s, z)$, we obtain

$$\psi(s, z) = \left[s - sz\int_0^{\infty} e^{-s\sigma}e^{-\beta\phi(\sigma)}\, d\sigma\right]^{-1}. \quad \text{(A5)}$$

Equation (A5) is valid for a general nearest-neighbor fluid. For a hard-core fluid, $w(x) = 0$, we obtain

$$\psi(s, z) = 1/(s - z\, e^{-sd}). \quad \text{(A6)}$$

Inverting the Laplace transform, we find

$$\Xi(L, z) = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} \frac{e^{sL}}{s - z\, e^{-sd}}\, ds, \quad \text{(A7)}$$

where a is to the right of all poles. The poles s_i in (A7) occur at the roots of the denominator, i.e.,

$$s_i = z\, e^{-s_i d}. \quad \text{(A8)}$$

The solutions of (A8) have the following properties:

(a) There is only one real positive root, labeled s_0, and $\mathrm{Re}\, s_i < s_0 < z$.

[7] For a discussion of the renewal equation, see R. Bellman and K. L. Cooke, *Differential-Difference Equations* (Academic Press Inc., New York, 1963), Chap. 7.

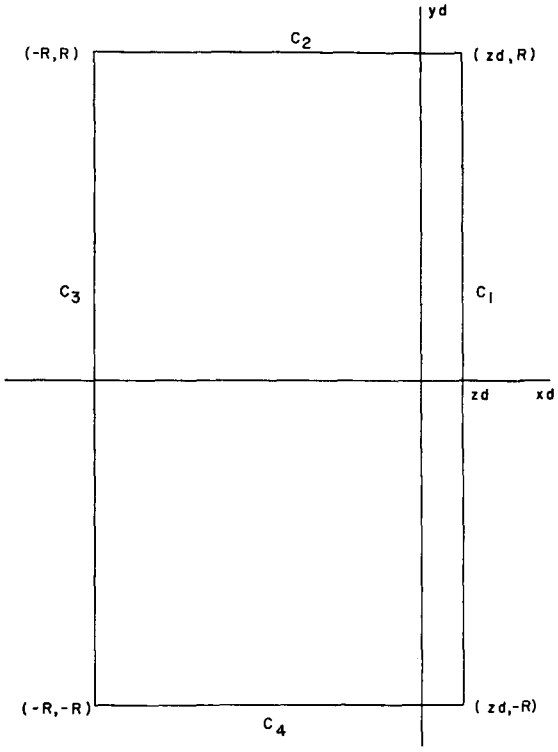

FIG. 3. A closed contour in the complex sd plane. The contour consists of four segments C_1, C_2, C_3, and C_4. A sequence of such contours is chosen such that for the nth contour $2\pi n < R < (2n+1)\pi$.

(b) The poles are located symmetrically about the real axis.

(c) For finite z, there are a finite number of s_i with positive real parts.

(d) $(2k-1)\pi \leq \mathrm{Im}\,(s_k d) \leq 2\pi k$, $k = 1, 2, \cdots$.

Choose a sequence of closed contours of the types shown in Fig. 3, where $2\pi n < R < (2n+1)\pi$. For n large it can be shown that

$$\int_{C_2+C_3+C_4} \frac{e^{sL}}{x - z\, e^{-sd}}\, ds \xrightarrow[n\to\infty]{} 0.$$

In this manner the contour in Eq. (A7) can be closed and $\Xi(L, z)$ is simply the sum of the residues of all poles. The residue of the pole s_k is found to be

$$\lim_{s\to s_k} \frac{e^{sL}(s - s_k)}{s - z\, e^{-sd}} = \frac{e^{s_k L}}{1 + zd\, e^{-s_k d}}, \quad \text{(A9)}$$

using l'Hôpital's rule. The grand partition function can now be written, using property (b) and Eq. (A8), as

$$\Xi'(L, \{s_i\}) = \frac{e^{s_0 L}}{1 + s_0 d} + 2\,\mathrm{Re}\sum_{i=1}^{\infty} \frac{e^{s_i L}}{1 + s_i d}. \quad \text{(A10)}$$

The prime indicates that the function is written in terms of the set of poles $\{s_i\}$. The fugacity z is related to $\{s_i\}$ by Eq. (A8).

Using properties (a), (c), and (d) it can be shown that, for large L, the residue of the pole s_0 dominates the sum of all other residues.[8] Hence, the grand partition function can be written as

$$\Xi'(L, \{s_i\}) = [e^{s_0 L}/(1 + s_0 d)][1 + O(\epsilon^L)], \quad L \to \infty, \tag{A11}$$

where

$$0 \leq \epsilon < 1.$$

The grand canonical potential $\pi(\beta, z)$ in the thermodynamic limit is defined by

$$\pi(\beta, z) = \lim_{L\to\infty} \frac{\ln \Xi(L, z)}{L}.$$

The β dependence of $\Xi(L, z)$ has been suppressed. For the hard-core fluid the grand canonical potential is

$$\pi'(\beta, s_0) = s_0.$$

where s_0 is determined by Eq. (A8) with i equal to zero. The grand canonical pressure and density are determined from the grand canonical potential[9] and Eq. (A8):

$$\beta P = \pi'(\beta, s_0) = s_0, \tag{A12}$$

$$\rho = z \frac{\partial \pi(\beta, z)}{\partial z} = z \frac{\partial \pi'(\beta, s_0)}{\partial s_0} \frac{\partial s_0}{\partial z} = \frac{s_0}{1 + s_0 d}. \tag{A13}$$

Equations (A12) and (A13) can be combined to obtain the equation of state:

$$\rho/(1 - \rho d) = \beta P. \tag{A14}$$

This is just the equation of state for a one-dimensional hard-core fluid.

[8] Using property (d), it can be shown that the infinite sum of all residues corresponding to poles with $\mathrm{Re}\, s_i < 0$ vanishes in the thermodynamic limit. Properties (a) and (c) imply that the residue of the pole at s_0 dominates the finite number of remaining residues.

[9] Taking the thermodynamic limit before obtaining the equations of state follows the definitions of P and ρ given by M. E. Fisher, Arch. Ratl. Mech. 17, 377 (1964).

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Instability of Transverse Waves in a Relativistic Plasma*

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Linearized equations are set up to describe disturbances in an infinite, spatially uniform, relativistic plasma without an ambient magnetic field. It is shown that, as well as the usual electrostatic waves, there also exists a class of electromagnetic waves. The two sets of waves are coupled in general, but can still be classified as mainly longitudinal or mainly transverse. Under the assumption that the system is stable against the longitudinal disturbances it is shown that the relativistic plasma will be unstable to the transverse waves unless it is virtually isotropic.

1. INTRODUCTION

The average age of cosmic rays in the galactic disk is estimated to be of the order of 5×10^6 years. Also it is known from observation that cosmic rays are isotropic to better than 1%.[1]

These two facts, together with the supernovae theory of the origin of cosmic rays, make it important to find a mechanism which reduces an arbitrary amount of anisotropy (since presumably supernovae produce cosmic rays anisotropically) to less than about 1% in a time less than, or of the order of, the mean cosmic-ray lifetime.

It has been conjectured that interstellar magnetic-field irregularities produce some measure of isotropy due to pitch-angle scattering. However, not much is known about the scale size of such irregularities.

It is therefore of interest to examine other possible ways of producing some degree of isotropy in an initially anisotropic relativistic plasma. One such possibility is particle velocity redistribution due to the influence of plasma waves. It is well known that it is difficult to make plasma waves carry a significant amount of energy but for producing isotropy this is not a prime requirement. In fact, the plasma waves need only reorder the plasma distribution function in order to achieve some measure of isotropy. In this sense the waves take on the role of collisions in a classical gas.

* This work was supported by the National Aeronautics and Space Administration under grant NASA-NsG-96-60.

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In discussing the behavior of a plasma perturbed by a disturbance, attention is usually restricted to purely electrostatic waves since these grow in the order of a plasma period which, in the absence of an ambient magnetic field, is the shortest possible time for a dynamical process.

However there also exists a class of electromagnetic disturbances whose existence has been recognized by several authors.[2,3] Such electromagnetic waves have been considered in considerable detail for a nonrelativistic plasma.[4]

The main reason for considering such waves is essentially due to the conditions attached to making the plasma unstable against the electrostatic mode. These conditions are well known.[5] It has been shown[6] that the requirements for electrostatic instability are difficult to meet in several interesting astrophysical situations.

It is therefore worthwhile considering the electromagnetic waves since the requirements for instability of these waves are much easier to meet. It should be emphasized that these waves are *not* the familiar fast electromagnetic waves with phase velocities of the order of c, the velocity of light. In fact, if the rms velocity spread is σc, the electromagnetic waves to be considered generally have amplification rates of the order of σ times the plasma frequency. Consequently, they are not nearly as violent as the electrostatic waves. They do have the advantage that the plasma need not obey such stringent requirements as the electrostatic mode demands before they become unstable.

In this analysis we do not allow for a galactic magnetic field despite the observational evidence which indicates the existence of such a field with a mean strength of about 5×10^{-6} Γ.[7] The plethora of complications which arise when an ambient magnetic field is taken into account have been the subject of innumerable papers and books and we make no attempt to consider them.

In several recent papers[8–10] particular attention was paid to the electromagnetic and space-charge waves when the relativistic plasma was embedded in an infinite, homogeneous magnetic field. In all these papers the tacit assumption was made that there was no coupling between the two types of wave. We demonstrate in this paper that, in the absence of an ambient magnetic field, coupling exists but barely influences the space-charge wave. It is also shown that the coupling seriously perturbs the electromagnetic wave. Thus the assumption of no coupling in an ambient magnetic field is suspect and should be investigated. In particular, under the assumption of no coupling it can be shown[9] that the electromagnetic mode, in an ambient magnetic field, does grow at a physically significant rate for the cosmic-ray gas. This result may not be true when interference is allowed for.

Thus this paper cannot describe the behavior of the galactic cosmic-ray gas in the general galactic magnetic field. The motivation behind this work is essentially self-educative. We hope that the results presented here lead to a better understanding of the physical behavior of relativistic plasmas.

As remarked earlier, a similar calculation to the following has been performed for a nonrelativistic plasma.[4] It is not immediately obvious that Kahn's criteria for stability against the electromagnetic waves can be applied to a relativistic plasma. We show that while the physical sense of Kahn's criteria is preserved, the mathematical formalism changes due to the relativistic nature of the problem.

We make no attempt to calculate instability rates for the unstable situations. Such a calculation would require a detailed knowledge of the distribution function and in this paper we shall only be concerned with general properties that a distribution function must possess in order to avoid instability.

Further, since we do not include an ambient magnetic field in the calculations, even if we were to calculate e-folding times for particular distribution functions, we could not place any reliance on them as measures of the speed with which an instability occurs in the galactic cosmic-ray gas.

2. DISPERSION RELATION

We consider only the case of a mobile relativistic proton plasma without an ambient magnetic field. It suffices to consider one mobile species since the theory to be developed uses linearized equations. Thus more than one mobile species can easily be taken into account. Along with the proton plasma we assume that there exists a cold, smeared out, electron charge background which does not contribute to the motion and serves to preserve over-all space-charge neutrality.

We let the equilibrium relativistic proton distribution function be f_0 and the first-order linear perturbation to f_0 be f_1. It is then a simple matter to show that f_1 satisfies the linearized relativistic Vlasov

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[8] I. Lerche, Phys. Fluids **9**, 1073 (1966).
[9] I. Lerche, Phys. Fluids **10**, 1071 (1967).
[10] I. Lerche, Phys. Fluids **10**, 2271 (1967).

equation

$$\frac{\partial f_1}{\partial t} + \frac{c\mathbf{p}}{(1+p^2)^{\frac{1}{2}}} \cdot \frac{\partial f_1}{\partial \mathbf{x}} + \frac{\epsilon}{mc}\left[-\nabla\varphi - c^{-1}\frac{\partial \mathbf{A}}{\partial t} + \frac{\mathbf{p}\times(\nabla\times\mathbf{A})}{(1+p^2)^{\frac{1}{2}}}\right] \cdot \frac{\partial f_0}{\partial \mathbf{p}} = 0, \tag{1}$$

where ϵ and m are the charge and rest mass of a proton, respectively. The normalized momentum $\mathbf{p}$ is defined in terms of the real momentum $\mathbf{P}$, through the relation $mc\mathbf{p} = \mathbf{P}$. Here φ and $\mathbf{A}$ are the scalar-electrostatic and vector-electromagnetic potentials, respectively.

We must also satisfy the Maxwell equations

$$\nabla^2\varphi - c^{-2}\frac{\partial^2\varphi}{\partial t^2} = -4\pi\epsilon\int f_1\, d^3p, \tag{2}$$

$$\nabla^2\mathbf{A} - c^{-2}\frac{\partial^2\mathbf{A}}{\partial t^2} = -4\pi\epsilon\int \frac{f_1\mathbf{p}\, d^3p}{(1+p^2)^{\frac{1}{2}}}. \tag{3}$$

In addition, we must ensure the preservation of the gauge condition

$$\nabla\cdot\mathbf{A} + \frac{1}{c}\frac{\partial\varphi}{\partial t} = 0. \tag{4}$$

We choose a particular Cartesian coordinate system and allow all first-order perturbation quantities to vary as

$$\exp\,[ik(x - c\beta t)]. \tag{5}$$

We let k be real and positive and β complex without any loss of generality.

Making use of (5) it can easily be shown that the solution to (1) is given by

$$f_1 = \frac{\epsilon}{mc^2}\left(A_y\frac{\partial f_0}{\partial p_y} + A_z\frac{\partial f_0}{\partial p_z}\right) + \frac{\epsilon[\varphi(1-\beta^2) - (p_yA_y + p_zA_z)(1+p^2)^{-\frac{1}{2}}]}{mc^2[p_x(1+p^2)^{-\frac{1}{2}} - \beta]}\frac{\partial f_0}{\partial p_x}, \tag{6}$$

where use has been made of the gauge condition in the form

$$A_x = \beta\varphi.$$

We now normalize f_0 so that

$$\int f_0\, d^3p = 1, \tag{7}$$

when it can be shown that, with the aid of (5), Eq. (2) becomes

$$k^2(1-\beta^2)\varphi = \frac{4\pi\epsilon^2N}{mc^2}\int dp_x\, dp_y\, dp_z\left\{A_y\frac{\partial f_0}{\partial p_y} + A_z\frac{\partial f_0}{\partial p_z} + \frac{[\varphi(1-\beta^2) - (p_yA_y + p_zA_z)(1+p^2)^{-\frac{1}{2}}]}{[p_x(1+p^2)^{-\frac{1}{2}} - \beta]}\frac{\partial f_0}{\partial p_x}\right\}, \tag{8}$$

and the range of integration in (7) and (8) is

$$-\infty \le p_x \le \infty, \quad -\infty \le p_y \le \infty, \quad -\infty \le p_z \le \infty.$$

With the help of (5) it may also be shown that (3) can be written

$$k^2(1-\beta^2)A_y = \frac{4\pi\epsilon^2N}{mc^2}\int \frac{p_y}{(1+p^2)^{\frac{1}{2}}}\{\ \}\, dp_x\, dp_y\, dp_z, \tag{9}$$

$$k^2(1-\beta^2)A_z = \frac{4\pi\epsilon^2N}{mc^2}\int \frac{p_z}{(1+p^2)^{\frac{1}{2}}}\{\ \}\, dp_x\, dp_y\, dp_z, \tag{10}$$

where the curly brackets in (9) and (10) denote the factor in curly brackets occurring in (8). Here N is the number density of relativistic particles.

Defining

$$\Phi = \varphi(1-\beta^2), \quad k_0^2 = 4\pi\epsilon^2N/(mc^2), \quad \kappa^2 = k^2k_0^{-2},$$

and noting that (8), (9), and (10) are all linear in Φ, A_y, and A_z, we see that for a solution to exist to these three equations we must demand that

$$\begin{vmatrix} \kappa^2 - I_1(\beta) & I_y(\beta) & I_z(\beta) \\ -I_y(\beta) & \kappa^2(1-\beta^2) + g_x + g_z + I_{yy}(\beta) & I_{yz}(\beta) - h_{yz} \\ -I_z(\beta) & I_{yz}(\beta) - h_{yz} & \kappa^2(1-\beta^2) + g_x + g_y + I_{zz}(\beta) \end{vmatrix} = 0, \tag{11}$$

where

$$g_x = \int \frac{f_0(1+p_x^2)\, d^3p}{(1+p^2)^{\frac{3}{2}}}, \quad (g_y, g_z) = \int \frac{f_0(p_y^2, p_z^2)\, d^3p}{(1+p^2)^{\frac{3}{2}}},$$

$$h_{yz} = \int \frac{f_0p_yp_z\, d^3p}{(1+p^2)^{\frac{3}{2}}}, \quad I_1(\beta) = \int \frac{(1+p^2)^{\frac{1}{2}}\partial f_0/\partial p_x\, d^3p}{[p_x - \beta(1+p^2)^{\frac{1}{2}}]},$$

$$(I_y, I_z, I_{yz}, I_{yy}, I_{zz}) = \int \frac{f_0\, d^3p}{[p_x - \beta(1+p^2)^{\frac{1}{2}}]} \times \left(p_y, p_z, \frac{p_yp_z}{(1+p^2)^{\frac{1}{2}}}, \frac{p_y^2}{(1+p^2)^{\frac{1}{2}}}, \frac{p_z^2}{(1+p^2)^{\frac{1}{2}}}\right).$$

We have also assumed that f_0 satisfies the usual convergence conditions as p_x, p_y, or $p_z \to \pm\infty$.

From the dispersion equation (11) we have a relation between k and β. An unstable situation will develop if, and only if, a real, positive k exists for which β has a positive imaginary part.

3. SOME ASPECTS OF THE DISPERSION RELATION

One point, which is immediately obvious from (11), is that if β is real, positive and greater than, or equal

to, unity, all the integrals in (11) are completely real since, for all values of p_x, p_y, and p_z, we have $p_x < \beta(1 + p_x^2 + p_y^2 + p_z^2)^{\frac{1}{2}}$. This merely states that waves with phase velocities greater than, or equal to, c, do not resonate with the finite rest-mass protons which always have subluminous velocities.

Also it can readily be shown that, provided f_0 is not pathological, all the integrals in (11) are analytic functions of β in any one half-plane. Since we are looking for temporal instability we choose to define k real and positive and β in the upper half-plane. It is then well known that as Im $(\beta) \to 0+$ from above the resulting functions of β are also analytic on the real β axis.[11]

Suppose we now choose the zero velocity to be the mean particle velocity, say. Then if the equilibrium distribution has a mean velocity half-width σc, we see that when $\beta \gg \sigma$, we have

$$I_1(\beta) = O(\beta^{-2}).$$

Likewise,

$$I_y(\beta) = O(\sigma\beta^{-2}),$$

and so on.

For those waves with phase velocities close to c, we have $\sigma \ll |\beta|$ in most physical situations. Neglecting terms of order $\sigma^2\beta^{-2}$, we see that in such a case (11) reduces to just its diagonal elements, and the electrostatic and electromagnetic waves completely decouple. We then obtain the usual relation

$$\kappa^2 - I_1(\beta) = 0 \tag{12}$$

for the electrostatic mode. The corresponding relation for the electromagnetic mode is

$$k^2\beta^2 = k^2 + k_0^2. \tag{13}$$

However we are interested in the situation where $|\beta| \ll 1$. In this case we can replace the factor $(1 - \beta^2)$ by unity in the electromagnetic diagonal terms of (11). Then the dispersion relation becomes

$$\begin{vmatrix} \kappa^2 - I_1(\beta) & I_y(\beta) & I_z(\beta) \\ -I_y(\beta) & \kappa^2 + g_x + g_z + I_{yy}(\beta) & I_{yz}(\beta) - h_{yz} \\ -I_z(\beta) & I_{yz}(\beta) - h_{yz} & \kappa^2 + g_x + g_y + I_{zz}(\beta) \end{vmatrix} = 0. \tag{14}$$

It may happen that a situation is chosen with sufficient symmetry so that

$$I_y(\beta) = 0 = I_z(\beta). \tag{15}$$

[11] J. D. Jackson, Space Technology Laboratories Report GM-TR-0165-00535, 1958; see also J. D. Jackson, J. Nucl. Energy Pt. C 1, 178 (1960).

In this case the electrostatic and electromagnetic modes completely decouple. In general, however, the integrals in (15) do not vanish and they introduce cross coupling between the two different types of modes. From (12) we see that the order-of-magnitude calculation shows that we are predominantly interested in those electrostatic modes for which

$$\kappa^2 = O(\beta^{-2}), \quad |\beta| \gg \sigma,$$
$$\kappa^2 = O(\sigma^{-2}), \quad |\beta| \ll \sigma.$$

In the present situation we are looking at $|\beta| \ll 1$ and, in particular, we assume that $\sigma \gg |\beta|$. Thus we expect κ^2 to be of the order σ^{-2} for the electrostatic mode. This is much larger than $\kappa^2 = O(1)$ which we expect for the electromagnetic mode. Thus as far as the electrostatic mode is concerned the coupling can be represented to a good enough approximation by

$$\begin{vmatrix} \kappa^2 - I_1(\beta) & I_y(\beta) & I_z(\beta) \\ -I_y(\beta) & \kappa^2 & 0 \\ -I_z(\beta) & 0 & \kappa^2 \end{vmatrix} = 0. \tag{16}$$

Setting

$$\kappa^2 = I_1(\beta)$$

in the second and third diagonal terms, which is accurate to the order required, we see that (16) becomes

$$\kappa^2 - I_1(\beta) \simeq -I_1^{-1}(\beta)[I_y^2(\beta) + I_z^2(\beta)]. \tag{17}$$

Thus an extra term of order σ^2 times the dominant term has been introduced. This hardly affects the electrostatic mode at all and consequently the usual electrostatic dispersion equation is a good enough approximation to the correct relation.

However the coupling of the electrostatic mode to the electromagnetic waves is not negligible. For the transverse waves, we are interested in values of κ^2 of the order of unity, while

$$I_1(\beta) = O(\sigma^{-2})$$

for the slow electrostatic wave. Thus as far as the transverse wave is concerned, a good enough approximation to the dispersion relation is

$$\begin{vmatrix} I_1(\beta) & I_y(\beta) & I_z(\beta) \\ I_y(\beta) & \kappa^2 + g_x + g_z + I_{yy}(\beta) & I_{yz}(\beta) - h_{yz} \\ I_z(\beta) & I_{yz}(\beta) - h_{yz} & \kappa^2 + g_x + g_y + I_{zz}(\beta) \end{vmatrix} = 0. \tag{18}$$

It is then a simple matter to show that (18) can be written as

$$[q + \tfrac{1}{2}(\mathfrak{I}_{yy} + \mathfrak{I}_{zz})]^2 = \tfrac{1}{4}(\mathfrak{I}_{yy} - \mathfrak{I}_{zz})^2 + \mathfrak{I}_{yz}^2, \tag{19}$$

where

$$q = \kappa^2 + g_x, \quad \mathfrak{I}_{yy} = g_z + I_{yy} - I_y^2 I_1^{-1},$$
$$\mathfrak{I}_{zz} = g_y + I_{zz} - I_z^2 I_1^{-1}, \quad \mathfrak{I}_{yz} = I_{yz} - h_{yz} - I_y I_z I_1^{-1}.$$

4. STABILITY CONSIDERATIONS

As has been done in the nonrelativistic case,[4] we now demonstrate that the class of electromagnetic waves whose dispersion relation is given by (19) is unstable unless the equilibrium relativistic proton distribution function satisfies some rather restrictive conditions.

We consider only the case of even parity distribution functions, i.e.,

$$f_0(p_x, p_y, p_z) = f_0(-p_x, -p_y, -p_z). \tag{20}$$

Making use of (20) it can easily be shown that I_1, I_{yy}, I_{zz}, I_{yz} are real, and I_y, I_z are pure imaginary when β is pure imaginary. We note also that g_x, g_y, and g_z are real and positive.

A sufficient condition for electromagnetic instability is that there exist a real, positive k whose β has a positive imaginary part. Since the right-hand side of (20) is real and positive and since $q = g_x + k^2 k_0^{-2}$, this means that there exists a β in the upper half complex plane whose corresponding q is real and greater than g_x. This is so if $\mathfrak{I}_{yy} + \mathfrak{I}_{zz}$ is real and less than $-2g_x$ somewhere on the imaginary β axis in the upper half-plane.

Hence, by continuity,

$$\mathfrak{I}_{yy} + \mathfrak{I}_{zz} < -2g_x \tag{21}$$

when $\beta = 0$. We can also ignore the class of situation for which I_1 is real and positive anywhere in the upper half complex β plane, since it follows that the plasma is then unstable against electrostatic waves. These dominate over the slow electromagnetic waves.

Thus the physically interesting situation is that in which I_1 and $I_y^2 + I_z^2$ are negative on $\beta = i\xi$ $(\xi > 0)$.

On $\beta = i\xi$ we have, therefore,

$$\mathfrak{I}_{yy} + \mathfrak{I}_{zz} = g_y + g_z + I_{yy} + I_{zz} - (I_y^2 + I_z^2) I_1^{-1} < -2g_x$$

and

$$\mathfrak{I}_{yy} + \mathfrak{I}_{zz} \leq g_y + g_z + I_{yy} + I_{zz} < -2g_x.$$

To avoid instability we require that

$$I_{yy}(0) + I_{zz}(0) \geq -2g_x - g_y - g_z, \tag{22}$$

with equality if and only if $I_y(0) = 0 = I_z(0)$. Now

$$I_{yy}(0) + I_{zz}(0) = \int \frac{(p_y^2 + p_z^2)}{p_x(1 + p^2)^{\frac{1}{2}}} \frac{\partial f_0}{\partial p_x} d^3p \equiv M(0), \text{ say.} \tag{23}$$

We now change to spherical momentum coordinates defined by

$$p_y = p \cos\theta, \quad p_y = p \sin\theta \cos\varphi, \quad p_z = p \sin\theta \sin\varphi$$

so that

$$\frac{\partial}{\partial p_x} = \cos\theta \frac{\partial}{\partial p} - \frac{\sin\theta}{p} \frac{\partial}{\partial \theta}.$$

Setting

$$\int_0^{2\pi} f_0(p, \theta, \varphi)\, d\varphi = 2\pi F(p, \theta),$$

we see that (23) becomes

$$M(0) = 2\pi \int_0^\infty \frac{p^2\, dp}{(1 + p^2)^{\frac{1}{2}}} \int_{-1}^{+1} (1 - \mu^2) \times \left[p \frac{\partial F}{\partial p} + \mu^{-1}(1 - \mu^2) \frac{\partial F}{\partial \mu} \right] d\mu, \tag{24}$$

where $\mu = \cos\theta$.

We note that

$$\int_0^\infty \frac{p^3}{(1 + p^2)^{\frac{1}{2}}} \frac{\partial F}{\partial p}\, dp = -3 \int_0^\infty \frac{p^2 F\, dp}{(1 + p_2)^{\frac{1}{2}}} + \int_0^\infty \frac{p^4 F\, dp}{(1 + p^2)^{\frac{3}{2}}}.$$

We now expand $F(p, \theta)$ in terms of Legendre polynomials

$$F(p, \theta) = \sum_{n=0}^{\infty} R_{2n}(p) P_{2n}(\mu), \tag{25}$$

where the assumption of even parity ensures that only even polynomials in μ enter (25).

Setting

$$r_{2n} = \int_0^\infty \frac{p^2 R_{2n}(p)\, dp}{(1 + p^2)^{\frac{1}{2}}}$$

and

$$J_{2n} = \int_0^\infty \frac{p^4 R_{2n}(p)\, dp}{(1 + p^2)^{\frac{3}{2}}},$$

we see that (24) can be written

$$M(0) = 2\pi \sum_{n=0}^{\infty} r_{2n} \int_{-1}^{+1} [-3(1 - \mu^2) P_{2n}(\mu) + \mu^{-1}(1 - \mu^2)^2 P'_{2n}(\mu)]\, d\mu + 2\pi \sum_{n=0}^{\infty} J_{2n} \int_{-1}^{+1} (1 - \mu^2) P_{2n}(\mu)\, d\mu, \tag{26}$$

where the prime denotes differentiation with respect to the argument.

It can be shown[4] that

$$\int_{-1}^{+1} [-3(1 - \mu^2) P_{2n}(\mu) + \mu^{-1}(1 - \mu^2)^2 P'_{2n}(\mu)]\, d\mu \equiv i_n, \text{ say,}$$
$$= -4, \quad n = 0,$$
$$= \frac{(-1)^{n-1} 2^{2n+1} (n!)^2}{(2n)!}, \quad n \geq 1,$$

so that

$$M(0) = -8\pi r_0 + 2\pi \sum_{n=1}^{\infty} i_n r_{2n} + \frac{8\pi}{3}\left(J_0 - \frac{J_2}{5}\right). \quad (27)$$

It can easily be shown that

$$g_y + g_z = (8\pi/3)(J_0 - J_2/5)$$

and

$$g_x + g_y + g_z = 4\pi r_0.$$

Thus the condition that instability be avoided can be written

$$\sum_{n=1}^{\infty} i_n r_{2n} \geq 0. \quad (28)$$

To avoid instability, this result must hold true not only for the one particular direction of the wave chosen, namely along the x axis, but for *any* direction of the wave normal.

We therefore define a basic direction with respect to which a given wave normal points into the direction (λ_0, ν_0). With respect to this basic direction we can write

$$f_0(\mathbf{p}) = f_0(p, \lambda, \nu) = \psi_0(p) + \sum_{n=1}^{\infty} \sum_{m=0}^{2n} \psi_{2n}^{(m)}(p) S_{2n}^{(m)}(\lambda, \nu), \quad (29)$$

where the $S_{2n}^{(m)}$ are spherical harmonics and the assumption of even parity ensures that only even harmonics enter (29).

Expressed with respect to a line parallel to the particular wave normal which points into (λ_0, ν_0), we can write

$$f_0(\mathbf{p}) = \sum_{n=0}^{\infty} \sum_{m=0}^{2n} f_{2n}^{(m)}(p) P_{2n}^{(m)}(\mu) \cos(m\varphi + \epsilon_{m,n}), \quad (30)$$

where the $\epsilon_{m,n}$ are suitably chosen constants and $P_{2n}^{(m)}(\mu)$ is the associated Legendre polynomial.

It follows that $\mu = 1$ when $\lambda = \lambda_0$, $\nu = \nu_0$, and then we have

$$P_{2n}^{(0)}(1) = 1; \quad P_{2n}^{(m)}(1) = 0, \quad m \neq 0.$$

Equating harmonics of the same order in (29) and (30) we have

$$f_{2n}^{(0)}(p) = \sum_{m=0}^{2n} \psi_{2n}^{(m)}(p) S_{2n}^{(m)}(\lambda_0, \nu_0),$$

when $\lambda = \lambda_0$, $\nu = \nu_0$.

Thus

$$R_{2n}(p) = \sum_{m=0}^{2n} \psi_{2n}^{(m)}(p) S_{2n}^{(m)}(\lambda_0, \nu_0).$$

Defining

$$\Psi_{2n}^{(m)} = \int_0^{\infty} \frac{\psi_{2n}^{(m)}(p) p^2 \, dp}{(1 + p^2)^{\frac{1}{2}}},$$

we have

$$r_{2n} = \sum_{m=0}^{2n} \Psi_{2n}^{(m)} S_{2n}^{(m)}(\lambda_0, \nu_0).$$

Thus the requirement that instability be avoided can be written

$$\sum_{n=1}^{\infty} \sum_{m=0}^{2n} i_n \Psi_{2n}^{(m)} S_{2n}^{(m)}(\lambda_0, \nu_0) \geq 0. \quad (31)$$

Now the average value of any spherical harmonic, of order unity or greater, over a sphere is zero. Therefore, if the sum in (31) must not be negative for *any* values of λ_0 and ν_0, it must vanish for *all* λ_0, ν_0. Since none of the i_n vanishes, it follows that

$$\Psi_{2n}^{(m)} = 0, \quad n \geq 1.$$

Making use of (29) we see that this demands

$$\int_0^{\infty} \frac{p^2}{(1 + p^2)^{\frac{1}{2}}} f_0(p, \lambda_0, \nu_0) \, dp = F_0, \quad \text{say,} \quad (32)$$

and F_0 must be independent of λ_0 and ν_0.

Denoting the solid-angle element by $d\Omega$ it can be shown[12] that

$$p^2 \, dp \, d\Omega (1 + p^2)^{-\frac{1}{2}}$$

is invariant under a Lorentz transformation.

Thus from (32) we can say that if electromagnetic instability is to be avoided then the number of relativistic particles moving into any given solid angle must be independent of the orientation of the solid angle.

When this is the case it can easily be seen that

$$M(0) = -8\pi r_0 + (8\pi/3)(J_0 - J_2/5),$$

for all directions of the wave normal. We also have

$$I_{yy}(0) = I_{zz}(0), \quad I_{yz}(0) = 0,$$

in this case.

The requirement for avoiding electromagnetic instability can be made even stronger since we have that

$$\mathfrak{I}_{yy} + \mathfrak{I}_{zz} \leq g_y + g_z + I_{yy} + I_{zz}, \quad (33)$$

with equality if and only if $I_y = 0 = I_z$.

Now at best the right-hand side of (33) equals $-2g_x$ for all directions of the wave normal. Thus I_y and I_z must vanish for *all* directions of the wave normal, in order that $\mathfrak{I}_{yy} + \mathfrak{I}_{zz}$ never be smaller than $-2g_x$, and thus that instability be avoided.

Both I_y and I_z are pure imaginary at $\beta = 0$ and hence at $p_x = 0$. Thus,

$$(I_y, I_z) = i\pi \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} (p_y, p_z) \frac{\partial f_0}{\partial p_x}\bigg|_{p_x=0} dp_z. \quad (34)$$

Changing to spherical momentum coordinates we

[12] L. Landau and E. Lifschitz, *Classical Theory of Fields* (Pergamon Press, London, 1951), Chap. 2, p. 31.

have

$$(I_y, I_z) = -i\pi \int_0^\infty p\,dp \int_0^{2\pi} (\cos\varphi, \sin\varphi) \frac{\partial f_0}{\partial \theta}\bigg|_{\theta=\pi/2} d\varphi. \tag{35}$$

With f_0 given by (30) it can easily be seen that

$$[I_y(0), I_z(0)] = i\pi^2 \sum_{n=0}^{\infty} \frac{dP_{2n}^{(1)}(\mu)}{d\mu}\bigg|_{\mu=0} \int_0^\infty p f_{2n}^{(1)}(p) \times dp(\cos\epsilon_{1,n}, -\sin\epsilon_{1,n}).$$

We again compare the two representations (29) and (30). We consider a particular wave normal through $\lambda = \lambda_0$, $\nu = \nu_0$, and let φ be measured in the plane containing the wave normal and the basic line.

Then, near $\lambda = \lambda_0$, $\nu = \nu_0$:

$$\begin{aligned} \frac{\partial}{\partial\lambda} &\equiv \frac{\partial}{\partial\theta}, & \varphi &= 0, \\ \frac{\partial}{\partial\theta} &\equiv \operatorname{cosec}\lambda \frac{\partial}{\partial\nu}, & \varphi &= \frac{\pi}{2}. \end{aligned} \tag{36}$$

Equating harmonics of equal order in (29) and (30), we see that

$$\sum_{m=0}^{2n} f_{2n}^{(m)}(p) P_{2n}^{(m)}(\mu) \cos(m\varphi + \epsilon_{m,n}) = \sum_{m=0}^{2n} \psi_{2n}^{(m)}(p) S_{2n}^{(m)}(\lambda, \nu). \tag{37}$$

Hence, near $\lambda = \lambda_0$, $\nu = \nu_0$ we have

$$\sum_{m=0}^{2n} \psi_{2n}^{(m)}(p) \frac{\partial S_{2n}^{(m)}}{\partial\lambda}\bigg|_{\lambda_0,\nu_0} = f_{2n}^{(1)}(p) \frac{dP_{2n}^{(1)}(\cos\theta)}{d\theta}\bigg|_{\theta=0} \cos\epsilon_{1,n},$$

$$\sum_{m=0}^{2n} \psi_{2n}^{(m)}(p) \operatorname{cosec}\lambda \frac{\partial S_{2n}^{(m)}}{\partial\nu}\bigg|_{\lambda_0,\nu_0} = -f_{2n}^{(1)}(p) \frac{dP_{2n}^{(1)}(\cos\theta)}{d\theta}\bigg|_{\theta=0} \sin\epsilon_{1,n},$$

where we have made use of the fact that

$$\frac{dP_{2n}^{(m)}(\cos\theta)}{d\theta} = 0 \quad \text{at} \quad \theta = 0 \quad \text{for} \quad m \neq 1.$$

Let

$$X_{2n}^{(m)} = \int_0^\infty p\psi_{2n}^{(m)}(p)\,dp,$$

then

$$I_y(0) = \partial G/\partial\lambda, \quad I_z(0) = \operatorname{cosec}\lambda \cdot \partial G/\partial\nu,$$

where

$$G = i\pi^2 \sum_{n=0}^{\infty} \sum_{m=0}^{2n} \frac{(dP_{2n}^{(1)}(\mu)/d\mu)_{\mu=0}}{(dP_{2n}^{(1)}(\mu)/d\theta)_{\theta=0}} X_{2n}^{(m)} S_{2n}^{(m)}(\lambda, \nu)$$

We require that $I_y(0)$ and $I_z(0)$ vanish for *all* values of λ, ν. Hence a similar argument to that employed previously shows that

$$X_{2n}^{(m)} = 0, \quad \forall\, n, m.$$

Thus it follows that we must demand

$$\int_0^\infty p f_0(p, \lambda, \nu)\,dp = L_0, \quad \text{say,} \tag{38}$$

where L_0 is a constant independent of λ, ν.

Thus if a relativistic plasma has a distribution function which satisfies (32) and (38), then there is no unstable electromagnetic disturbance with a real nonzero wavenumber and zero phase velocity.

We can rewrite (38) as

$$\int_0^\infty \frac{p^2\,dp}{(1+p^2)^{\frac{1}{2}}} \left[\frac{(1+p^2)^{\frac{1}{2}}}{p} f_0(p, \lambda, \nu)\right] = L_0, \tag{39}$$

and we note that $p(1+p^2)^{-\frac{1}{2}} = Vc^{-1}$ where V is the particle velocity. Thus (38) demands that the harmonic mean velocity of those particles moving in a given solid angle be independent of the spatial orientation of the solid angle. When (32) and (38) are satisfied we can show that no electromagnetic disturbance with a small imaginary β and real wavenumber can exist. To prove this we consider the values of $\mathfrak{I}_{yy}$, $\mathfrak{I}_{zz}$, and $\mathfrak{I}_{yz}$ near $\xi = 0$ ($\beta = i\xi$).

Now

$$\mathfrak{I}_{yy}(i\xi) = \mathfrak{I}_{yy}(0) + \xi \frac{\partial \mathfrak{I}_{yy}}{\partial\xi}\bigg|_{\xi=0} + \tfrac{1}{2}\xi^2 \frac{\partial^2 \mathfrak{I}_{yy}}{\partial\xi^2}\bigg|_{\xi=0} + \cdots$$

and, since $I_y(0) = 0$,

$$\frac{\partial \mathfrak{I}_{yy}}{\partial\xi}\bigg|_{\xi=0} = \frac{\partial I_{yy}}{\partial\xi}\bigg|_{\xi=0}.$$

Likewise,

$$\frac{\partial^2 \mathfrak{I}_{yy}}{\partial\xi^2}\bigg|_{\xi=0} = \frac{\partial^2 I_{yy}}{\partial\xi^2}\bigg|_{\xi=0} - 2I_1^{-1}(0)\left(\frac{\partial I_y}{\partial\xi}\right)^2_{\xi=0}.$$

Making use of the fact that I_{yy}, I_1 are real and I_y is pure imaginary when β is pure imaginary, it can be shown that

$$\frac{\partial \mathfrak{I}_{yy}}{\partial\xi}\bigg|_{\xi=0} = 0$$

and

$$\frac{1}{2}\frac{\partial^2 \mathfrak{I}_{yy}}{\partial\xi^2}\bigg|_{\xi=0} = -\int \frac{p_y^2(1+p^2)^{\frac{1}{2}}}{p_x^3} \frac{\partial f_0}{\partial p_x}\,d^3p + \left[\int \frac{p_y(1+p^2)^{\frac{1}{2}}}{p_x^2} \frac{\partial f_0}{\partial p_x}\,d^3p\right]^2 I_1^{-1}(0). \tag{40}$$

Now,

$$I_1(0) < 0$$

by definition. Thus, in order that $\partial^2 \mathfrak{I}_{yy}/\partial\xi^2$ be positive,

it is both necessary and sufficient that

$$\int \frac{p_y^2(1+p^2)^{\frac{1}{2}}}{p_x^3} \frac{\partial f_0}{\partial p_x} d^3p < 0. \tag{41}$$

It is algebraically complicated, but quite straightforward, to show that (41) is obeyed. The method of proof consists of changing to spherical momentum coordinates, making use of (32), and expanding $f_0(\mathbf{p})$ as in (29) and (30). Consequently,

$$\left.\frac{\partial^2 \mathfrak{I}_{yy}}{\partial \xi^2}\right|_{\xi=0} > 0$$

and thus

$$\mathfrak{I}_{yy}(i\xi) > -g_x.$$

Likewise it can be shown that $\mathfrak{I}_{zz}(i\xi) > -g_x$ and $\mathfrak{I}_{yy}(i\xi) = \mathfrak{I}_{zz}(i\xi)$, to order ξ^2. It can also be shown that $\mathfrak{I}_{yz}(i\xi) = O(\xi^4)$. As a result, to order ξ^2, the dispersion relation becomes

$$[q + \tfrac{1}{2}(\mathfrak{I}_{yy} + \mathfrak{I}_{zz})]^2 = 0. \tag{42}$$

Since $\mathfrak{I}_{yy}(i\xi) + \mathfrak{I}_{zz}(i\xi) > -2g_x$, it follows that the q corresponding to $\beta = i\xi$ ($\xi > 0$) is less than g_x. Consequently no real k exists for the given β value. Thus there are no unstable transverse waves which have an imaginary, but small, phase velocity and a positive wavenumber.

5. CONCLUSION

Under the assumption that the plasma is stable against electrostatic waves, it has been shown that the plasma supports a class of growing transverse waves unless the number of protons moving into a given solid angle and their harmonic mean velocity are independent of the spatial orientation of the solid angle. This physical statement is identical to the result which obtains in the case of a nonrelativistic, even parity, plasma[4] except that the statement is now true for all plasmas both relativistic and nonrelativistic. The mathematical formalism of the statement is changed in the relativistic case so that the conditions for stability remain invariant under a Lorentz transformation.

There are three interesting points worth noting.

First, in principle it is possible to have pressure isotropy in the relativistic plasma and still have an electromagnetically unstable situation. In practice it is difficult to conceive of a physical situation where this will occur.

Secondly, we cannot state definitely that a relativistic plasma will be stable if its distribution function satisfies (32) and (38) since no account has been given of those values of k for which the phase velocity is different from zero. We can however, state that if the distribution function does *not* satisfy (32) and (38) then the plasma will be unstable.

Thirdly, we have considered only those waves for which $|> \sigma \gg |\beta|$. There still remains the class of slow electromagnetic waves for which $|\beta| \ll 1$ but $|\beta| \gtrsim \sigma$. No account has been given of these waves. Also we have not considered distribution functions which are not of even parity.

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Unitary Representations of $SL(2, C)$ in an $E(2)$ Basis

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Starting from the functional representation of Gel'fand and Naimark, the unitary irreducible representations of $SL(2, C)$ are described in a basis of the subgroup $E(2) \otimes D$, where $E(2) \otimes D$ is the subgroup of all 2×2 matrices of the form $\begin{pmatrix} \alpha & 0 \\ \gamma & \delta \end{pmatrix}$, $\alpha\delta = 1$. Physically, this is the subgroup into which $SL(2, C)$ degenerates at infinite momentum and may be thought of as the 2-dimensional Euclidean group together with its dilations. Advantages to using the $E(2) \otimes D$ basis are: (1) It is convenient to calculate form factors; (2) the generators of $E(2) \otimes D$ are represented either multiplicatively or by first-order differential operators and are independent of the values of the $SL(2, C)$ Casimir operators; (3) the principal and supplementary series of $SL(2, C)$ are treated on the same footing and, in particular, have the same inner product; and (4) the transformation coefficients to the usual angular-momentum basis are related to Bessel functions. The $E(2) \otimes D$ is used to compute explicitly the finite matrix elements of an arbitrary Lorentz transformation and to investigate the structure of vector operators in unitary representation of $SL(2, C)$.

1. INTRODUCTION

The infinite-dimensional unitary irreducible representations of $SL(2, C)$ have been studied in general by Gel'fand and Naimark[1,2] using a space of infinitely differentiable functions $f(z)$, where $z = x + iy$, and x, y are two real independent variables. In this paper we start from this space and describe the unitary irreducible representations of $SL(2, C)$ in a basis which is diagonal with respect to the subgroup $E(2) \otimes D$ consisting of all 2×2 matrices of the form $\begin{pmatrix} \alpha & 0 \\ \gamma & \delta \end{pmatrix}$, $\alpha\delta = 1$. There are several reasons for using the $E(2) \otimes D$ basis.[3] Physically, $E(2) \otimes D$ is the subgroup into which $SL(2, C)$ degenerates in the infinite-momentum limit suggested for the saturation-of-current algebra.[4,5] [$E(2)$ may be thought of as the 2-dimensional Euclidean group and D as its dilation group.] The $E(2) \otimes D$ basis is also a convenient basis to calculate form factors at any momentum in those theories in which particles are assigned to representations of $SL(2, C)$.[6] Mathematically, in this basis the $E(2) \otimes D$ generators are either multiplicative operators or differential operators of first order and they are independent of the values of the Casimir operators of $SL(2, C)$. [The latter feature reflects the fact that it is the same unique unitary representation of $E(2) \otimes D$ which occurs in all unitary representations of $SL(2, C)$.] Furthermore, in the $E(2) \otimes D$ basis the principal and supplementary series of unitary representations of $SL(2, C)$ are treated on the same footing. In particular, the $E(2) \otimes D$ inner product is local and is the same for both series.

In Sec. 2 we describe the physical meaning of the $E(2) \otimes D$ subgroup, and in Sec. 3, the relationship between the $E(2) \otimes D$ basis and Gel'fand–Naimark's functional representation is established. In Sec. 4 the transformation functions between the $E(2) \otimes D$ basis and the usual angular-momentum basis are given explicitly. In Secs. 5 and 6, the $E(2) \otimes D$ basis is used to compute the finite matrix elements for an arbitrary Lorentz transformation in the angular-momentum basis and to study the general structure of vector operators in unitary representations of $SL(2, C)$.

2. MOTIVATION FOR $E(2)$

The exploration of the $E(2)$ basis is motivated by the theory of current algebra at infinite momentum of Dashen and Gell-Mann[4] and of Fubini and Furlan,[5] who suggested that the current algebra should be saturated by one-particle states at infinite momentum. It is known that in the infinite-momentum limit the homogeneous Lorentz group $SL(2, C)$ degenerates into a 4-parameter group $E(2) \otimes D$.[7] Mathematically, if we represented the $SL(2, C)$ by its fundamental 2-dimensional representation

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \tag{1}$$

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[1] I. M. Gel'fand and M. A. Naimark, Izv. Akad. Nauk SSSR **11**, 411 (1947).

[2] I. M. Gel'fand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Applications* (Pergamon Press, Inc., London, 1963).

[3] S. J. Chang, J. G. Kuriyan, and L. O'Raifeartaigh, Phys. Rev. **169**, 1275 (1968).

[4] R. F. Dashen and M. Gell-Mann, Phys. Rev. Letters **17**, 340 (1966); in *Proceedings of the Third* (also *Fourth*) *Coral Gables Conference on Symmetry Principles at High Energy, University of Miami, 1966 (1967)* (W. H. Freeman and Co., San Francisco, California, 1966, 1967).

[5] S. Fubini and G. Furlan, Physics **1**, 229 (1965).

[6] For theories based on the unitary representations of $SL(2, C)$, see A. O. Barut and H. Kleinert, Phys. Rev. **156**, 1546 (1967); C. Fronsdal Phys. Rev. **156**, 1653 (1967); Y. Nambu, Progr. Theoret. Phys. (Kyoto) **37**, 368 (1966); Phys. Rev. **160**, 1171 (1967).

[7] See for example, H. Bacry and N. P. Chang, Ann. Phys. (N.Y.) **47**, 407 (1968).

with $\alpha\delta - \beta\gamma = 1$, the $E(2) \otimes D$ subgroup is the subgroup $\beta = 0$. A simple physical interpretation is the following: For large momentum the mass term is small in comparison with the momentum, and, in the limit $p_3 = \infty$, it becomes zero. The $E(2)$ group in $E(2) \otimes D$ is just the little group of the massless particle,[8] and the D in $E(2) \otimes D$ is the group of dilations of the (lightlike) momentum which leaves the direction unchanged. To understand how the group $SL(2, C)$ degenerates at $p_3 \to \pm\infty$ into this subgroup, we consider the acceleration along the z axis. Under this acceleration any operator O transforms according to

$$O \to e^{i\lambda K_3} O e^{-i\lambda K_3}. \tag{2}$$

It is easy to see that the six generators of $SL(2, C)$ can be classified into three pairs according to their transformation laws:

$$\begin{aligned} E_{1,2} &\to e^{\lambda} E_{1,2}, \\ L_3, K_3 &\to L_3, K_3, \\ F_{1,2} &\to e^{-\lambda} F_{1,2}, \end{aligned} \tag{3}$$

where

$$E_1 = K_1 + L_2, \quad E_2 = K_2 - L_1, \tag{4}$$

$$F_1 = K_1 - L_2, \quad F_2 = K_2 + L_1, \tag{5}$$

and

$$\begin{aligned} [L_i, L_j] = i\epsilon_{ijk} L_k, \quad [L_i, K_j] = i\epsilon_{ijk} K_k, \\ [K_i, K_j] = -i\epsilon_{ijk} L_k \end{aligned} \tag{6}$$

form the conventional basis for the $SL(2, C)$ algebra. Since there are no elements of the algebra which are multiplied by a factor $e^{\pm 2\lambda}$ in (3), it follows that the E's and F's, respectively, must commute among themselves. A similar argument leads to the conclusion that the commutator of an $E(F)$ with L_3 or K_3 is again an $E(F)$. This is why $E_{1,2}$, L_3, and K_3 close to form a subalgebra. A similar argument applies for any vector V_μ, such as the current or the 4-momentum. The transformation (2) yields

$$\begin{aligned} V_{1,2} &\to V_{1,2}, \\ V_0 \pm V_3 &\to e^{\pm\lambda}(V_0 \pm V_3), \end{aligned}$$

so that $(E, V_0 + V_3)$ and $(F, V_0 - V_3)$ form commuting sets.

3. CONSTRUCTION OF THE $E(2)$ BASIS

In this section, we consider the unitary representation of $SL(2, C)$ in the infinite-momentum $E(2)$ basis. We choose our vectors $\langle \epsilon_1, \epsilon_2 |$ as the eigenstates of the generators E_1 and E_2 with corresponding eigenvalues ϵ_1, ϵ_2. The spectrum of E_1 and E_2 is the continuum $(-\infty, \infty)$, and the usefulness of $E(2)$ rests on the fact that, because the ϵ's are continuous, the usual algebraic equations reduce in the $E(2)$ basis to differential equations. To construct the explicit representations for the generators of the $SL(2, C)$ in the $E(2)$ basis, we start from Gel'fand and Naimark's classical approach of representing $SL(2, C)$ by transformations on infinitely differentiable functions. Gel'fand and Naimark showed that it is always possible to describe an irreducible representation of $SL(2, C)$ by proper transformations on a set of infinitely differentiable test functions $\phi(z, \bar{z})$, where $z = x + iy$, $\bar{z} = x - iy$, x and y being two real independent variables, and for notational convenience we write $\phi(z, \bar{z})$ as $\phi(z)$. If the Lorentz transformation g is defined by the 2×2 unimodular matrix

$$g = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix},$$

then, in a general irreducible representation of $SL(2, C)$, it is represented by the transformation[9]

$$T(g)\phi(z) = (\beta z + \delta)^{n_1 - 1}(\bar{\beta} z + \bar{\delta})^{n_2 - 1} \phi\left(\frac{\alpha z + \gamma}{\beta z + \delta}\right), \tag{7}$$

where

$$n_1 = j_0 + c, \quad n_2 = -j_0 + c$$

are Casimir operators.[10] To find the connection between this functional representation and our $E(2)$ representation, we write Eq. (7) in infinitesimal form:

$$\begin{aligned} E_+ &= 2i \frac{\partial}{\partial \bar{z}}, \\ E_- &= 2i \frac{\partial}{\partial z}, \\ L_3 &= \left[z \frac{\partial}{\partial z} - \bar{z} \frac{\partial}{\partial \bar{z}} + \frac{1}{2}(n_2 - n_1) \right], \\ K_3 &= i\left[1 + z \frac{\partial}{\partial z} + \bar{z} \frac{\partial}{\partial \bar{z}} - \frac{1}{2}(n_1 + n_2) \right], \\ F_+ &= \frac{1}{i}\left[2z^2 \frac{\partial}{\partial z} - 2(n_1 - 1)z \right], \\ F_- &= \frac{1}{i}\left[2\bar{z}^2 \frac{\partial}{\partial \bar{z}} - 2(n_2 - 1)\bar{z} \right], \end{aligned}$$

where

$$E_\pm = E_1 \pm iE_2, \quad F_\pm = F_1 \pm iF_2.$$

[8] E. Wigner, Ann. Math. **40**, 149 (1939).

[9] I. M. Gel'fand, M. I. Graev, and N. Ya. Vilenkin, *Generalized Functions* (Academic Press Inc., New York, 1966), Vol. 5, Chap. III.

[10] The Casimir operator j_0 is the smallest value of l (spin) in the decomposition of the irreducible representation of $SL(2, C)$ into the representations of $SU(2)$. The Casimir operator c is chosen to be imaginary for the principal series.

So far, we have not discussed scalar products. We now wish to emphasize that in the z space the scalar products for principal series ($n_1 = -\bar{n}_2$) and supplementary series ($n_1 = n_2 =$ real number c, $0 < |c| < 1$) of unitary representations of $SL(2, C)$ are quite different. The positive scalar product[9] for the principal series is given by

$$(\psi, \varphi) = \frac{i}{2}\int \varphi(z)\bar{\psi}(z)\, dz\, d\bar{z}$$

and for the supplementary series it is given by

$$(\psi, \varphi) = \left(\frac{i}{2}\right)^2 \int |z_1 - z_2|^{-2c-2}\, \varphi(z_1)\bar{\psi}(z_2)\, dz_1\, d\bar{z}_1\, dz_2\, d\bar{z}_2 .$$

The highly nonlocal structure of the scalar product in the supplementary series indicates that the z space is not suitable for actual computation.

The infinite-momentum $E(2)$ basis is characterized by the condition that E_1 and E_2 are represented multiplicatively. Now since in the z basis E_1 and E_2 are represented by two independent first-order differential operators, this suggests that to reach the $E(2)$ basis we should make a Fourier transformation. Making the Fourier transformation

$$\phi(w) = \int \frac{i}{2}\frac{dz\, d\bar{z}}{2\pi}\, e^{\frac{1}{2}i(w\bar{z}+\bar{w}z)}\phi(z),$$
$$w = w_1 + iw_2,$$

we find the following realization in the Fourier-transformed space:

$$E_+ = w,$$
$$E_- = \bar{w},$$
$$L_3 = \left[w\frac{\partial}{\partial w} - \bar{w}\frac{\partial}{\partial \bar{w}} + \frac{1}{2}(n_2 - n_1)\right],$$
$$K_3 = \frac{1}{i}\left[1 + w\frac{\partial}{\partial w} + \bar{w}\frac{\partial}{\partial \bar{w}} + \frac{1}{2}(n_1 + n_2)\right],$$
$$F_+ = 4\left(\frac{\partial}{\partial \bar{w}}\bar{w}\frac{\partial}{\partial \bar{w}} + n_1\frac{\partial}{\partial \bar{w}}\right),$$
$$F_- = 4\left(\frac{\partial}{\partial w}w\frac{\partial}{\partial w} + n_2\frac{\partial}{\partial w}\right).$$

The scalar product in the w space reduces to

$$(\psi, \varphi) = \frac{i}{2}\int \varphi(w)\bar{\psi}(w)\, dw\, d\bar{w} \tag{8}$$

for the principal series, and

$$(\psi, \varphi) \sim \frac{i}{2}\int |w|^{2c}\, \varphi(w)\bar{\psi}(w)\, dw\, d\bar{w}$$

for the supplementary series. E_1 and E_2 (also $E_\pm$) are represented multiplicatively in this space, as required. However, the w basis is not the final basis that we are looking for. The reasons are: (1) the additional terms $(1/2)(n_2 - n_1)$ and $(1/2i)(n_1 + n_2)$ appearing in the representations of L_3 and K_3 should be removed in order to give a simpler basis for the subgroup $E(2) \otimes D$; (2) although the scalar products for the principal and supplementary series are now local, they are still different. The nice feature, however, is that by making the similarity transformation

$$\phi(\epsilon_\pm) = \bar{w}^{\frac{1}{2}n_1} w^{\frac{1}{2}n_2}\phi(w), \quad \epsilon_\pm = \epsilon_1 \pm i\epsilon_2 = (w, \bar{w}), \tag{9}$$

these two disadvantages can be removed simultaneously. The transformation (9) yields

$$E_\pm = \epsilon_\pm,$$
$$L_3 = \left(\epsilon_+\frac{\partial}{\partial \epsilon_+} - \epsilon_-\frac{\partial}{\partial \epsilon_-}\right),$$
$$K_3 = \frac{1}{i}\left(1 + \epsilon_+\frac{\partial}{\partial \epsilon_+} + \epsilon_-\frac{\partial}{\partial \epsilon_-}\right), \tag{10}$$
$$F_+ = 4\frac{\partial}{\partial \epsilon_-}\epsilon_-\frac{\partial}{\partial \epsilon_-} - \frac{n_1^2}{\epsilon_-},$$
$$F_+ = 4\frac{\partial}{\partial \epsilon_+}\epsilon_+\frac{\partial}{\partial \epsilon_+} - \frac{n_2^2}{\epsilon_+},$$

for the infinitesimal generators, and

$$(\psi, \varphi) = \int d\epsilon_1\, d\epsilon_2 \varphi(\epsilon_\pm)\bar{\psi}(\epsilon_\pm)$$

for the inner product for both the principal and supplementary series. It is now natural to introduce a Dirac basis[11] $\langle \epsilon_1, \epsilon_2|$ such that

$$\phi(\epsilon_\pm) = \langle \epsilon_1, \epsilon_2 \,|\, \phi\rangle,$$
$$\langle \epsilon_1', \epsilon_2' \,|\, \epsilon_1, \epsilon_2\rangle = \delta(\epsilon_1' - \epsilon_1)\delta(\epsilon_2' - \epsilon_2).$$

In terms of ϵ_1, ϵ_2 basis, Eqs. (10) can be written as

$$\langle \epsilon_1, \epsilon_2| E_{1,2} = \epsilon_{1,2}\langle \epsilon_1, \epsilon_2|,$$
$$\langle \epsilon_1, \epsilon_2| L_3 = \frac{1}{i}\left(\epsilon_1\frac{\partial}{\partial \epsilon_2} - \epsilon_2\frac{\partial}{\partial \epsilon_1}\right)\langle \epsilon_1, \epsilon_2|,$$
$$\langle \epsilon_1, \epsilon_2| L_3 = \frac{1}{i}\left(1 + \epsilon_1\frac{\partial}{\partial \epsilon_1} + \epsilon_2\frac{\partial}{\partial \epsilon_2}\right)\langle \epsilon_1, \epsilon_2|,$$
$$\langle \epsilon_1, \epsilon_2| F_1 = \left[\epsilon_1\frac{\partial^2}{\partial \epsilon_1^2} + 2\epsilon_2\frac{\partial^2}{\partial \epsilon_1 \partial \epsilon_2} - \epsilon_1\frac{\partial^2}{\partial \epsilon_2^2} + 2\frac{\partial}{\partial \epsilon_1} - \frac{(j_0^2 + c^2)\epsilon_1 + 2ij_0 c\epsilon_2}{\epsilon^2}\right]\langle \epsilon_1, \epsilon_2|,$$
$$\langle \epsilon_1, \epsilon_2| F_2 = \left[\epsilon_2\frac{\partial^2}{\partial \epsilon_2^2} - \epsilon_2\frac{\partial^2}{\partial \epsilon_1^2} + 2\epsilon_1\frac{\partial^2}{\partial \epsilon_1 \partial \epsilon_2} + 2\frac{\partial}{\partial \epsilon_2} - \frac{(j_0^2 + c^2)\epsilon_2 - 2ij_0 c\epsilon_1}{\epsilon^2}\right]\langle \epsilon_1, \epsilon_2|,$$
$$\epsilon^2 = \epsilon_1^2 + \epsilon_2^2, \tag{11}$$

[11] See, for example, P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, London, 1958).

with the same inner product; and in terms of the polar coordinates ϵ, $L_3' = m$, Eq. (10) takes the form

$$\langle \epsilon, m|\, E_\pm = \epsilon\, \langle \epsilon, m \mp 1|,$$
$$\langle \epsilon, m|\, L_3 = m\, \langle \epsilon, m|,$$
$$\langle \epsilon, m|\, K_3 = \frac{1}{i}\left(1 + \epsilon \frac{\partial}{\partial \epsilon}\right)\langle \epsilon, m|,$$
$$\langle \epsilon, m|\, F_\pm = \left[\epsilon \frac{\partial^2}{\partial \epsilon^2} + (3 \mp 2m)\frac{\partial}{\partial \epsilon} + \frac{(m \mp 1)^2 - (j_0 \pm c)^2}{\epsilon}\right]\langle \epsilon, m \mp 1|, \quad (12)$$

where the inner product is now

$$\langle \epsilon', m' \mid \epsilon, m\rangle = \delta_{m'm}(1/\epsilon)\delta(\epsilon' - \epsilon)$$

for both series. The bases (11) and (12) are the Cartesian and polar forms, respectively, of the required $E(2) \otimes D$ basis. The $E(2) \otimes D$ basis has the following features:

(i) The generators $E_{1,2}$ and L_3, K_3 of $E(2) \otimes D$ are multiplicative and first-order differential operators, respectively.

(ii) These four generators are independent of the values of the Casimir operators j_0, c of $SL(2, C)$.

(iii) The inner products are the same for the principal and supplementary series.

(iv) The transformation functions from the (ϵ, m) to the angular-momentum basis are related to Bessel functions (Sec. 4).

These are the advantages of the $E(2) \otimes D$ basis. Of course, in this basis, the two extra $SL(2, C)$ generators $F_\pm$ are quite complicated second-order differential operators and are strongly dependent on the Casimir numbers, but for many purposes this is not a serious complication.

We conclude this section with the following observation: By making an appropriate similarity transformation in the original z basis, one can obtain a k basis $k = k_1 + ik_2$ in which all the $SL(2, C)$ generators are represented by first-order differential operators, and the dependence on the Casimir operators has been removed from L_3 and K_3. In this basis, we have for the Cartesian form

$$\langle k_1, k_2|\, E_1 = \left(i\frac{\partial}{\partial k_1} + \frac{ak_1 + bk_2}{2k^2}\right)\langle k_1, k_2|,$$
$$\langle k_1, k_2|\, E_2 = \left(i\frac{\partial}{\partial k_2} + \frac{ak_2 - bk_1}{2k^2}\right)\langle k_1, k_2|,$$
$$\langle k_1, k_2|\, L_3 = \frac{1}{i}\left(k_1\frac{\partial}{\partial k_2} - k_2\frac{\partial}{\partial k_1}\right)\langle k_1, k_2|,$$
$$\langle k_1, k_2|\, K_3 = i\left(1 + k_1\frac{\partial}{\partial k_1} + k_2\frac{\partial}{\partial k_2}\right)\langle k_1, k_2|,$$
$$\langle k_1, k_2|\, F_1 = \left\{\frac{1}{i}\left[(k_1^2 - k_2^2)\frac{\partial}{\partial k_1} + 2k_1k_2\frac{\partial}{\partial k_2} + 2k_1\right] + \frac{1}{2}(ak_1 - bk_2)\right\}\langle k_1, k_2|,$$
$$\langle k_1, k_2|\, F_2 = \left\{\frac{1}{i}\left[(k_2^2 - k_1^2)\frac{\partial}{\partial k_2} + 2k_1k_2\frac{\partial}{\partial k_1} + 2k_2\right] + \frac{1}{2}(ak_2 + bk_1)\right\}\langle k_1, k_2|, \quad (13)$$

where a, b are real, satisfying

$$\tfrac{1}{4}(b^2 - a^2) = j_0^2 + c^2, \quad \tfrac{1}{4}ab = j_0 ic.$$

For the polar form we have

$$\langle k, m|\, E_\pm = \left(i\frac{\partial}{\partial k} \mp \frac{i(m \mp 1)}{k} + \frac{a \mp ib}{2k}\right)\langle k, m \mp 1|,$$
$$\langle k, m|\, L_3 = m\, \langle k, m|,$$
$$\langle k, m|\, K_3 = i\left(1 + k\frac{\partial}{\partial k}\right)\langle k, m|,$$
$$\langle k, m|\, F_\pm = \left\{\frac{1}{i}\left[k^2\frac{\partial}{\partial k} \pm (m \pm 1)k\right] + \frac{k}{2}(a \pm ib)\right\}\langle k, m \mp 1|. \quad (14)$$

Furthermore, the inner product in the k basis takes the simple form

$$\langle k' \mid k\rangle = \delta(k_1' - k_1)\delta(k_2' - k_2),$$
$$\langle k', m' \mid k, m\rangle = \delta_{m'm}(1/k)\delta(k' - k),$$

for both the principal and supplementary series. Thus the principal and supplementary series can also be described simultaneously in a basis which is closely related to the z basis. Of course, in the k basis, the $E(2)$ translations are not represented multiplicatively and are not independent of the Casimir numbers. On the other hand, the k basis has the advantage that the self-adjointness of the $SL(2, C)$ operators can be verified *directly*, essentially because these operators are first-order differential operators. In fact, the self-adjointness of the generators is guaranteed in all the bases that we have used by construction, but it is not so easy to verify it in the ϵ basis for example, because of the complexity of $F_\pm$. In conclusion, we note that the transformation coefficients between the polar k and ϵ bases are

$$\langle k, m' \mid \epsilon, m\rangle = \delta_{m'm} i^{l-m}(k\epsilon)^{\frac{1}{2}ia} J_{m+\frac{1}{2}b}(k\epsilon),$$

and that in these bases the finite acceleration $\exp i\lambda K_3$

has the simple forms

$$\langle \epsilon, m| e^{i\lambda K_3} = e^{\lambda} \langle e^{\lambda}\epsilon, m|,$$
$$\langle k, m| e^{i\lambda K_3} = e^{-\lambda} \langle e^{-\lambda}k, m|, \tag{15}$$

which are very useful for computing its finite matrix elements in the angular-momentum basis (Sec. 4).

4. TRANSFORMATION COEFFICIENTS

In this section we find the transformation coefficients between the $E(2) \otimes D$ basis and the usual angular-momentum basis of $SL(2, C)$. Since in the angular-momentum basis

$$L_3 = \frac{1}{i}\left(\epsilon_1 \frac{\partial}{\partial \epsilon_2} - \epsilon_2 \frac{\partial}{\partial \epsilon_1}\right)$$

is diagonal, it is obviously most convenient to take the ϵ basis in its polar form.

To evaluate the transformation coefficients between the base vector $\langle \epsilon, m|$ and the usual angular-momentum base vector $\langle l, m|$, we use the standard technique first to evaluate $\langle \epsilon, l \,|\, l, l\rangle$. Recalling that

$$\langle \epsilon, l+1| L_+ |l, l\rangle = 0, \tag{16}$$

we have

$$\left[\epsilon \frac{d^2}{d\epsilon^2} + (1-2l)\frac{d}{d\epsilon} + \frac{l^2 - (j_0 + c)^2}{\epsilon} - \epsilon\right] \times \langle \epsilon, l \,|\, l, l\rangle = 0.$$

The only solution which is square-integrable at $\epsilon = \infty$ is

$$\langle \epsilon, l \,|\, l, l\rangle = c_l \epsilon^l K_{j_0+c}(\epsilon), \tag{17}$$

where $K_{j_0+c}(\epsilon)$ is the modified Bessel function of order $j_0 + c$,[12] and

$$c_l = 2^{-l}[2(2l+1)!]^{+\frac{1}{2}}[\Gamma(j_0 + l + 1)\Gamma(l + c + 1) \times \Gamma(l - c + 1)\Gamma(l - j_0 + 1)]^{-\frac{1}{2}}. \tag{18}$$

The general transformation function $\langle \epsilon, m \,|\, l, m\rangle$ can be obtained from $\langle \epsilon, l \,|\, l, l\rangle$ by the repeated use of the lowering operator L_-, giving

$$\begin{aligned}
&\langle \epsilon, m \,|\, l, m\rangle \\
&= [(l-m)(l+m+1)]^{-\frac{1}{2}} \langle \epsilon, m| L_- |l, m+1\rangle \\
&= \frac{i}{2}[(l-m)(l+m+1)]^{-\frac{1}{2}}\left[\epsilon \frac{d^2}{d\epsilon^2} + (2m+3)\frac{d}{d\epsilon} \right. \\
&\quad \left. + \frac{(m+1)^2 - (j_0 - c)^2}{\epsilon} - \epsilon\right]\langle \epsilon, m+1 \,|\, l, m+1\rangle \\
&= \left(\frac{i}{2}\right)^{l-m}\left[\frac{(l+m)!}{(l-m)!\,(2l)!}\right]^{\frac{1}{2}} \epsilon^{-m} B^{l-m}_{j_0-c}(\epsilon)\epsilon^l \langle \epsilon, l \,|\, l, l\rangle,
\end{aligned} \tag{19}$$

where

$$B_\nu(\epsilon) = \frac{d^2}{d\epsilon^2} + \frac{1}{\epsilon}\frac{d}{d\epsilon} - \frac{\nu^2}{\epsilon^2} - 1 \tag{20}$$

is the Bessel operator. Since these functions are related simply to Bessel functions, we can transform our result from one basis to another very easily. It is rather straightforward to verify that $\langle \epsilon, m' \,|\, l, m\rangle$ are square-integrable functions of ϵ, and that they form an orthonormal basis (see Appendices B and C).

The transformation function $\langle k, m \,|\, l, m\rangle$ can be computed analogously:

$$\begin{aligned}
&\langle k, m \,|\, l, m\rangle \\
&\quad = \frac{1}{\Gamma(m + \frac{1}{2}b + 1)} \\
&\qquad \times \left[\frac{(l+m)!\, 2(2l+1)\Gamma(l + \frac{1}{2}b + 1)}{(l-m)!\,\Gamma(l + 1 - \frac{1}{2}b)}\right]^{\frac{1}{2}} \\
&\qquad \times k^{m+\frac{1}{2}(b+ia)}(1+k^2)^{-l-1-\frac{1}{2}ia} \\
&\qquad \times F(-l+m, -l+\tfrac{1}{2}b; m+\tfrac{1}{2}b+1; -k^2) \\
&\quad = 2^{-m-1-\frac{1}{2}ia}\left[\frac{(l+m)!\,(l-m)!\,2(2l+1)}{\Gamma(l+1+\frac{1}{2}b)\Gamma(l+1-\frac{1}{2}b)}\right]^{\frac{1}{2}} \\
&\qquad \times (1-x)^{\frac{1}{2}m+\frac{1}{4}(b+ia)}(1+x)^{\frac{1}{2}m+1-\frac{1}{4}(b-ia)} \\
&\qquad \times P_{l-m}^{(m+\frac{1}{2}b, m-\frac{1}{2}b)}(x),
\end{aligned} \tag{21}$$

where $x = (1-k^2)/(1+k^2)$. The $F(a, b; c; z)$ are hypergeometric functions and $P_l^{(\alpha,\beta)}(x)$ are Jacobi polynomials.[12] The orthonormality condition can be verified easily by using the orthonormality conditions of the Jacobi polynomials. Note that the transformation functions between the $E(2)$ and the $SU(2)$ bases are related simply to Bessel functions; in the k basis and also in the $\theta - \varphi$ basis introduced by Ström,[13] these functions are related to the hypergeometric functions. This is one of the advantages of the $E(2)$ basis mentioned earlier.

We verify the conditions on the Casimir operators for which an irreducible representation of $SL(2, C)$ is unitary. The requirement that $\langle \epsilon, m \,|\, l, m\rangle$ be well-defined and square-integrable (see Appendix A) implies that

$$2j_0 \text{ and } l - j_0 \text{ are nonnegative integers,}$$

and

$$|\mathrm{Re}\, c| < 1.$$

The unitarity condition implies

$$(j_0 + c)^{*2} = (j_0 - c)^2. \tag{22}$$

These conditions lead immediately to the following

[12] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, Inc., New York, 1965).

[13] S. Ström, Arkiv Fysik **34**, 215 (1967).

two classes of unitary representations:

(1) Principal series: $j_0 =$ integer or half-integer, $c =$ pure imaginary;

(2) Supplementary series: $j_0 = 0$, c is real and $0 < |c| < 1$.

Finally, we should mention that, although we have confined ourselves here to the case of unitary representations of $SL(2, C)$, the $E(2) \otimes D$ basis actually has a somewhat wider domain of applicability. For example, it can be used for nonunitary representations of $SL(2, C)$, whose restrictions to $E(2) \otimes D$ are unitary.

5. FINITE MATRIX ELEMENTS

In this section, we wish to apply our infinite-momentum basis to some specific problems. In particular, we compute the matrix elements of a finite Lorentz transformation in the angular-momentum basis. It is known that an arbitrary Lorentz transformation can be reduced to the standard form

$$L = e^{-i\omega' \cdot \mathbf{J}} e^{-i\lambda K_3} e^{-i\omega \cdot \mathbf{J}},$$

where $e^{-i\omega' \cdot \mathbf{J}}$ and $e^{-i\omega \cdot \mathbf{J}}$ stand for the usual 3-dimensional rotations, and $e^{-i\lambda K_3}$ for an acceleration along the z axis. Since the operation of rotation on angular-momentum base vectors $\langle l, m|$ is well known, the only nontrivial matrix elements to be computed are

$$\langle l', m| e^{-i\lambda K_3} |l, m\rangle.$$

For definiteness, we assume $l' \geq l$. We first compute the special case of $m = l$. In evaluating these matrix elements, we transform the base vectors $\langle l, m|$ from the angular-momentum basis to the infinite-momentum basis, giving

$$\langle l', l| e^{-i\lambda K_3} |l, l\rangle = \int_0^\infty \epsilon \, d\epsilon \langle l', l \,|\, \epsilon, l\rangle \langle \epsilon, l| e^{-i\lambda K_3} |l, l\rangle. \quad (23)$$

Making use of Eqs. (15) and (19), we have

$$\begin{aligned}\langle l', l| e^{-i\lambda K_3} |l, l\rangle &= \left(\frac{1}{2i}\right)^{l'-l} \left[\frac{(l'+l)!}{(l'-l)!\,(2l')!}\right]^{\frac{1}{2}} c_l' c_l \beta^{l+1} \\ &\times \int_0^\infty \epsilon \, d\epsilon \{B_{j_0+c}(\epsilon)^{l'-l} [\epsilon^{2l'} K_{j_0-c}(\epsilon)]\} K_{j_0+c}(\beta\epsilon) \\ &= \left(\frac{1}{2i}\right)^{l'-l} \left[\frac{(l'+l)!}{(l'-l)!\,(2l')!}\right]^{\frac{1}{2}} c_l' c_l \beta^{l+1} \\ &\times \int_0^\infty \epsilon \, d\epsilon \, \epsilon^{2l'} K_{j_0-c}(\epsilon) B_{j_0+c}(\epsilon)^{l'-l} K_{j_0+c}(\beta\epsilon), \quad (24)\end{aligned}$$

where, in the derivation of the last equation, we have used integration by parts. It is easy to see that the surface terms always drop out automatically. Now, we use the property that

$$\begin{aligned}\beta_{j_0+c}(\epsilon) K_{j_0+c}(\beta\epsilon) &= [\beta^2 B_{j_0+c}(\beta\epsilon) + \beta^2 - 1] K_{j_0+c}(\beta\epsilon) \\ &= -(1-\beta^2) K_{j_0+c}(\beta\epsilon) \quad (25)\end{aligned}$$

and obtain

$$\begin{aligned}\langle l', l| e^{-i\lambda K_3} |l, l\rangle &= \left(\frac{i}{2}\right)^{l'-l} \left[\frac{(l'+l)!}{(l'-l)!\,(2l')!}\right]^{\frac{1}{2}} c_l' c_l \beta^{l+1} (1-\beta^2)^{l'-l} \\ &\times \int_0^\infty \epsilon \, d\epsilon \, \epsilon^{2l'} K_{j_0-c}(\epsilon) K_{j_0+c}(\beta\epsilon). \quad (26)\end{aligned}$$

The definite integral is well known[14] and leads to

$$\begin{aligned}\langle l', l| e^{-i\lambda K_3} |l, l\rangle = i^{l'-l} &\left[\frac{(l'+l)!\,(2l+1)!\,\Gamma(j_0+l'+1)\Gamma(l'+c+1)\Gamma(l'-c+1)\Gamma(l'-j_0+1)}{(l'-l)!\,(2l')!\,(2l'+1)!\,\Gamma(j_0+l+1)\Gamma(l+c+1)\Gamma(l-c+1)\Gamma(l-j_0+1)}\right]^{\frac{1}{2}} \\ &\times \beta^{j_0+c+l+1}(1-\beta^2)^{l'-l} F(j_0+l'+1, l'+c+1; 2l'+2; 1-\beta^2). \quad (27)\end{aligned}$$

The general matrix elements for $m \neq l$ can be obtained through the following recursion formula[15]:

$$\begin{aligned}&\alpha^{l'}_{m,m+1}\alpha^{l}_{m,m+1} \langle l', m| e^{-i\lambda K_3} |l, m\rangle \\ &= \alpha^{l'}_{m+1,m+2}\alpha^{l}_{m+1,m+2} \langle l', m+2| e^{-i\lambda K_3} |l, m+2\rangle \\ &+ \left[2(m+1)\sinh\lambda \frac{\partial}{\partial\lambda} + 2(m+1)\cosh\lambda \right. \\ &\left. + 2i(j_0 ic)\sinh\lambda\right] \langle l', m+1| e^{-i\lambda K_3} |l, m+1\rangle, \quad (28)\end{aligned}$$

where

$$\alpha^{l}_{m',m} = [(l-m')(l+m)]^{\frac{1}{2}}.$$

The results obtained here have been obtained also by Ström using a different method.

6. VECTOR OPERATORS

In this section, we wish to construct the vector operators in the infinite-dimensional representations of $SL(2, C)$.[2] Even though it is known in principle how to construct vector (and tensor) operators in the infinite-dimensional representation of $SL(2, C)$, it turns out that the actual explicit construction is quite easy in the $E(2)$ basis. Since it is well known that, in general, one can not construct a vector from a single irreducible representation of $SL(2, C)$, we start from

[14] W. Magnus and F. Oberhettinger, *Formulas and Theorems for Special Functions of Mathematical Physics* (Springer, New York, 1966), third ed.

[15] S. Ström, Arkiv Fysik **30**, 267 (1965).

a set of such representations. They are labeled by their Casimir operators j_0, c, but we suppress the j_0, c labels and interpret the numerical coefficients which relate states of different j_0, c as matrices in the j_0, c space. A general 4-vector V_μ satisfies the following commutator relations:

$$[V_0 + V_3, L_3] = [V_0 + V_3, E_\pm] = 0,$$
$$[V_0 + V_3, K_3] = i(V_0 + V_3), \tag{29}$$

$$V_\pm = V_1 \pm iV_2 = \frac{1}{2i}[V_0 + V_3, F_\pm],$$

$$V_0 - V_3 = \frac{1}{2i}[V_-, F_+] = \frac{1}{2i}[V_+, F_-], \tag{30}$$

$$[V_+, F_+] = [V_-, F_-] = 0,$$
$$[V_0 - V_3, F_\pm] = 0. \tag{31}$$

Equation (29) determines the structure of the matrix elements of $V_0 + V_3$ in the $E(2)$ basis, up to a constant matrix G in the (j_0, c) space. We have

$$\langle \epsilon, m| (V_0 + V_3) = G\epsilon \langle \epsilon, m|. \tag{32}$$

The corresponding expressions for $V_\pm$, $V_0 - V_3$ can be obtained from Eqs. (30) as

$$\langle \epsilon, m| V_\pm = \left\{ iG\left(\epsilon \frac{\partial}{\partial \epsilon} + \frac{3 \mp 2m}{2}\right) + \frac{i}{2}[G, (j_0 \pm c)^2]\right\} \langle \epsilon, m \mp 1|,$$

$$\langle \epsilon, m| (V_0 - V_3) = \left\{ -G\left(\epsilon \frac{\partial^2}{\partial \epsilon^2} + 2\frac{\partial}{\partial \epsilon} - \frac{4m^2 - 1}{4\epsilon}\right) - \tfrac{1}{2}[G, (j_0 + c)^2]\left(\frac{\partial}{\partial \epsilon} + \frac{2m + 1}{2\epsilon}\right) - \tfrac{1}{2}[G, (j_0 - c)^2]\left(\frac{\partial}{\partial \epsilon} + \frac{1 - 2m}{2\epsilon}\right) - \frac{1}{4\epsilon}[[G, (j_0 - c)^2], (j_0 + c)^2]\right\} \langle \epsilon, m|. \tag{33}$$

Equations (31) are the consistency requirements. They impose a restriction on G, namely,

$$[[G, \nu_\pm^2], \nu_\pm^2] = 2\{\nu_\pm^2 - \tfrac{1}{4}, G\}, \tag{34}$$

with $\nu_\pm = j_0 \pm c$.

It is straightforward to verify that these two equations are the necessary and sufficient conditions for V_μ transforming as a 4-vector. Equations (34) can be solved symbolically, giving

$$G = f_1(\nu_+, \nu_-) \exp\left(\frac{\partial}{\partial \nu_+} + \frac{\partial}{\partial \nu_-}\right) + f_2(\nu_+, \nu_-) \exp\left(-\frac{\partial}{\partial \nu_+} + \frac{\partial}{\partial \nu_-}\right) + f_3(\nu_+, \nu_-) \exp\left(\frac{\partial}{\partial \nu_+} - \frac{\partial}{\partial \nu_-}\right) + f_4(\nu_+, \nu_-) \exp\left(-\frac{\partial}{\partial \nu_+} - \frac{\partial}{\partial \nu_-}\right),$$

where $f(\nu_+, \nu_-) = f(j_0, c)$ is an arbitrary function of j_0 and c. Operating on the base vector $\langle \epsilon, m; j_0, c|$, we have

$$\langle j_0, c| G = f_1(j_0, c) \langle j_0 + 1, c| + f_2(j_0, c) \langle j_0, c - 1| + f_3(j_0, c) \langle j_0, c + 1| + f_4(j_0, c) \langle j_0 - 1, c|.$$

This indicates that a vector operator can only connect a state of (j_0, c) to other states with $\Delta j_0 = \pm 1$, $\Delta c = 0$, or $\Delta j_0 = 0$, $\Delta c = \pm 1$.[16] It is interesting to recall that the necessary condition for a single unitary irreducible representation to possess a vector operator is given by the requirement that Eq. (34) has $G =$ const as a solution. This leads to

$$G[(j_0 \pm c)^2 - \tfrac{1}{4}] = 0,$$

which implies that only the Majorana representations possess a vector operator.

Up to this point the construction of the vector operators is quite general. However, since the vector operators are very important in constructing infinite-component wave equations, we shall now construct the vector operators for a very special class of representations, namely, the class of parity-doubled unitary irreducible representations

$$(j_0, c) \oplus (j_0, -c).$$

The criterion that these two representations possess a vector operator is given by

$$j_0 - 1 = -j_0 \quad \text{or} \quad j_0 = \tfrac{1}{2}.$$

The matrix G is now given as a 2×2 matrix in the c space. For $c \neq 0$, there are only two linearly independent operators, and their G matrices can be chosen as

$$G_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad G_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{35}$$

[16] These selection rules can also be obtained easily by sandwiching Eqs. (34) between states with eigenvalues ν', ν, giving $(\nu' \pm \nu)^2 = 1$, as required.

The vector operators are then determined completely by Eq. (33), with

$$[G_1, (j_0 \pm c)^2] = \mp 2icG_2,$$
$$[G_2, (j_0 \pm c)^2] = \pm 2icG_1,$$
$$[[G_{1,2}, (j_0 + c)^2], (j_0 - c)^2] = 4(ic)^2 G_{1,2},$$

where G_1, G_2 are the 2×2 matrices in (35).

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APPENDIX A

In this appendix we wish to verify that the transformation functions $\langle \epsilon, m \mid l, m \rangle$ are well defined when we make the restrictions

$$2j_0 = \text{nonnegative integer},$$
$$l - j_0 = \text{nonnegative integer}, \qquad \text{(A1)}$$

and

$$|\mathrm{Re}\, c| < 1,$$

What this means is the following: according to the text, the transformation functions are determined by the requirements

$$\langle \epsilon, l + 1 | L_+ | l, l \rangle = 0 \qquad \text{(A2)}$$

and

$$\langle \epsilon, m \mid l, m \rangle = \text{const}\, \epsilon^{-m} B^{l-m}_{j_0-c}(\epsilon) \epsilon^l \langle \epsilon, l \mid l, l \rangle. \qquad \text{(A3)}$$

But we could also construct our transformation functions from the state of the lowest eigenvalue $m = -l$, using

$$\langle \epsilon, -l - 1 | L_- | l, -l \rangle = 0 \qquad \text{(A4)}$$

and step up, and these two procedures should lead to the same results. In other words, the transformation functions constructed according to Eqs. (A2) and (A3) should satisfy (A4) automatically. This is a consistency requirement which eventually determines the possible eigenvalues of the Casimir operator j_0. In the next two sections, we verify that, under these conditions, these transformation functions are square-integrable and form an orthonormal basis.

Let us now check the validity of Eq. (A4) under the assumption that we have constructed our transformation functions according to Eqs. (A1) and (A2), giving

$$\langle \epsilon, m \mid l, m \rangle = c_{lm} \epsilon^{-m} B_{j_0-c}(\epsilon)^{l-m} \epsilon^{2l} K_{j_0+c}(\epsilon).$$

Equation (A4) now takes the form

$$B_{j_0-c}(\epsilon)^{2l+1} \epsilon^{2l} K_{j_0+c}(\epsilon) = 0. \qquad \text{(A5)}$$

To check (A5), we make use of the identity

$$K_{j_0+c} = \epsilon^{j_0+c} \left(\frac{1}{\epsilon} \frac{d}{d\epsilon} \right)^{2j_0} (\epsilon^{j_0-c} K_{j_0-c}), \qquad \text{(A6)}$$

and have

$$\begin{aligned} B_{j_0-c}(\epsilon)^{2l+1} \epsilon^{2l} K_{j_0+c}(\epsilon) &= B_{j_0-c}(\epsilon)^{2l+1} \epsilon^{2l+j_0+c} \left(\frac{1}{\epsilon} \frac{d}{d\epsilon} \right)^{2j_0} (\epsilon^{j_0-c} K_{j_0-c}) \\ &= B_{j_0-c}(\epsilon)^{2l+1} \left(\epsilon \frac{d}{d\epsilon} - 2l - j_0 - c + 2 \right) \\ &\quad \times \left(\epsilon \frac{d}{d\epsilon} - 2l - j_0 - c + 4 \right) \cdots \\ &\quad \times \left(\epsilon \frac{d}{d\epsilon} - 2l - j_0 - c + 4j_0 \right) \epsilon^{2(l-j_0)} K_{j_0-c}(\epsilon). \end{aligned} \qquad \text{(A7)}$$

Next, we bring the Bessel operators to the Bessel function. Using the relations

$$\begin{aligned} B_\nu(\epsilon)^n \left(\epsilon \frac{d}{d\epsilon} + a \right) &= \left[\left(\epsilon \frac{d}{d\epsilon} + a + 2n \right) B_\nu + 2n \right] B_\nu^{n-1}, \\ B_\nu(\epsilon)^{2m+1} \epsilon^2 &= \left[\epsilon^2 B_\nu^2 + 4m \left(\epsilon \frac{d}{d\epsilon} + 2m + 3 \right) B_\nu \right. \\ &\quad \left. + 8m(m+1) \right] B_\nu^{2(m-1)+1}, \\ n, 2m &= \text{positive integers}, \end{aligned} \qquad \text{(A8)}$$

we find immediately that we can always bring the Bessel operators through the intermediate factors and have exactly one factor left over to operate directly on the Bessel function K_{j_0-c} and consequently annihilate it. This completes the proof that Eq. (A5), is indeed satisfied. Note that the proof depends critically on the fact that $2j_0$ and $l - j_0$ are nonnegative integers. We therefore conclude that these relations are not only sufficient, but also necessary for the consistency of Eqs. (A2)–(A4).

APPENDIX B

Next, we ask under what condition the transformation functions are square-integrable. Since the transformation functions are effectively the Bessel functions which are analytic between 0 and ∞, we only need to consider the behavior of the transformation functions near the origin and at infinity. For large ϵ, the modified Bessel function behaves asymptotically as

$$\lim_{\epsilon \to \infty} K_\nu(\epsilon) \sim \left(\frac{\pi}{2\epsilon} \right)^{\frac{1}{2}} e^{-\epsilon},$$

which implies that the transformation functions are always square-integrable at infinity. We then study the behavior of the transformation functions at the origin.

It is straightforward, though quite tedious, to verify that the transformation functions behave at the origin as

$$|\langle \epsilon, m \mid l, m\rangle| \sim \epsilon^{|j_0-|m||-|\mathrm{Re}\, c|} \tag{B1}$$

(with an extra $\log \epsilon$ factor in the case that $j_0 \pm c$ is integer). We therefore conclude that the transformation functions are square-integrable with respect to the metric $\epsilon\, d\epsilon$, if

$$|\mathrm{Re}\, c| < 1. \tag{B2}$$

It is worth noting that even though Gel'fand–Naimark's functional representation is applicable to all irreducible representation of $SL(2, C)$, our $E(2)$ basis is comparatively limited. The reason is that even though all the irreducible representations of $SL(2, C)$ can be represented by some classes of infinitely differentiable functions $\phi(z)$, only in certain representations do these functions have Fourier transforms. Equation (B2) is the criterion for them to have Fourier transforms. In particular, the finite-dimensional representations of $SL(2, C)$ are represented in the z basis by polynomials, which do not have proper Fourier transforms. This is understandable, since for finite-dimensional representations E^2 is nilpotent and, consequently, the $E(2)$ basis does not exist in any useful sense.

APPENDIX C

It is now a simple matter to verify that the transformation functions form an orthonormal basis. Since the orthogonality condition for different values of m is trivial, we consider only the transformation functions with the same value of m. Starting from the relations

$$\begin{aligned}
&\langle l, m \mid \epsilon, m\rangle \\
&\quad = \left(\pm \frac{1}{2i}\right)[(l \mp m)(l \pm m + 1)]^{-\frac{1}{2}} \\
&\qquad \times \left[\epsilon \frac{d^2}{d\epsilon^2} + (3 \pm 2m)\frac{d}{d\epsilon} - \epsilon \right. \\
&\qquad \left. + \frac{(m \pm 1)^2 - (j_0 \pm c)^2}{\epsilon}\right]\langle l, m \pm 1 \mid \epsilon, m \pm 1\rangle,
\end{aligned}$$

we have

$$\begin{aligned}
&\int \epsilon\, d\epsilon \langle l', m \mid \epsilon, m\rangle\langle \epsilon, m \mid l, m\rangle, \qquad l' \geq l, \\
&= \int \epsilon\, d\epsilon \frac{1}{2i}[(l' - m)(l' + m + 1)]^{-\frac{1}{2}}\left\{\left[\epsilon \frac{d^2}{d\epsilon^2}\right.\right. \\
&\qquad + (2m + 3)\frac{d}{d\epsilon} - \epsilon + \left.\frac{(m + 1)^2 - (j_0 + c)^2}{\epsilon}\right] \\
&\qquad \left.\times \langle l', m + 1 \mid \epsilon, m + 1\rangle\right\}\langle \epsilon, m \mid l, m\rangle \\
&= \int \epsilon\, d\epsilon \frac{1}{2i}[(l' - m)(l' + m + 1)]^{-\frac{1}{2}} \\
&\qquad \times \langle l', m + 1 \mid \epsilon, m + 1\rangle\left[\epsilon \frac{d^2}{d\epsilon^2} + (1 - 2m)\frac{d}{d\epsilon}\right. \\
&\qquad \left. - \epsilon + \frac{m^2 - (j_0 + c)^2}{\epsilon}\right]\langle \epsilon, m \mid l, m\rangle \\
&\qquad + \left[\frac{d}{d\epsilon}[\epsilon^2\langle l', m + 1 \mid \epsilon, m + 1\rangle]\langle \epsilon, m \mid l, m\rangle\right. \\
&\qquad - \epsilon^2\langle l', m + 1 \mid \epsilon, m + 1\rangle \frac{d}{d\epsilon}\langle \epsilon, m \mid l, m\rangle \\
&\qquad \left. + (2m - 1)\epsilon\langle l', m + 1 \mid \epsilon, m + 1\rangle\langle \epsilon, m \mid l, m\rangle\right]_0^\infty \\
&= \int \epsilon\, d\epsilon\left[\frac{(l - m)(l + m + 1)}{(l' - m)(l' + m + 1)}\right]^{\frac{1}{2}} \\
&\qquad \times \langle l', m + 1 \mid \epsilon, m + 1\rangle\langle \epsilon, m + 1 \mid l, m + 1\rangle \\
&\qquad + \text{surface terms.}
\end{aligned}$$

One can easily verify that the surface terms drop out. Setting $\beta = 1$ in Eq. (24), one sees that

$$\int \epsilon\, d\epsilon \langle l', l \mid \epsilon, l\rangle\langle \epsilon, l \mid l, l\rangle = \delta_{l'l}.$$

Hence, by the use of mathematical induction,

$$\int \epsilon\, d\epsilon \langle l', m \mid \epsilon, m\rangle\langle \epsilon, m \mid l, m\rangle = \delta_{l'l},$$

as required.

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Configuration-Space Approach to the Four-Particle Problem

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The configuration-space approach to the three-particle problem is generalized to the case of four particles. Special coordinates are defined which have simple symmetry properties with respect to the exchange of identical particles. The construction of a suitable orthogonal system is discussed. Some of these functions are given explicitly. It is pointed out that the use of this orthogonal system leads to a considerable simplification for a large number of four-particle problems, namely, the approximate reduction of the Schrödinger equation to a finite system of coupled differential equations for functions that depend on one variable only.

1. INTRODUCTION

The approach to the quantum-mechanical four-body problem represented in this paper is a generalization of an approach to the quantum-mechanical three-body problem discussed in earlier publications.[1–3] As the situation for the three-body problem is much more transparent, the main points of those earlier publications are discussed shortly in this introduction.

It is well known that the Schrödinger equation for the quantum-mechanical three-body problem can be reduced by separating the total orbital angular momentum.[2,4,5] One obtains a system of coupled differential equations for functions depending on three internal variables only. For three identical particles there is a most suitable choice of these internal coordinates[1,6] exhibiting simple symmetry properties with respect to the exchange of particles. They can also be used for nonidentical particles (for example, the ground state of the Helium atom[2]), but they seem to be most powerful in the case of three identical particles.[1,2,7,8] Therefore the discussion is restricted to this case. The whole transformation of the original Schrödinger equation in the center-of-mass system to the new coordinates can be done the following way (showing the properties of the coordinates mentioned above):

In terms of the vectors

$$\mathbf{x}_1 = \mathbf{r}_2 - \mathbf{r}_1,$$
$$\mathbf{x}_2 = (\tfrac{4}{3})^{\frac{1}{2}}[\mathbf{r}_3 - \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)], \tag{1}$$

where $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ are the space vectors of the three particles, the Schrödinger equation in the center-of-mass system contains the sum of the two Δ operators

$$\Delta_1 + \Delta_2. \tag{2}$$

A so-called kinematic rotation[9] is now performed.

$$\mathbf{y}_1 = \mathbf{x}_1 \cos\gamma + \mathbf{x}_2 \sin\gamma,$$
$$\mathbf{y}_2 = -\mathbf{x}_1 \sin\gamma + \mathbf{x}_2 \cos\gamma. \tag{3}$$

Equation (2) would be invariant under this rotation if γ were not dependent on $\mathbf{x}_1$ and $\mathbf{x}_2$. In our case γ depends on $\mathbf{x}_1$ and $\mathbf{x}_2$. It is chosen in such a way that $\mathbf{y}_1$ and $\mathbf{y}_2$ are perpendicular to each other. It can be shown that the directions of $\mathbf{y}_1$ and $\mathbf{y}_2$ coincide with the principal axis of the moment of inertia in the plane of the three particles. Three external coordinates are defined now by the Euler angles ψ, ϑ, φ of the three axes $\mathbf{y}_1$, $\mathbf{y}_2$ and $\mathbf{y}_1 \times \mathbf{y}_2$ in the center-of-mass system. The separation of the orbital angular momentum mentioned above means separation of the dependence of the wavefunction on ψ, ϑ, φ. A possible set for the internal coordinates is

$$y_1, y_2, \gamma. \tag{4}$$

In the preceding publications,[1–3,7,8] y, α, β were chosen instead with the following properties.

$$y_1 = y \sin(\alpha/2),$$
$$y_2 = y \cos(\alpha/2), \tag{5}$$
$$\beta = \pi/2 - 2\gamma.$$

β is the only coordinate which is changed when two identical particles are exchanged. With the use of these special coordinates it was possible, for example, to compute the ground states of three inert gas atoms interacting by van der Waals forces.[7] This calculation was done to a high precision after Ref. 7 was published.[10]

In many cases a further reduction of the Schrödinger equation can be accomplished by expanding the wavefunction as a series of the eigenfunctions of the

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operator

$$y^2\left\{\Delta_1 + \Delta_2 - \left[\frac{\partial^2}{\partial y^2} + \frac{5}{y}\frac{\partial}{\partial y}\right]\right\}. \tag{6}$$

The eigenfunctions of (6) have the form[2]

$$\sum_K e^{i\mu\beta} f^{L\lambda}_{K\mu}(\alpha) D^L_{MK}(\varphi, \vartheta, \psi) \tag{7}$$

and they belong to eigenvalues

$$-4\lambda(\lambda + 2). \tag{8}$$

The coefficients of the expansion are functions $h^{L\lambda}_\mu(y)$ for which one obtains an infinite coupled system of differential equations. In these equations, terms like $-4\lambda(\lambda + 2)/y^2$ occur which resemble the centrifugal term in the two-body problem. As a consequence one can expect that only functions with low values of λ are of importance. Thus one can break the series off after a few values of λ. Then one has only a finite number of functions $h^{L\lambda}_\mu$ and the same number of coupled differential equations. The validity of this approximation depends, of course, also on the interaction between the particles and it has to be tested for every application. So far arguments have been given for good convergence in the nuclear three-body problem[1,3] provided the interaction has no hard core, but rather a soft core.[1,3] This means strong repulsive but finite forces for small distances. In the case of a hard core it is very difficult to express the boundary condition (vanishing of the wavefunction at the hard-core radius) in terms of the three-body coordinates y, α, β. The same is true for the four-particle coordinates defined in this paper, the method does not work for hard-core interactions.

The three-particle method has been successful in describing the state of three α particles from the decay of ^{12}C.[8]

2. DEFINITION OF FOUR-PARTICLE COORDINATES

The coordinates for the quantum-mechanical four-body problem defined in this section enable us to construct a simple orthogonal system of functions for four particles. The possibility of such a simple representation of four-particle states was pointed out also by Lévy-Leblond.[11] He used group-theoretical arguments.

To define the four-particle coordinates we again start from the Schrödinger equation in the center-of-mass system in its ordinary form. A convenient choice for the vectors in this system are

$$\begin{aligned}\mathbf{x}_1 &= \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_3 - \mathbf{r}_4),\\ \mathbf{x}_2 &= \tfrac{1}{2}(-\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_3 + \mathbf{r}_4),\\ \mathbf{x}_3 &= \tfrac{1}{2}(-\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3 - \mathbf{r}_4).\end{aligned} \tag{9}$$

[11] J. M. Lévy-Leblond, J. Math. Phys. 7, 2217 (1966).

The vectors $\mathbf{r}_i$ are, again, the space vectors of the four particles. The Schrödinger equation contains the sum

$$(\hbar^2/2m)(\Delta_1 + \Delta_2 + \Delta_3). \tag{10}$$

Here m is the mass of the particles. [All masses are again equal. The generalization to nonidentical masses is no problem.[2] The definition of the vectors in (9) changes somewhat then.]

We now perform a kinematic rotation

$$\mathbf{y}_i = \sum_{k=1}^{3} a_{ik}\mathbf{x}_k, \quad i = 1, 2, 3. \tag{11}$$

Here the a_{ik} form an orthogonal matrix. Such a three-dimensional orthogonal matrix can be represented by three Euler angles. The a_{ik} are simple functions of these Euler angles which are called α, β, γ. It is now required that the vectors $\mathbf{y}_i$ are perpendicular to each other. It can be shown easily again that their directions coincide with the directions of the three principal axes of the moment of inertia. Instead of the vectors $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, the following nine coordinates are now chosen to describe the four-particle system:

(a) Three "external" Euler angles ψ, ϑ, φ which describe the positions of the three axes $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ in the center-of-mass system.

(b) Three "internal" Euler angles α, β, γ. As stated above, they are chosen such as to make $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ perpendicular vectors. Hence they are functions of the original vectors $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$.

(c) The three lengths y_1, y_2, y_3.

The moments of inertia of the four-particle system are proportional to $y_1^2 + y_2^2$, $y_2^2 + y_3^2$, and $y_3^2 + y_1^2$.

3. TRANSFORMATION OF THE SCHRÖDINGER EQUATION

The transformation of the Schrödinger equation to the new coordinates is facilitated by introducing, at first, complex variables t^k_j instead of the vectors $\mathbf{x}_i$. These coordinates t^k_j are defined in the following way:

$$\begin{aligned}t^1_1 &= (x_{11} + ix_{21} + ix_{12} - x_{22})/2,\\ t^1_0 &= -(x_{13} + ix_{23})/2^{\frac{1}{2}},\\ t^1_{-1} &= (-x_{11} - ix_{21} + ix_{12} - x_{22})/2,\\ t^0_1 &= -(x_{31} + ix_{32})/2^{\frac{1}{2}},\\ t^0_0 &= x_{33},\\ t^0_{-1} &= (x_{31} - ix_{32})/2^{\frac{1}{2}},\\ t^{-1}_1 &= (-x_{11} + ix_{21} - ix_{12} - x_{22})/2,\\ t^{-1}_0 &= (x_{13} - ix_{23})/2^{\frac{1}{2}},\\ t^{-1}_{-1} &= (x_{11} - ix_{21} - ix_{12} - x_{22})/2\end{aligned} \tag{12}$$

(components of the vector $\mathbf{x}_i$ are called x_{i1}, x_{i2}, x_{i3}). With these variables, the sum of the three Δ operators has the form

$$\Delta_1 + \Delta_2 + \Delta_3 = \sum_{j=-1}^{+1} \sum_{k=-1}^{+1} (-)^{j+k} \frac{\partial^2}{\partial t_j^k \partial t_{-j}^{-k}}. \quad (13)$$

The relation between t_j^k and the new coordinates introduced in Sec. 2 is very simple now,

$$t_j^k = \sum_{p=-1}^{+1} \sum_{q=-1}^{+1} D^1_{pk}(\alpha, \beta, \gamma) D^1_{qj}(\psi, \vartheta, \varphi)(t_q^p)'. \quad (14)$$

The relations between $(t_q^p)'$ and $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ are the same as between t_j^k and $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$. The directions of $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ are perpendicular to each other and form the coordinate system to which the $(t_q^p)'$ are referred. Thus,

$$\begin{aligned} (t_1^1)' &= (t_{-1}^{-1})' = \tfrac{1}{2}(y_1 - y_2), \\ (t_{-1}^1)' &= (t_1^{-1})' = -\tfrac{1}{2}(y_1 + y_2), \\ (t_0^0)' &= y_3, \\ (t_0^1)' &= (t_1^0)' = (t_{-1}^0)' = (t_0^{-1})' = 0. \end{aligned} \quad (15)$$

The transformation of (13) to the new coordinates is discussed in the Appendix. The result is

$$\begin{aligned} &\Delta_1 + \Delta_2 + \Delta_3 \\ &= \frac{\partial^2}{\partial y_1^2} + 2y_1\left(\frac{1}{y_1^2 - y_2^2} + \frac{1}{y_1^2 - y_3^2}\right)\frac{\partial}{\partial y_1} \\ &\quad + \frac{\partial^2}{\partial y_2^2} + 2y_2\left(\frac{1}{y_2^2 - y_3^2} + \frac{1}{y_2^2 - y_1^2}\right)\frac{\partial}{\partial y_2} \\ &\quad + \frac{\partial^2}{\partial y_3^2} + 2y_3\left(\frac{1}{y_3^2 - y_1^2} + \frac{1}{y_3^2 - y_2^2}\right)\frac{\partial}{\partial y_3} \\ &\quad - \frac{y_2^2 + y_3^2}{(y_2^2 - y_3^2)^2}(L_{i1}^2 + L_{e1}^2) - \frac{y_3^2 + y_1^2}{(y_3^2 - y_1^2)^2}(L_{i2}^2 + L_{e2}^2) \\ &\quad - \frac{y_1^2 + y_2^2}{(y_1^2 - y_2^2)^2}(L_{i3}^2 + L_{e3}^2) - \frac{4y_2y_3}{(y_2^2 - y_3^2)^2} L_{i1}L_{e1} \\ &\quad - \frac{4y_3y_1}{(y_3^2 - y_1^2)^2} L_{i2}L_{e2} - \frac{4y_1y_2}{(y_1^2 - y_2^2)^2} L_{i3}L_{e3}. \end{aligned} \quad (16)$$

In Eq. (16), the operators L_{e1}, L_{e2}, L_{e3} are the components of the total orbital angular momentum with respect to the body-fixed coordinate system whose axes coincide with the directions of $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$.

$$\begin{aligned} L_{e1} &= i\hbar\left[\cos\psi\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi} - \cot\vartheta\frac{\partial}{\partial\psi}\right) - \sin\psi\frac{\partial}{\partial\vartheta}\right], \\ L_{e2} &= -i\hbar\left[\sin\psi\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi} - \cot\vartheta\frac{\partial}{\partial\psi}\right) + \cos\psi\frac{\partial}{\partial\vartheta}\right], \\ L_{e3} &= -i\hbar\frac{\partial}{\partial\psi}. \end{aligned} \quad (17)$$

The expressions for L_{i1}, L_{i2}, L_{i3} are completely analogous to (17), where ψ, ϑ, φ are replaced simply by α, β, γ.

4. CONSTRUCTION OF A SUITABLE ORTHOGONAL SYSTEM FOR THE FOUR-PARTICLE PROBLEM

The Schrödinger equation of the four-particle system can always be reduced by separating the orbital angular momentum. If only central interactions are assumed, the eigenfunctions of the Schrödinger equation can be chosen to be eigenfunctions of $\mathbf{L}_e^2$ and L_{ez} also. (L_{ez} is the z component of $\mathbf{L}_e$.) In this case the wavefunction is a sum over $D^L_{KM}(\psi, \vartheta, \varphi)$. It is summed over K, the coefficients of D^L_{KM} depend on y_1, y_2, y_3, α, β, γ. Similarly as for the three-body problem one proceeds now by expanding the wavefunction as a series over eigenfunctions of suitable operators. These operators are

$$\mathbf{L}_i^2,$$

$$L_{i\zeta} = -i\hbar\frac{\partial}{\partial\gamma} \quad (18)$$

which is analogous to L_{ez},

$$\Lambda^2 = y^2\left[(\Delta_1 + \Delta_2 + \Delta_3) - \frac{\partial^2}{\partial y^2} - \frac{8}{y}\frac{\partial}{\partial y}\right], \quad (19)$$

where

$$y = [x_1^2 + x_2^2 + x_3^2]^{\frac{1}{2}} = [y_1^2 + y_2^2 + y_3^2]^{\frac{1}{2}}.$$

The five operators $\mathbf{L}_e^2$, L_{ez}, $\mathbf{L}_i^2$, $L_{i\zeta}$, Λ^2 form a set of commutable operators. There are of course four more operators, which could be constructed, that are commutable with each other and the five operators above. One of these could be taken as $\partial^2/\partial y^2 + (8/y)\partial/\partial y$, for example. The remaining three operators are complicated and it is not useful to derive them. It is probably easier to construct eigenfunctions for the above five operators only. They depend on eight dimensionless variables (the only length is y) and in the general case one finds several independent eigenfunctions for fixed eigenvalues of $\mathbf{L}_e^2$, L_{ez}, $\mathbf{L}_i^2$, $L_{i\zeta}$, Λ^2. These eigenfunctions have to be orthogonalized. When expanding the solution of the Schrödinger equation as a series over these functions, the coefficients depend on y and they contain all the information about the interaction of the particles. It might be useful in some cases to expand these y-dependent parts also in a complete orthogonal system, but this point is not discussed here. Why is it convenient to choose the above five operators for constructing an orthogonal system? This is discussed shortly. The quantum numbers for the orbital angular momentum and its z component are called L_e and M_e and in complete analogy L_i and M_i for the operators $\mathbf{L}_i^2$ and

$L_{i\zeta}$. For the moment it is assumed that the interaction of the four particles depends only on y. This would be the case, for instance, for oscillatory interactions of equal strength between all particle pairs. But such an interaction is far from reality and it is used for the moment only to show the convenience of the operators chosen. The arguments are correct also for other interaction as will be seen.

The operator Λ^2 has the following form:

$$\begin{aligned}\Lambda^2 = &\frac{y^2}{x_1^2}\left[\frac{\partial^2}{\partial\vartheta_1^2} + \frac{\cos\vartheta_1}{\sin\vartheta_1}\frac{\partial}{\partial\vartheta_1} + \frac{1}{\sin^2\vartheta_1}\frac{\partial^2}{\partial\varphi_1^2}\right]\\ &+ \frac{y^2}{x_2}\left[\frac{\partial^2}{\partial\vartheta_2^2} + \frac{\cos\vartheta_2}{\sin\vartheta_2}\frac{\partial}{\partial\vartheta_2} + \frac{1}{\sin^2\vartheta_2}\frac{\partial^2}{\partial\varphi_2^2}\right]\\ &+ \frac{y^2}{x_3^2}\left[\frac{\partial^2}{\partial\vartheta_3^2} + \frac{\cos\vartheta_3}{\sin\vartheta_3}\frac{\partial}{\partial\vartheta_3} + \frac{1}{\sin^2\vartheta_3}\frac{\partial^2}{\partial\varphi_3^2}\right]\\ &+ \frac{\partial^2}{\partial\chi^2} + \left(5\frac{\cos\chi}{\sin\chi} - 2\frac{\sin\chi}{\cos\chi}\right)\frac{\partial}{\partial\chi}\\ &+ \frac{\partial^2}{\partial\xi^2} + 4\frac{\cos 2\xi}{\sin 2\xi}\frac{\partial}{\partial\varphi}. \end{aligned} \tag{20}$$

The polar angles of the vector $\mathbf{x}_1$ are ϑ_1, φ_1; ϑ_2, φ_2 and ϑ_3, φ_3 are the same for $\mathbf{x}_2$ and $\mathbf{x}_3$, respectively, and

$$\begin{aligned} x_1 &= y\sin\chi\cos\xi,\\ x_2 &= y\sin\chi\sin\xi,\\ x_2 &= y\cos\chi. \end{aligned} \tag{21}$$

The eigenfunctions for Λ^2 are

$$\begin{aligned} &Y_{l_1m_1}(\vartheta_1\varphi_1)Y_{l_2m_2}(\vartheta_2\varphi_2)Y_{l_3m_3}(\vartheta_3\varphi_3)\\ &(\cos\xi)^{l_1}(\sin\xi)^{l_2}\\ &\quad\times F(-\tfrac{1}{2}(\nu - l_1 - l_2), \tfrac{1}{2}(\nu + l_1 + l_2 + 4);\\ &\qquad -l_1 - \tfrac{3}{2}; \cos^2\xi)\\ &(\cos\chi)^{l_3}(\sin\chi)^{\nu}\\ &\quad\times F(-\tfrac{1}{2}(\lambda - l_3 - \nu), \tfrac{1}{2}(\lambda + l_3 + \nu + 7);\\ &\qquad -l_3 - \tfrac{3}{2}; \cos^2\chi), \end{aligned} \tag{22}$$

$$\nu - l_1 - l_2 \geq 0 \quad \text{and even},$$

$$\lambda - l_3 - \nu \geq 0 \quad \text{and even}.$$

The solution of the Schrödinger equation for a y-dependent interaction $V(y)$ is Eq. (22) multiplied by a factor $h_\lambda(y)$. For $h_\lambda(y)$ one obtains the equation

$$\left\{\frac{h^2}{2m}\left[\frac{\partial^2}{\partial y^2} + \frac{8}{y}\frac{\partial}{\partial y} - \frac{\lambda(\lambda+7)}{y^2}\right] + E - V(y)\right\}h_\lambda(y) = 0. \tag{23}$$

The term $\lambda(\lambda + 7)/y^2$ has the same effect as the centrifugal term in the ordinary two-body problem. The ground state has $\lambda = 0$; states with larger values of λ are higher in energy. For arbitrary interactions, (23) is replaced by an infinite system of coupled differential equations for y-dependent functions, but centrifugal terms $\lambda(\lambda + 7)/y^2$ occur in all these equations and they have the same effect in many cases as for the simple case above. For the total wavefunction of the four-particle system this means, then, that only low values of λ are important. Thus one may ignore the higher values of λ, that is, one may break off the series for the total wavefunction and one has only a few coupled differential equations. As in the case of the three-body problem, one has to, of course, test whether this approximation is good or not. There are interactions for which one cannot use it, for example, inert-gas atoms interacting according to van der Waals forces.[7]

The eigenfunctions for Λ^2 in the form (22) are not suitable for calculations with four identical particles. The separation of the orbital angular momentum is difficult and the functions (22) have complicated properties with respect to exchange of identical particles. Therefore the eigenfunctions of Λ^2 constructed below are eigenfunctions to $\mathbf{L}_e^2$, L_{ez}, $\mathbf{L}_i^2$, $L_{i\zeta}$. They have the form

$$\begin{aligned} &F_{\lambda,L_e,M_e,L_i,M_i}(\alpha,\beta,\gamma,\psi,\vartheta,\varphi,y_1/y,y_2/y)\\ &= \sum_{K_eK_i} D^{L_e}_{K_eM_e}(\psi,\vartheta,\varphi)D^{L_i}_{K_iM_i}(\alpha,\beta,\gamma)\,{}_\lambda G^{L_i,K_i}_{L_e,K_e}\left(\frac{y_1}{y},\frac{y_2}{y}\right) \end{aligned} \tag{24}$$

(with $K_e + K_i$ even, as is shown below).

The main problem consists in finding the functions ${}_\lambda G^{L_iK_i}_{L_eK_e}$. This can be done by transforming (22) to the new coordinates and writing it as a sum over functions (24). One property of (24) can be derived without further calculation. The eigenfunctions of Λ^2 can be written in terms of t_j^k/y, where the t_j^k are defined as in (12) and y as in (19). They are sums over products of the t_j^k/y. The transformation of t_j^k to the new coordinates is given by (14). Only terms with $p + q$ even contribute to the sum in (14) as is seen from (15). Replacing t_j^k in the eigenfunctions of Λ^2 by (14) and using the well-known formula for the multiplication of the rotation matrices, one can conclude immediately that $K_e + K_i$ in (24) must be even also.

When one has constructed the functions ${}_\lambda G^{L_iK_i}_{L_eK_e}$ from (22), one can check on their correctness by placing them in the coupled system of differential equations to which they belong. It is obtained from

$$[\Lambda^2 + \lambda(\lambda+7)]F_{\lambda,L_e,M_e,L_i,M_i} = 0 \tag{25}$$

and has the following form:

$$\left\{\frac{\partial^2}{\partial y_1^2}+2y_1\left(\frac{1}{y_1^2-y_2^2}+\frac{1}{y_1^2-y_3^2}\right)\frac{\partial}{\partial y_1}+\frac{\partial^2}{\partial y_2^2}+2y_2\left(\frac{1}{y_2^2-y_3^2}+\frac{1}{y_2^2-y_1^2}\right)\frac{\partial}{\partial y_2}+\frac{\partial^2}{\partial y_3^2}+2y_3\left(\frac{1}{y_3^2-y_1^2}+\frac{1}{y_3^2-y_2^2}\right)\frac{\partial}{\partial y_3}\right.$$
$$-\tfrac{1}{2}[L_e(L_e+1)+L_i(L_i+1)-K_e^2-K_i^2]\left[\frac{y_2^2+y_3^2}{(y_2^2-y_3^2)^2}+\frac{y_3^2+y_1^2}{(y_3^2-y_1^2)^2}\right.$$
$$\left.\left.-\frac{y_1^2+y_2^2}{(y_1^2-y_2^2)^2}(K_e^2+K_i^2)-\frac{4y_1y_2}{(y_1^2-y_2^2)^2}K_eK_i+\frac{\lambda(\lambda+7)}{y^2}\right]{}_\lambda G_{L_e,K_e}^{L_i,K_i}\right.$$
$$=\frac{1}{4}\left[\frac{y_2^2+y_3^2}{(y_2^2-y_3^2)^2}-\frac{y_3^2+y_1^2}{(y_3^2-y_1^2)^2}\right][g_{K_e+2}^{L_e}g_{K_e+1}^{L_e}{}_\lambda G_{L_e,K_e+2}^{L_i,K_i}+g_{-K_e+2}^{L_e}g_{-K_e+1}^{L_e}{}_\lambda G_{L_e,K_e-2}^{L_i,K_i}$$
$$+g_{K_i+2}^{L_i}g_{K_i+1}^{L_i}{}_\lambda G_{L_e,K_e}^{L_i,K_i+2}+g_{-K_i+2}^{L_i}g_{-K_i+1}^{L_i}{}_\lambda G_{L_e,K_e}^{L_i,K_i-2}]$$
$$+\left[\frac{y_2y_3}{(y_2^2-y_3^2)^2}-\frac{y_3y_1}{(y_3^2-y_1^2)^2}\right][g_{K_i+1}^{L_i}g_{K_e+1}^{L_e}{}_\lambda G_{L_e,K_e+1}^{L_i,K_i+1}+g_{-K_i+1}^{L_i}g_{-K_e+1}^{L_e}{}_\lambda G_{L_e,K_e-1}^{L_i,K_i-1}]$$
$$+\left[\frac{y_2y_3}{(y_2^2-y_3^2)^2}+\frac{y_3y_1}{(y_3^2-y_1^2)^2}\right][g_{K_i+1}^{L_i}g_{-K_e+1}^{L_e}{}_\lambda G_{L_e,K_e-1}^{L_i,K_i+1}+g_{-K_i+1}^{L_i}g_{K_e+1}^{L_e}{}_\lambda G_{L_e,K_e+1}^{L_i,K_i-1}], \quad (26)$$

with $g_K^L=[(L+K)(L-K+1)]^{\frac{1}{2}}$ (it was multiplied by $1/y^2$ and the operator $\partial^2/\partial y^2+(8/y)\partial/\partial y$ was included. This does not matter, because there is no y dependence in the functions considered).

The eigenfunctions have been derived for $\lambda=0$, 1, 2. The result is given below; the functions are not normalized:

$$\lambda=0,\quad L_e=L_i=0,\qquad {}_0G_{00}^{00}=1, \quad (27)$$

$$\lambda=1,\quad L_e=L_i=1,\qquad {}_1G_{1K_e}^{1K_i}=(t_{K_e}^{K_i})'/y, \quad (28)$$

$$\lambda=2,\quad L_e=0,\quad L_i=2,\qquad {}_2G_{00}^{22}={}_2G_{00}^{2-2}=(y_1^2-y_2^2)/y^2,$$
$${}_2G_{00}^{20}=(2y_3^2-y_1^2-y_2^2)(\tfrac{2}{3})^{\frac{1}{2}}y^{-2}, \quad (29)$$

$$L_e=2,\quad L_i=0,_2\qquad G_{2K}^{00}={}_2G_{00}^{2K}, \quad (30)$$

$$L_e=L_i=2,\qquad {}_2G_{22}^{22}={}_2G_{2-2}^{2-2}=(y_1-y_2)^2/y^2,$$
$${}_2G_{2-2}^{22}=G_{22}^{2-2}=(y_1+y_2)^2/y^2,$$
$${}_2G_{20}^{22}={}_2G_{22}^{20}={}_2G_{20}^{2-2}={}_2G_{2-2}^{20}$$
$$=-(y_1^2-y_2^2)(\tfrac{2}{3})^{\frac{1}{2}}y^{-2}, \quad (31)$$

$$L_e=L_i=2,\qquad {}_2G_{21}^{21}={}_2G_{2-1}^{2-1}=2y_3(y_1-y_2)/y^2,$$
$${}_2G_{21}^{2-1}={}_1G_{2-1}^{21}=-2y_3(y_1+y_2)/y^2,$$
$${}_2G_{20}^{20}=(4y_3^2+y_1^2+y_2^2)\tfrac{2}{3}y^{-2},$$
$$L_e=L_i=2,\qquad {}_2G_{21}^{21}={}_2G_{2-1}^{2-1}=y_3(y_1-y_2)/y^2,$$
$${}_2G_{2-1}^{21}={}_2G_{21}^{2-1}=y_3(y_1+y_2)/y^2,$$
$${}_2G_{20}^{20}=-2y_1y_2/y^2. \quad (32)$$

These functions are complete up to $\lambda=2$ as one can find simply by counting. It is remarkable that one finds a single eigenfunction only for fixed values of λ, L_e, L_i, M_e, M_i. As there are three more operators commutable with Λ^2, $\mathbf{L}_e$, $\mathbf{L}_i$, L_{ez}, $L_{i\zeta}$, one would expect more than one eigenfunction. But this is the case only for higher values of λ just as in the case of three particles.[2]

5. PARITY AND SYMMETRY PROPERTIES

In this section parity and symmetry properties of the four-particle functions are discussed without further proof.

The parity operation means that t_j^k is replaced by $-t_j^k$. In the new coordinates this replacement corresponds to replacing y_i by $-y_i$ while α, β, γ, ψ, ϑ, φ are unchanged.

The exchange of identical particles can be represented in the new coordinates by the reflection of $y_i (y_i \to -y_i)$ plus a kinematic rotation. This is illustrated for the exchange of particles 1 and 2. This exchange means that the vectors $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$ of (9) are transformed to vectors $\mathbf{x}_1'$, $\mathbf{x}_2'$, $\mathbf{x}_3'$ with

$$\begin{aligned} \mathbf{x}_1' &= \mathbf{x}_1, \\ \mathbf{x}_2' &= -\mathbf{x}_3, \\ \mathbf{x}_3' &= -\mathbf{x}_2. \end{aligned} \tag{33}$$

For t_j^k of (12) this means a transformation to $\tilde{t}_j^k$ with

$$\tilde{t}_j^k = \sum_i a_{ik} t_j^i. \tag{34}$$

The matrix a_{ik} can be derived from (33) and the definitions of the t_j^k from (12):

$$\begin{aligned} &a_{11} = a_{-1-1} = -a_{1-1} = -a_{-11} = 1/2, \\ &a_{10} = a_{-10} = -a_{01} = -a_{0-1} = i/2^{\frac{1}{2}}, \\ &a_{00} = 0, \end{aligned} \tag{35}$$

In the new coordinates the exchange alters α, β, γ to α', β', γ' and $(t_q^p)'$ to $(t_q^p)''$, while ψ, ϑ, φ are unchanged. That means that

$$\tilde{t}_j^k = \sum_{pq} D^1_{pk}(\alpha', \beta', \gamma') D^1_{qj}(\psi, \vartheta, \varphi)(t_q^p)''. \tag{36}$$

For $(t_q^p)''$ one finds

$$(t_q^p)'' = -(t_q^p)'. \tag{37}$$

Thus,

$$\tilde{t}_j^k = -\sum_{pq} D^1_{pk}(\alpha', \beta', \gamma') D^1_{qj}(\psi, \vartheta, \varphi)(t_q^p)'. \tag{38}$$

Equations (34) and (38) give

$$\sum_i a_{ik} \sum_{pq} D^1_{pi}(\alpha, \beta, \gamma) D^1_{qj}(\psi, \vartheta, \varphi)(t_q^p)' = -\sum_{pq} D^1_{pk}(\alpha', \beta', \gamma') D^1_{qj}(\psi, \vartheta, \varphi)(t_q^p)'. \tag{39}$$

Hence,

$$\sum_i a_{ik} \sum_p D^1_{pi}(\alpha, \beta, \gamma)(t_q^p)' = -\sum_p D^1_{pk}(\alpha', \beta', \gamma')(t_q^p)'. \tag{40}$$

In Eq. (40), q is fixed. The $(t_q^p)'$ for different values of p are independent. Thus,

$$\sum_i a_{ik} D^1_{pi}(\alpha, \beta, \gamma) = -D^1_{pk}(\alpha', \beta', \gamma'). \tag{41}$$

From (35) and the formulas for D^1_{ik},[12] one finds

$$a_{ik} = -D^1_{ik}(\alpha_1, \beta_1, \gamma_1), \tag{42}$$

with

$$\alpha_1 = \tfrac{3}{2}\pi, \quad \beta_1 = \tfrac{1}{2}\pi, \quad \gamma_1 = \tfrac{3}{2}\pi. \tag{43}$$

Equation (41) is now

$$D^1_{pk}(\alpha', \beta', \gamma') = \sum_i D^1_{ik}(\alpha_1, \beta_1, \gamma_1) D^1_{pi}(\alpha, \beta, \gamma) \tag{44}$$

and represents a kinematic rotation, that is, a rotation in the α, β, γ space. Thus it was confirmed that the exchange of particles 1 and 2 means reflection of y_i [Eq. (37)] and a kinematic rotation [(43) and (44)]. For the other exchanges, one finds

$$\begin{aligned} &1 \leftrightarrow 2: \quad \alpha_1 = \tfrac{3}{2}\pi, \quad \beta_1 = \tfrac{1}{2}\pi, \quad \gamma_1 = \tfrac{3}{2}\pi, \\ &3 \leftrightarrow 4: \quad \alpha_1 = \tfrac{1}{2}\pi, \quad \beta_1 = \tfrac{1}{2}\pi, \quad \gamma_1 = \tfrac{1}{2}\pi, \\ &3 \leftrightarrow 1: \quad \alpha_1 = 0, \quad \beta_1 = \tfrac{1}{2}\pi, \quad \gamma_1 = \pi, \\ &2 \leftrightarrow 4: \quad \alpha_1 = \pi, \quad \beta_1 = \tfrac{1}{2}\pi, \quad \gamma_1 = 0, \\ &1 \leftrightarrow 4: \quad \alpha_1 = \tfrac{1}{2}\pi, \quad \beta_1 = \pi, \quad \gamma_1 = 0, \\ &2 \leftrightarrow 3: \quad \alpha_1 = \tfrac{3}{2}\pi, \quad \beta_1 = \pi, \quad \gamma_1 = 0. \end{aligned} \tag{45}$$

(For completeness, exchange $1 \leftrightarrow 2$ is also included.)

As in the case of three particles,[2] one can choose a representation of the orthogonal system in which every function has definite symmetry properties for one exchange, for example, the exchange of particles 1 and 2. Every function of the system is either symmetric or antisymmetric with respect to this exchange. In general, these functions exhibit a complicated behavior with respect to any other exchange. There are only a few functions which exhibit the same behavior with respect to any of the exchanges, that is, completely symmetric or completely antisymmetric functions. To construct such functions one has to take combinations

$$\sum_M b_{M_i} F_{\lambda, L_e, M_e, L_i, M_i} \tag{46}$$

of the functions defined in (24). The coefficients b_{M_i} are determined from the requirement that (46) is either invariant under all particle exchanges or that it changes sign under all exchanges. Completely symmetric space functions would be needed in the case of four bosons, e.g., four α particles. The lowest values of L_i for which one finds such functions are $L_i = 0, 4, 6$. For completely antisymmetric functions one finds $L_i = 4, 6$. They would be needed in the case of four nucleons. But other space functions are needed in that case, too, because they have to be combined with spin–isospin functions to form completely antisymmetric functions. It is not the purpose of this paper to discuss these functions.

6. REDUCTION OF THE SCHRÖDINGER EQUATION FOR FOUR PARTICLES WITH CENTRAL INTERACTIONS

The solutions of the Schrödinger equation for four particles with central interactions are eigenfunctions of the orbital angular-momentum operators L_e^2 and L_{ez}:

$$\Psi = \sum_{\lambda=0}^{\infty} \sum_{L_i=0}^{\lambda} \sum_{M_i=-L_i}^{+L_i} h_{\lambda, L_i, M_i}(y) F_{\lambda, L_e, M_e, L_i, M_i}. \tag{47}$$

If, as we assume, only a few values of λ bring a considerable contribution, the sum over λ can be broken

[12] G. Breit, "Theory of Resonance Reactions and Allied Topics" in *Handbuch der Physik, Vol. XLI*, Part 1, S. Flügge, Ed. (Springer-Verlag, Berlin, 1959).

off and Ψ is replaced by the approximate function Ψ_a:

$$\Psi_a = \sum_{\lambda=0}^{\lambda_m} \sum_{L_i=0}^{\lambda} \sum_{M_i=-L_i}^{+L_i} h_{\lambda,L_i,M_i}(y) F_{\lambda,L_e,M_e,L_i,M_i}. \quad (48)$$

Equation (48) is put into the Schrödinger equation which is multiplied by $F_{\lambda',L_e,M_e,L_i',M_i'}$. The integraton over the eight angular coordinates is carried out yielding a coupled system of differential equations for the functions h_{λ,L_i,M_i}. The matrix elements containing the interaction can be simplified considerably. The matrix element

$$(F_{\lambda,L_e,M_e,L_i,M_i}|\, V(r_{12})\, |F_{\lambda',L_e,M_e,L_i',M_i'}) \quad (49)$$

is considered as an example. The distance of particles 1 and 2 in (49) is r_{12}. With respect to the vectors,

$$\begin{aligned} \mathbf{Z}_1 &= [\mathbf{r}_4 - \tfrac{1}{3}(\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)](\tfrac{3}{4})^{\frac{1}{2}}, \\ \mathbf{Z}_2 &= [\mathbf{r}_3 - \tfrac{1}{3}(\mathbf{r}_1 + \mathbf{r}_2)](\tfrac{2}{3})^{\frac{1}{2}}, \\ \mathbf{Z}_3 &= (\mathbf{r}_1 - \mathbf{r}_2)2^{-\frac{1}{2}}. \end{aligned} \quad (50)$$

The Schrödinger equation contains again the sum of the three Δ operators $\Delta_1 + \Delta_2 + \Delta_3$. Introducing as new coordinates the polar angles ϑ_1', φ_1', ϑ_2', φ_2', ϑ_3', φ_3', of the vector $\mathbf{Z}_1$, $\mathbf{Z}_2$, $\mathbf{Z}_3$, respectively, and y, χ', ξ' with

$$\begin{aligned} Z_1 &= y \sin\chi' \cos\xi', \\ Z_2 &= y \sin\chi' \sin\xi', \\ Z_3 &= y \cos\chi', \end{aligned} \quad (51)$$

one can again construct a complete orthogonal system in the angular coordinates which has exactly the same form as (22) except that all the angles have to get primes. (λ has the same meaning as throughout the whole paper.)

The functions $F_{\lambda,L_e,M_e,L_i,M_i}$ are linear combinations of these orthogonal functions. The interaction $V(r_{12})$ depends on $y \cos\chi'$ only and thus seven of the eight integrations can be carried out without difficulty.

APPENDIX

To transform (10) to the new coordinates, the derivatives of the new coordinates with respect to t_j^k are needed. To obtain these, the derivative of Eq. (14) with respect to $t_{j'}^{k'}$ is formed,

$$\begin{aligned} \delta_{jj'}\delta_{kk'} = \sum_{pq} \Bigg\{ & \left[ip \frac{\partial\alpha}{\partial t_{j'}^{k'}} + ik \frac{\partial\gamma}{\partial t_{j'}^{k'}} + iq \frac{\partial\psi}{\partial t_{j'}^{k'}} + ij \frac{\partial\varphi}{\partial t_{j'}^{k'}} \right] \\ & \times D^1_{pk}(\alpha\beta\gamma) D^1_{qj}(\psi\vartheta\varphi)(t_q^p)' \\ & + \left[\frac{\partial}{\partial\beta} D^1_{pk}(\alpha\beta\gamma) \right] D^1_{qj}(\psi\vartheta\varphi) \frac{\partial\beta}{\partial t_{j'}^{k'}} (t_q^p)' \\ & + D^1_{pk}(\alpha\beta\gamma) \left[\frac{\partial}{\partial\vartheta} D^1_{qj}(\psi\vartheta\varphi) \right] \frac{\partial\vartheta}{\partial t_{j'}^{k'}} (t_p^p)' \\ & + D^1_{pk}(\alpha\beta\gamma) D^1_{qj}(\psi\vartheta\varphi) \frac{\partial (t_q^p)'}{\partial t_{j'}^{k'}} \Bigg\}. \end{aligned} \quad (A1)$$

Multiplication of (A1) with $D^{1*}_{p'k}(\alpha, \beta, \gamma) D^{1*}_{q'j}(\psi, \vartheta, \varphi)$ and summation over k and j yields

$$\begin{aligned} & D^{1*}_{p'k'}(\alpha, \beta, \gamma) D^{1*}_{q'j'}(\psi, \vartheta, \varphi) \\ & = ip'(t_{q'}^{p'})' \frac{\partial\alpha}{\partial t_{j'}^{k'}} + iq'(t_{q'}^{p'})' \frac{\partial\psi}{\partial t_{j'}^{k'}} + \frac{\partial (t_{q'}^{p'})'}{\partial t_{j'}^{k'}} \\ & \quad + \frac{\partial\gamma}{\partial t_{j'}^{k'}} \sum_p \sum_k ik D^{1*}_{p'k}(\alpha, \beta, \gamma) D^1_{pk}(\alpha, \beta, \gamma)(t_{q'}^p)' \\ & \quad + \frac{\partial\varphi}{\partial t_{j'}^{k'}} \sum_q \sum_j ij D^{1*}_{q'j}(\psi, \vartheta, \varphi) D^1_{qj}(\psi, \vartheta, \varphi)(t_q^{p'})' \\ & \quad + \frac{\partial\beta}{\partial t_{j'}^{k'}} \sum_p \sum_k D^{1*}_{p'k}(\alpha, \beta, \gamma) \left[\frac{\partial}{\partial\beta} D^1_{pk}(\alpha, \beta, \gamma) \right] (t_{q'}^p)' \\ & \quad + \frac{\partial\vartheta}{\partial t_{j'}^{k'}} \sum_q \sum_j D^{1*}_{q'j}(\psi, \vartheta, \varphi) \left[\frac{\partial}{\partial\vartheta} D^1_{qj}(\psi, \vartheta, \varphi) \right] (t_q^{p'})'. \end{aligned} \quad (A2)$$

These nine equations for the derivatives with respect to $t_{j'}^{k'}$ can be simplified considerably by putting in the known forms of the rotation matrices. The coefficients of $\partial\alpha/\partial t_{j'}^{k'}$, $\partial\psi/\partial t_{j'}^{k'}$ can be taken from (15) directly. The coefficients of $\partial\gamma/\partial t_{j'}^{k'}$, $\partial\varphi\partial t/_{j'}^{k'}$, $\partial\beta/\partial t_{j'}^{k'}$, $\partial\vartheta/\partial t_{j'}^{k'}$ in (A2) are called $\Gamma_{p'q'}$, $\Phi_{p'q'}$, $B_{p'q'}$, $\Theta_{p'q'}$, respectively. One finds

$$\begin{aligned} \Gamma_{11} &= \Gamma^*_{-1-1} = [i(y_1 - y_2)\cos\beta]/2, \\ \Gamma_{10} &= -\Gamma^*_{-10} = -ie^{-i\alpha} \sin\beta y_3/2^{\frac{1}{2}}, \\ \Gamma_{1-1} &= \Gamma^*_{-11} = -[i(y_1 + y_2)\cos\beta]/2, \\ \Gamma_{01} &= -\Gamma^*_{0-1} \\ &= i \sin\beta[-(y_1 - y_2)e^{i\alpha} + (y_1 + y_2)e^{-i\alpha}]/2^{\frac{3}{2}}, \\ \Gamma_{00} &= 0; \end{aligned} \quad (A3)$$

$$\begin{aligned} \Phi_{11} &= \Phi^*_{-1-1} = [i(y_1 - y_2)\cos\vartheta]/2, \\ \Phi_{10} &= -\Phi^*_{-10} \\ &= i \sin\vartheta[-(y_1 - y_2)e^{i\psi} + (y_1 + y_2)e^{-i\psi}]/2^{\frac{3}{2}}, \\ \Phi_{1-1} &= \Phi^*_{-11} = [i(y_1 + y_2)\cos\vartheta]/2, \\ \Phi_{01} &= -\Phi^*_{0-1} = -ie^{-i\psi} \sin\vartheta y_3/2^{\frac{1}{2}}, \\ \Phi_{00} &= 0; \end{aligned} \quad (A4)$$

$$\begin{aligned} B_{11} &= B_{1-1} = B_{00} = B_{-11} = B_{-1-1} = 0, \\ B_{10} &= -B^*_{-10} = -y_3 e^{-i\alpha}/2^{\frac{1}{2}}, \\ B_{01} &= -B^*_{0-1} = [(y_1 - y_2)e^{i\alpha} + (y_1 + y_2)e^{-i\alpha}]/2^{\frac{3}{2}}; \end{aligned} \quad (A5)$$

$$\begin{aligned} \Theta_{11} &= \Theta_{1-1} = \Theta_{00} = \Theta_{-11} = \Theta_{-1-1} = 0, \\ \Theta_{10} &= -\Theta^*_{-10} = [(y_1 - y_2)e^{i\psi} + (y_1 + y_1)e^{-i\psi}]/2^{\frac{3}{2}}, \\ \Theta_{01} &= -\Theta^*_{0-1} = -y_3 e^{-i\psi}/2^{\frac{1}{2}}. \end{aligned} \quad (A6)$$

Equation (A2) can be solved now. The results are

$$\frac{\partial(t_0^0)'}{\partial t_{j'}^{k'}} = D_{0k'}^{1*}(\alpha, \beta, \gamma) D_{0j'}^{1*}(\psi, \vartheta, \varphi), \tag{A7}$$

$$\frac{\partial(t_1^1)'}{\partial t_{j'}^{k'}} = \tfrac{1}{2}[D_{1k'}^{1*}(\alpha, \beta, \gamma) D_{1j'}^{1*}(\psi, \vartheta, \varphi) + D_{-1k'}^{1*}(\alpha, \beta, \gamma) D_{-1j'}^{1*}(\psi, \vartheta, \varphi)], \tag{A8}$$

$$\frac{\partial(t_{-1}^1)'}{\partial t_{j'}^{k'}} = \tfrac{1}{2}[D_{1k'}^{1*}(\alpha, \beta, \gamma) D_{-1j'}^{1*}(\psi, \vartheta, \varphi) + D_{-1k'}^{1*}(\alpha, \beta, \gamma) D_{1j'}^{1*}(\psi, \vartheta, \varphi)], \tag{A9}$$

$$\begin{aligned}
&-\frac{\partial \varphi}{\partial t_{j'}^{k'}} i 2^{\frac{3}{2}} \sin\vartheta (y_2^2 - y_3^2)(y_3^2 - y_1^2) \\
&= y_3 D_{0k'}^{1*}(\alpha, \beta, \gamma)\{D_{1j'}^{1*}(\psi, \vartheta, \varphi)[e^{-i\psi}(y_1^2 - y_2^2) \\
&\quad + e^{i\psi}(y_1^2 + y_2^2 - 2y_3^2)] + D_{-1j'}^{1*}(\psi, \vartheta, \varphi) \\
&\quad \times [e^{i\psi}(y_1^2 - y_2^2) + e^{-i\psi}(y_1^2 + y_2^2 - 2y_3^2)]\} \\
&\quad + \tfrac{1}{2} D_{1k'}^{1*}(\alpha, \beta, \gamma) D_{0j'}^{1*}(\psi, \vartheta, \varphi) \\
&\quad \times \{(y_1 + y_2)[e^{-i\psi}(y_1^2 - y_2^2) + e^{i\psi}(y_1^2 + y_2^2 - 2y_3^2)] \\
&\quad - (y_1 - y_2)[e^{i\psi}(y_1^2 - y_2^2) + e^{-i\psi}(y_1^2 + y_2^2 - 2y_3^2)]\} \\
&\quad + \tfrac{1}{2} D_{-1k'}^{1*}(\alpha, \beta, \gamma) D_{0j'}^{1*}(\psi, \vartheta, \varphi) \\
&\quad \times \{-(y_1 - y_2)[e^{-i\psi}(y_1^2 - y_2^2) + e^{i\psi}(y_1^2 + y_2^2 - 2y_3^2)] \\
&\quad + (y_1 + y_2)[e^{i\psi}(y_1^2 - y_2^2) + e^{-i\psi}(y_1^2 + y_2^2 - 2y_3^2)]\}.
\end{aligned} \tag{A10}$$

For $(\partial\vartheta/\partial t_{j'}^{k'}) 2^{\frac{3}{2}}(y_2^2 - y_3^2)(y_3^2 - y_1^2)$, one obtains an expression which is almost the same as the right-hand side in Eq. (A10). The only change consists in a change of sign of $e^{i\psi}$; $e^{-i\psi}$ has the same sign as in Eq. (A10):

$$\begin{aligned}
\frac{\partial \psi}{\partial t_{j'}^{k'}} &= -\cos\vartheta \frac{\partial \varphi}{\partial t_{j'}^{k'}} - i[D_{1k'}^{1*}(\alpha, \beta, \gamma) D_{1j'}^{1*}(\psi, \vartheta, \varphi) \\
&\quad - D_{-1k'}^{1*}(\alpha, \beta, \gamma) D_{-1j'}^{1*}(\psi, \vartheta, \varphi)]/2(y_1 - y_2) \\
&\quad - i[D_{1k'}^{1*}(\alpha, \beta, \gamma) D_{-1j'}^{1*}(\psi, \vartheta, \varphi) \\
&\quad - D_{-1k'}^{1*}(\alpha, \beta, \gamma) D_{1j'}^{1*}(\psi, \vartheta, \varphi)]/2(y_1 + y_2).
\end{aligned} \tag{A11}$$

The expressions for $\partial\gamma/\partial t_{j'}^{k'}$, $\partial\beta/\partial t_{j'}^{k'}$, $\partial\alpha/\partial t_{j'}^{k'}$ are obtained from the expressions for $\partial\varphi/\partial t_{j'}^{k'}$, $\partial\vartheta/\partial t_{j'}^{k'}$, $\partial\psi/\partial t_{j'}^{k'}$ by exchanging

$$\begin{aligned}
(\alpha, \beta, \gamma) &\leftrightarrow (\psi, \vartheta, \varphi), \\
k' &\leftrightarrow j'.
\end{aligned} \tag{A12}$$

To transform the Schrödinger equation to the new coordinates, extensive use is made of the properties of the rotation matrices. The first step of this transformation is illustrated. The new coordinates are called v_i now:

$$(v_1, \cdots, v_9) = (t_0^0, t_1^1, t_{-1}^1, \alpha, \beta, \gamma, \psi, \vartheta, \varphi). \tag{A13}$$

The expressions for the first derivatives derived in this appendix can be written as

$$\frac{\partial v_m}{\partial t_{j'}^{k'}} = \sum_n \sum_p D_{nk'}^{1*}(\alpha, \beta, \gamma) D_{pj'}^{1*}(\psi, \vartheta, \varphi) a_{np}^m. \tag{A14}$$

The a_{np}^m do not depend on $\alpha, \beta, \gamma, \psi, \vartheta, \varphi$. Thus one obtains for (13):

$$\begin{aligned}
\sum_{jk} (-)^{j+k} \frac{\partial^2}{\partial t_j^k \partial t_{-j}^{-k}} &= \sum_{jk} \sum_{nn'p} \sum_{m'n'p'} (-)^{j+k} D_{nk}^{1*}(\alpha, \beta, \gamma) D_{pj}^{1*}(\psi, \vartheta, \varphi) a_{np}^m \\
&\quad \times \left[\frac{\partial}{\partial v_m} D_{n'-k}^{1*}(\alpha, \beta, \gamma) D_{p'-j}^{1*}(\psi, \vartheta, \varphi) a_{n'p'}^{m'} \frac{\partial}{\partial v_{m'}}\right].
\end{aligned} \tag{A15}$$

The coefficients $f_{mm'}$ of the second derivatives $\partial^2/\partial v_m \partial v_{m'}$ in the transformed Schrödinger equation are then

$$\begin{aligned}
f_{mm'} &= \sum_{jk} \sum_{np} \sum_{n'p'} (-)^{j+k} D_{nk}^{1*}(\alpha, \beta, \gamma) D_{pj}^{1*}(\psi, \vartheta, \varphi) \\
&\quad \times D_{n'-k}^{1*}(\alpha, \beta, \gamma) D_{p'-j}^{1*}(\psi, \vartheta, \varphi) a_{np}^m a_{n'p'}^{m'} (2 - \delta_{mm'}) \\
&= (2 - \delta_{mm'}) \sum_{np} (-)^{n+p} a_{np}^m a_{-n-p}^{m'}.
\end{aligned} \tag{A16}$$

The final result of the transformation is given in Eq. (16).

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Solutions of the Zero-Rest-Mass Equations

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By means of contour integrals involving arbitrary analytic functions, general solutions of the zero-rest-mass field equations in flat space-time can be generated for each spin. If the contour surrounds only a simple (respectively, low-order) pole of the function, the resulting field is null (respectively, algebraically special).

1. THE CONTOUR INTEGRAL

It is possible to generate a very wide class of solutions to the zero-rest-mass field equations for each spin, $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$, in flat space–time by means of a certain contour-integral expression. By choosing the integrand and contour suitably, the resulting field can be made to have certain prescribed properties, e.g., it may be made null or algebraically special. The expression arises naturally in the theory of twistors,[1] but the result can be given quite readily without using twistors. The present note gives the main results without going into the general theory.

Let x^0, x^1, x^2, x^3 be standard Minkowskian coordinates and set

$$u = 2^{-\frac{1}{2}}(x^0 + x^1), \quad v = 2^{-\frac{1}{2}}(x^0 - x^1),$$
$$\zeta = 2^{-\frac{1}{2}}(x^2 + ix^3), \tag{1.1}$$

so that the metric becomes $ds^2 = 2du\,dv - 2d\zeta\,d\bar{\zeta}$. Let f be an analytic function of three complex variables. Choose a nonnegative integer $2s$ and, for $r = 0, 1, \cdots, 2s$, put

$$\phi_r = \frac{1}{2\pi i}\oint \lambda^r f(\lambda, u + \lambda\bar{\zeta}, \zeta + \lambda v)\,d\lambda, \tag{1.2}$$

where the contour surrounds (but does not encounter) singularities of f and varies continuously with u, v, and ζ. Then we have

$$\frac{\partial\phi_r}{\partial\bar{\zeta}} = \frac{\partial\phi_{r+1}}{\partial u}, \frac{\partial\phi_r}{\partial v} = \frac{\partial\phi_{r+1}}{\partial\zeta}, \quad r = 0, \cdots, 2s-1, \tag{1.3}$$

(if $s > 0$) and

$$\left\{\frac{\partial^2}{\partial u\partial v} - \frac{\partial^2}{\partial\zeta\partial\bar{\zeta}}\right\}\phi_r = 0, \quad r = 0, \cdots, 2s. \tag{1.4}$$

Equations (1.4) is simply the wave equation in the coordinates (1.1) while Eqs. (1.3) are the spin-s zero-rest-mass equations in a suitable notation. For if we put

$$\phi_0 = \phi_{000\cdots0}, \quad \phi_1 = \phi_{100\cdots0}, \quad \phi_2 = \phi_{110\cdots0}, \cdots, \quad \phi_{2s} = \phi_{111\cdots1}, \tag{1.5}$$

where $\phi_{ABC\cdots K}$ has $2s$ indices and is symmetric: $\phi_{AB\cdots K} = \phi_{(AB\cdots K)}$; then Eqs. (1.3) can be written

$$\frac{\partial}{\partial x_{AP'}}\phi_{ABC\cdots K} = 0 \tag{1.6}$$

(summation convention assumed), where the 2-spinor notation $x_{00'} = v$, $x_{01'} = -\bar{\zeta}$, $x_{10'} = -\zeta$, and $x_{11'} = u$ is being used. Equation (1.6) is simply the Dirac–Fierz spinor equation[2,3] for mass zero and spin s. If $s = 1$, we can put

$$\phi_0 = \tfrac{1}{2}(F^{12} - F^{02} - iF^{13} + iF^{03}),$$
$$\phi_1 = \tfrac{1}{2}(F^{01} - iF^{23}),$$
$$\phi_2 = \tfrac{1}{2}(F^{12} + F^{02} + iF^{13} + iF^{03}),$$

and Eqs. (1.3) become Maxwell's equations

$$\frac{\partial}{\partial x^a}F^{ab} = 0, \quad \frac{\partial}{\partial x^a}F_{bc} + \frac{\partial}{\partial x^b}F_{ca} + \frac{\partial}{\partial x^c}F_{ab} = 0.$$

Similarly, for $s = 2$, we can get the linearized Einstein equations in gauge-invariant ("curvature-tensor") form.[3,4,5]

2. NULL AND ALGEBRAICALLY SPECIAL FIELDS

Suppose the contour in (1.2) surrounds only a k-order pole of the function f. Let $\lambda = \eta$ be the pole for given u, v, ζ (so η is a function of u, v, ζ, $\bar{\zeta}$). Then

$$\oint (\lambda - \eta)^k\lambda^r f(\lambda, u + \lambda\bar{\zeta}, \zeta + \lambda v)\,d\lambda = 0.$$

Thus, if $2s \geq k$,

$$\phi_{r+k} - k\phi_{r+k-1}\eta + \tfrac{1}{2}k(k-1)\phi_{r+k-2}\eta^2 - \cdots + \phi_r(-\eta)^k = 0, \quad r = 0, \cdots, 2s-k \tag{2.1}$$

[see (1.2)]. We can rewrite Eqs. (2.1), using the notation (1.5), as

$$\phi_{AB\cdots DE\cdots K}\xi^A\xi^B\cdots\xi^D = 0, \tag{2.2}$$

where $A, B, \cdots, D$ are k in number and where

$$\xi^0 = -\eta, \quad \xi^1 = 1. \tag{2.3}$$

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Equation (2.2) is, in fact, precisely the condition for a spinor ξ^A to represent a $(2s - k + 1)$-fold *principal null direction*[5] for the field $\phi_{AB\dots K}$. Thus, when $k = 1$, so that the contour surrounds only a simple pole of f, all $2s$ principal null directions coincide in the direction of ξ^A so that we get a *null field*.[5] [In the Maxwell case this means $F_{ab}F^{ab} = 0 = F_{ab}F_{cd}\epsilon^{abcd}$ i.e., $\phi_0\phi_2 = (\phi_1)^2$.] More generally, whenever $k < 2s$ *at least two* principal null directions coincide (in the direction of ξ^A), that is to say, the field is algebraically special. (Such fields, when $s = 2$, are of interest in gravitation theory.[6,7])

The direction of ξ^A is given by the vector translation $\xi^A\bar{\xi}^{B'}$, i.e., by

$$du : d\zeta : d\bar{\zeta} : dv = \xi^0\bar{\xi}^{0'} : \xi^0\bar{\xi}^{1'} : \xi^1\bar{\xi}^{0'} : \xi^1\bar{\xi}^1$$
$$= \eta\bar{\eta} : -\eta : -\bar{\eta} : 1.$$

Thus η defines the null direction[8] given by

$$du + \eta\, d\bar{\zeta} = 0 = d\zeta + \eta\, dv. \qquad (2.4)$$

It is known[5–7,9] that the multiple principal null direction of an algebraically special field is tangential to a shear-free congruence of null geodesics (here, straight lines). In the above case, this follows also by a theorem of Kerr[1] which states that such a congruence is defined by (2.4) if we *specify an analytic relation connecting* η, $u + \eta\bar{\zeta}$, and $\zeta + \eta v$. In the present situation, the analytic equation $\{f(\lambda, u + \lambda\bar{\zeta}, \zeta + \lambda v)\}^{-1} = 0$ defines the poles $\lambda = \eta$ of f, verifying that the directions (2.4) are indeed geodetic and shear free.

In addition, Kerr's theorem states that, conversely, *any* shear-free geodetic null congruence in flat space–time (except for certain rather special limiting cases) can be obtained from such a analytic relation. This indicates the generality of expression (1.2) for the construction of null fields. Robinson[9] showed how, *starting* from any shear-free geodetic null congruence, it is possible to construct all the corresponding null solutions of Maxwell's equations by the arbitrary specification of an analytic function of two complex variables. The integral (1.2) achieves effectively the same thing (in flat space–time, but now for fields of arbitrary spin $s \geq 1$). For, by Kerr's result, the given shear-free congruence can (normally) be defined by (2.4) subject to $h(\eta, u + \eta\xi, \zeta + \eta v) = 0$, where h is some analytic function with simple zeros. Into the integrand of (1.2) we can substitute $f = gh^{-1}$, where g is an analytic function regular at the (relevant) zeros of h. The freedom of choice for the residues in (1.2) at the poles of f is, h being given, simply the freedom in the choice of g at $h = 0$. This is essentially one complex function of two complex variables ($h = 0$ being a two-complex-dimensional set) in agreement with Robinson's result.

Indeed, we can go somewhat further since algebraically special fields can also be treated by the method given here. For example, if $s = 2$, an expression gh^{-3} yields, when substituted into (1.2), a general type of algebraically special linearized gravitational field. (Here it is the values of g and its first and second derivatives, at $h = 0$, which are relevant.) We can also consider the slightly more general fields given when $k = 2s$ in (1.2). The directions (2.4) are evidently (by Kerr's theorem) still geodetic and shear free but they are now just *simple* principal null directions and the field is not algebraically special. Since, for a general field, the principal null directions are neither shear free nor geodetic, it follows that the fields given by $k = 2s$ in (1.2) are still of a rather special type. (The case $k = 2s = 1$ defines what we might tentatively call a "null neutrino field.") However, more general fields are generated if the contour surrounds a pole of higher order than $2s$ [for then (2.4) will not even be a principal null direction of the field], or more than one pole of f (in which case the resulting field will be a finite linear combination of fields of the type we have just been considering), or singularities or singular regions of more complicated types.

It is not hard to construct a function f for most of the simple types of fields normally encountered (e.g., plane waves, monopole, or multipole solutions, etc.). Also, provided the contour can be chosen consistently, we can obtain linear combinations of such fields in the form (1.2) simply by taking the corresponding linear combinations of f's. This process may fail if too extensive (continuous) linear combinations of f's are taken, since the resulting singularities may leave no room for the contour. Nevertheless, it is evident that there is considerable generality in the expression (1.2).

The full discussion of (1.2) and of its transformation properties is best carried out in terms of twistors.[1] The twistor description will be given elsewhere.[10]

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[6] I. Robinson and A. Trautman, Proc. Roy. Soc. (London) **A265**, 463 (1962).

[7] J. N. Goldberg and R. K. Sachs, Acta Phys. Polon. **22**, 13 (1962).

[8] The value $\eta = \infty$ also gives a well-defined null direction, although this would not arise from the integral (1.2) as given. To obtain null and algebraically special fields in a way similar to the above, but in which this exceptional null direction could also be represented, we would have to transform (1.2) suitably. It is in the transformation properties of (1.2) that the different spin values play a role. [Equation (1.2) is curiously oblivious to the value of s here!] The complete manifestly (conformally) covariant expression, of which (1.2) is a particular realization, requires the use of twistors.

[9] I. Robinson, J. Math. Phys. **2**, 290 (1960).

[10] *Note Added in Proof.* Due to the delay in the publishing of this paper, this description has already appeared; see R. Penrose, Intern. J. Theoret. Phys. **1**, 61 (1968).

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Many-Neighbored Ising Chain

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Using a method suggested by Montroll, we extend the well-known matrix formulation of the nearest-neighbor one-dimensional Ising problem to allow for interactions with an arbitrary finite range n, general spin l, and an applied magnetic field B. We exhibit the relevant matrix element explicitly and hence formally obtain the partition function via an eigenvalue problem of order $(2l+1)^n$. For the case $B=0$, $l=\frac{1}{2}$ we introduce a change of variable which simplifies the partition function while still allowing a matrix formulation. Using this approach we have computed specific-heat curves for infinite, ferromagnetic Ising chains with interactions of range n ($n \leq 7$). We prove in an appendix that open and cyclic boundary conditions are equivalent for the system under consideration.

1. INTRODUCTION

The partition function for an infinite chain of spins was originally calculated by Ising.[1] Kramers and Wannier[2] reformulated the problem in terms of 2×2 matrices. Both of these calculations are restricted to the nearest-neighbor problem. When the interaction is allowed to have an arbitrary finite range, the partition function is harder to calculate; however, Montroll[3] has shown that, in principle, the matrix approach can be applied to this more general problem. Other exact formulations have also been given.[4]

The present paper is devoted in part to an explicit matrix formulation of the many-neighbor problem, based on Montroll's suggestion. The nonsymmetry of the matrices was considered an obstacle by Montroll; this difficulty is removed by a theorem proved in the Appendix.

In Sec. 2 we introduce a change of variable in order to exhibit a relation between the spin-$\frac{1}{2}$ open-chain Ising partition functions for two distinct situations, namely,

(i) no external B field, nearest- and second-nearest-neighbor interactions, and

(ii) external B field applied, nearest-neighbor interactions only.

This relation was first demonstrated by Frankel[5] in another context.

Section 3 deals with the many-neighbored chain of arbitrary spins in an applied B field. We explicitly calculate the general element of a matrix whose largest eigenvalue determines the partition function.

In Sec. 4 we impose the restriction $B=0$, but otherwise retain the generality of Sec. 3. The eigenvalue problem of Sec. 3 is reduced to two eigenvalue problems of lower order.

In Sec. 5 we restrict our attention further to the spin-$\frac{1}{2}$ chain ($l=\frac{1}{2}$) in zero B field. The range (n) of the interaction is still general. We reformulate the problem in terms of the variables described in Sec. 2, and the reduction used in Sec. 4 becomes superfluous.

In Sec. 6 we present computed values of specific heat for the system described in Sec. 5.

In Sec. 7 we discuss other treatments of the one-dimensional Ising problem, particularly those which deal with *infinite*-ranged interactions. We attempt to relate the results of this paper to predictions of critical behavior given by other authors.

Finally, in the Appendix, we prove a theorem to justify a statement made in Sec. 3. The theorem has wider applicability, however, and it amounts to a proof that boundary conditions do not affect the thermodynamic behavior of infinite chains, at least when the interactions have finite range.

2. SIMPLE TREATMENT OF THE CASE $l=\frac{1}{2}$, $B=0$, $n=2$

We consider the spin-$\frac{1}{2}$ chain in zero B field, assuming that spin–spin interactions are negligible except for nearest and second-nearest neighbors. The partition function for a chain of length N is

$$\bar{Q}_N(\beta, J_1, J_2) = \sum_{s_1=-1}^{1} \cdots \sum_{s_N=-1}^{1} \exp \beta \left(J_1 \sum_{i=1}^{N-1} s_i s_{i+1} + J_2 \sum_{i=1}^{N-2} s_i s_{i+2} \right), \quad (2.1)$$

where the coupling constants J_1 and J_2 are positive for a ferromagnetic chain.

[1] E. Ising, Z. Phys. **31**, 253 (1925).

[2] H. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252 (1941). These authors use cyclic boundary conditions leading to an expression for the partition function as the trace of a matrix.

[3] E. W. Montroll, J. Chem. Phys. **10**, 61 (1942). See particularly pp. 68–70.

[4] H. S. Green and J. Liepnik [Rev. Mod. Phys. **32**, 129 (1960)], have developed a "matrix-spinor" approach which has been modified by M. E. Fisher and H. N. V. Temperley, Rev. Mod. Phys. **32**, 1029 (1960). The recursion relations they obtain may well be suited to an exact numerical treatment of the many-neighbored Ising chain.

[5] N. E. Frankel and D. Rapaport (to be published).

We define a new set of variables $\{t_i\}$ with possible values ± 1:

$$t_0 = s_1$$
$$t_i = s_i s_{i+1}, \quad i = 1, 2, \cdots, N-1. \tag{2.2}$$

In the spin-$\frac{1}{2}$ case this transformation can be uniquely inverted since $s_i^2 \equiv 1$ so that

$$s_i = s_i s_{i-1} s_{i-1} s_{i-2} s_{i-2} \cdots s_2 s_1 s_1 = t_{i-1} t_{i-2} \cdots t_1 t_0. \tag{2.3}$$

Thus for each set of values $\{s_i\}$ there is exactly one set $\{t_i\}$ and vice versa. Hence the partition function becomes

$$\bar{Q}_N(\beta, J_1, J_2) = 2 \sum_{t_1=-1}^{1} \cdots \sum_{t_{N-1}=-1}^{1} \exp \beta \left(J_1 \sum_{i=1}^{N-1} t_i + J_2 \sum_{i=1}^{N-2} t_i t_{i+1} \right), \tag{2.4}$$

where $s_i s_{i+2} = s_i (s_{i+1})^2 s_{i+2} = t_i t_{i+1}$, and the factor 2 arises from the sum over t_0.

Now the partition function for the spin-$\frac{1}{2}$ nearest-neighbor chain in a magnetic field B is given by

$$Q_N(\beta, J, B) = \sum_{s_1=-1}^{1} \cdots \sum_{s_N=-1}^{1} \exp \beta \left(\mu B \sum_{i=1}^{N} s_i + J \sum_{i=1}^{N-1} s_i s_{i+1} \right). \tag{2.5}$$

Hence, from comparison of (2.4) and (2.5),

$$\bar{Q}_N(\beta, J_1, J_2) = 2 Q_{N-1}(\beta, J, B), \tag{2.6}$$

where $J = J_2$ and $\mu B = J_1$.

Thus the second-nearest-neighbor result can be transcribed from the well-known nearest-neighbor result.[6] The relation (2.6) was first noticed by Frankel[5] in another context.

The transformation (2.2) can only be used in the spin-$\frac{1}{2}$ case for which the unique inverse (2.3) exists; a further restriction is that the applied field B is zero. However the technique is *not* restricted to the second-nearest-neighbor problem and we use (2.2) in Sec. 5 in the context of long-ranged interactions.

3. GENERAL PARTITION FUNCTION

We consider the case of general spin with an external magnetic field B.

Let each site have spin l so that the spin projection s_i can take $2l + 1$ values.

We consider an n-neighbor chain; thus the interaction energy of two spins is

$$E(s_i, s_{i\pm k}) = \begin{cases} -J_k s_i s_{i\pm k}, & \text{when } 0 < k \leq n, \\ 0, & \text{when } k > n. \end{cases}$$

In order to write down the energy of the chain in any given configuration we divide the chain into blocks of length n and consider a chain of total length Nn. This procedure was suggested by Montroll[3] who performed the calculation explicitly for the case $l = \frac{1}{2}$, $n = 2$, $B = 0$.

The division is as follows:

1st block	2nd block	$\cdots$	jth block	$\cdots$	Nth block
$[s_1 \ s_2 \ \cdots \ s_n]$	$[s_{n+1} \ s_{n+2} \ \cdots \ s_{2n}]$	$\cdots$	$[s_{(j-1)n+1} \ \cdots \ s_{jn}]$	$\cdots$	$[s_{(N-1)n+1} \ \cdots \ s_{Nn}]$
or $[s_1^{(1)} \ \cdots \ s_n^{(1)}]$	$[s_1^{(2)} \ \cdots \ s_n^{(2)}]$	$\cdots$	$[s_1^{(j)} \ \cdots \ s_n^{(j)}]$	$\cdots$	$[s_1^{(N)} \ \cdots \ s_n^{(N)}]$,

where the second alternative is merely a convenient relabeling of the first.

Each block has $(2l + 1)^n$ possible configurations, so that the configuration of the jth block can be specified by a single integer c_j where $1 \leq c_j \leq (2l + 1)^n$. Because the interaction has range n, a spin in the jth block can interact only with spins in the $(j-1)$th, jth, and $(j+1)$th blocks. Hence the energy of the chain is the sum of three types of term:

(i) interaction energies with the external B field,

(ii) mutual energies of spins which are in the same block, and

(iii) mutual energies of spins from two adjacent blocks.

The contributions of types (i) and (ii) from the jth block are

$$X_{c_j} \equiv X(s_1^{(j)}, s_2^{(j)}, \cdots, s_n^{(j)}) = -\mu B \sum_{i=1}^{n} s_i^{(j)} - \sum_{k=1}^{n} J_k \left(\sum_{i=1}^{n-k} s_i^{(j)} s_{i+k}^{(j)} \right). \tag{3.1}$$

The contribution of type (iii) from the jth and $(j+1)$th blocks is

$$Y_{c_j, c_{j+1}} \equiv Y(s_1^{(j)}, \cdots, s_n^{(j)}; s_1^{(j+1)}, \cdots, s_n^{(j+1)}) = -\sum_{k=1}^{n} J_k \left(\sum_{i=1}^{k} s_{n+1-i}^{(j)} s_{k-i+1}^{(j+1)} \right). \tag{3.2}$$

Note that if the configurations of blocks j and $(j+1)$ are interchanged their mutual energy is *not* invariant; that is, the matrix Y is nonsymmetric.

The total energy of the chain in configuration $(c_1, c_2, \cdots, c_N)$ is

$$H(c_1, \cdots, c_N) = X_{c_1} + Y_{c_1, c_2} + X_{c_2} + Y_{c_2, c_3} + \cdots + Y_{c_{N-1}, c_N} + X_{c_N}.$$

[6] The simplest derivation of the nearest-neighbor result (that of Ref. 2) uses cyclic boundary conditions whereas we use open-chain conditions to derive (2.6). However the appendix to this paper is a rigorous proof that the boundary conditions are unimportant. See also the remarks at the end of Sec. 3.

Defining a matrix V and a vector $\mathbf{U}$ by the relations

$$V_{c_i,c_j} = \exp -\beta(\tfrac{1}{2}X_{c_i} + Y_{c_i,c_j} + \tfrac{1}{2}X_{c_j}),$$
$$U_{c_i} = \exp -\tfrac{1}{2}\beta X_{c_i}, \tag{3.3}$$

we find that the partition function is

$$\begin{aligned} Q_{Nn} &= \sum_{c_1}\cdots\sum_{c_N} \exp -\beta H(c_1,\cdots,c_N) \\ &= \sum_{c_1}\cdots\sum_{c_N} U_{c_1}V_{c_1,c_2}V_{c_2,c_3}\cdots V_{c_{N-1},c_N}U_{c_N} \\ &= \mathbf{U}^{\mathrm{T}}V^{N-1}\mathbf{U} \end{aligned} \tag{3.4}$$

The vector $\mathbf{U}$ can be regarded as representing end effects due to a deficiency of neighbors for the spins near the ends of the chain.

Because V is, in general, nonsymmetric, it may not be similar to any diagonal matrix and the rigorous evaluation of (3.4) is not quite straightforward, even in the limit $N \to \infty$. For example, Montroll, in calculating the second-nearest-neighbor partition function from a formula similar to (3.4), was obliged to exhibit a full orthonormal set of left and right eigenvectors for his matrix; the existence of such a set is not automatic for a nonsymmetric matrix.

We overcome this difficulty in a completely general fashion in the Appendix, where we show that the Q_{Nn} of Eq. (3.4) has the following property:

$$(\log Q_{Nn})/(N-1) \to \log \lambda_1, \quad \text{as} \quad N \to \infty, \tag{3.5}$$

where λ_1 is the positive, nondegenerate, largest eigenvalue of V. The *only* conditions necessary for this result are that V and $\mathbf{U}$ are of finite size and have positive elements.

If we had applied cyclic boundary conditions[2] to the chain, the formula (3.4) would have been

$$Q_{Nn} = \mathrm{Tr}\, V^N.$$

Now it is easily proved that, for *any* $M \times M$ matrix V,

$$\mathrm{Tr}\, V^N = \sum_{i=1}^{M} \lambda_i^N,$$

where λ_i are the M (possibly degenerate) eigenvalues of V. Hence, for cyclic boundary conditions

$$Q_{Nn} \sim \lambda_1^N,$$

where λ_1 is the dominant eigenvalue of V.

Therefore, the appendix is actually a rigorous demonstration that open and cyclic boundary conditions lead to the same thermodynamic behavior for the type of system we have been considering.

4. REDUCTION OF THE GENERAL EIGENVALUE PROBLEM[7]

When there is no external B field the energy of the chain is unaltered by a complete "spin flip"; in fact the matrix V of (3.3) has the following property:

$$\begin{aligned} &V(s_1,\cdots,s_N;s_1',\cdots,s_N') \\ &\quad = V(-s_1,\cdots,-s_N;-s_1',\cdots,-s_N'), \\ &\qquad \text{for} \quad B = 0. \end{aligned} \tag{4.1}$$

Also, if the spin l is an integer, s_i may take the value zero and clearly

$$V(0,\cdots,0;s_1,\cdots,s_N) = V(s_1,\cdots,s_N;0,\cdots,0). \tag{4.2}$$

From (4.1) and (4.2) it follows that, by suitably ordering the configurations c_j, we can cast V into the following partitioned form:

$$V = \left(\begin{array}{c|c} A & B \\ \hline B & A \end{array}\right), \quad \text{for half-integral } l,$$

or

$$V = \left(\begin{array}{c|c|c} C & \mathbf{x} & D \\ \hline \mathbf{x}^{\mathrm{T}} & 1 & \mathbf{x}^{\mathrm{T}} \\ \hline D & \mathbf{x} & C \end{array}\right), \quad \text{for integral } l.$$

Here A, B, C, and D are square matrices whose dimension is the greatest integer l' not exceeding $(2l+1)^n/2$. $\mathbf{x}$ is a column vector of dimension l'.

Defining the orthogonal matrices

$$T_1 = 2^{-\frac{1}{2}}\left(\begin{array}{c|c} I & I \\ \hline I & -I \end{array}\right) = T_1^{-1},$$

$$T_2 = 2^{-\frac{1}{2}}\left(\begin{array}{c|c|c} I & \mathbf{O} & I \\ \hline \mathbf{O}^{\mathrm{T}} & 2^{\frac{1}{2}} & \mathbf{O}^{\mathrm{T}} \\ \hline I & \mathbf{O} & -I \end{array}\right) = T_2^{-1},$$

we find that

$$T_1 V T_1^{-1} = \left(\begin{array}{c|c} A+B & 0 \\ \hline 0 & A-B \end{array}\right), \quad \text{for half-integral } l,$$

$$T_2 V T_2^{-1} = \left(\begin{array}{c|c|c} C+D & 2^{\frac{1}{2}}\mathbf{x} & 0 \\ \hline 2^{\frac{1}{2}}\mathbf{x}^{\mathrm{T}} & 1 & \mathbf{O}^{\mathrm{T}} \\ \hline 0 & \mathbf{O} & C-D \end{array}\right), \quad \text{for integral } l. \tag{4.3}$$

Equation (4.3) shows that the dominant eigenvalue of V is equal to the dominant eigenvalue of one of two smaller matrices, each of approximately one-half the

[7] This paragraph generalizes the work of Montroll (Ref. 3) and includes as a special case the reduction of M. Suzuki, B. Tsujiyama, and S. Katsura, J. Math. Phys. **8**, 124 (1967).

dimension of V. With reference to the right-hand side of (4.3), we believe that it is always the *upper* submatrix which contributes the dominant eigenvalue of V, but we have not proved this.

5. REDUCTION OF EIGENPROBLEM FOR SPIN $\frac{1}{2}$

In the case $B = 0$, $l = \frac{1}{2}$, the entire problem may be reformulated in terms of the variables t_i defined by (2.2). The result is a *single* eigenproblem of order 2^{n-1} instead of *two* such problems as in Sec. 4.

For an interaction of range n we consider a chain of length $N(n-1)+1$. When $B = 0$, the energy of the chain is independent of t_0:

$$\begin{aligned} H(t_1, \cdots, t_{Nm}) &= -J_1\{t_1 + t_2 + \cdots + t_{Nm}\} \\ &\quad - J_2\{t_1t_2 + \cdots + t_{Nm-1}t_{Nm}\} - \cdots \\ &\quad - J_n\{t_1t_2\cdots t_m + \cdots + t_{m(N-1)+1}\cdots t_{Nm}\}, \end{aligned} \tag{5.1}$$

where we have temporarily put $(n-1) \equiv m$.

Again we impose a grouping of the variables into blocks:

$$[t_1^{(1)}, \cdots, t_{n-1}^{(1)}]\,[t_1^{(2)}, \cdots, t_{n-1}^{(2)}]\cdots[t_1^{(N)}, \cdots, t_{n-1}^{(N)}].$$

The products $t_it_{i+1}\cdots t_{i+k}$ occurring in (5.1) are of two types:

(i) t_i and t_{i+k} may be in the same block,
(ii) t_i and t_{i+k} may be in adjacent blocks.

The contribution of type (i) from the jth block is

$$\begin{aligned} \bar{X}_{c_j} &\equiv \bar{X}(t_1^{(j)}, \cdots, t_{n-1}^{(j)}) \\ &= -\sum_{k=1}^{n-1} J_k \sum_{i=1}^{n-k} t_i^{(j)} t_{i+1}^{(j)} \cdots t_{i+k-1}^{(j)} \end{aligned} \tag{5.2}$$

and the contribution of type (ii) from blocks j and $(j+1)$ is

$$\begin{aligned} \bar{Y}_{c_j,c_{j+1}} &\equiv \bar{Y}(t_1^{(j)}, \cdots, t_{n-1}^{(j)}; t_1^{(j+1)}, \cdots, t_{n-1}^{(j+1)}) \\ &= -\sum_{k=2}^{n} J_k \sum_{i=1}^{k-1} t_{n-i}^{(j)} t_{n-i+1}^{(j)} \cdots t_{n-1}^{(j)} t_1^{(j+1)} \cdots t_{k-i}^{(j+1)}. \end{aligned} \tag{5.3}$$

As in Sec. 3, we define

$$\begin{aligned} \bar{V}_{c_j,c_{j+1}} &= \exp -\beta(\tfrac{1}{2}\bar{X}_{c_j} + \bar{Y}_{c_j,c_{j+1}} + \tfrac{1}{2}\bar{X}_{c_{j+1}}), \\ \bar{U}_{c_j} &= \exp -\tfrac{1}{2}\beta\bar{X}_{c_j}, \end{aligned} \tag{5.4}$$

and once more the partition function has the form

$$\bar{Q}_{Nm+1} = 2\bar{\mathbf{U}}^{\mathrm{T}}\bar{V}^{N-1}\bar{\mathbf{U}}, \quad 2 \equiv \sum_{t_0=-1}^{1}, \tag{5.5}$$

where the dimension of $\bar{\mathbf{U}}$ and $\bar{V}$ is 2^{n-1} and both have positive elements. The result of the Appendix is again applicable:

$$(\log \bar{Q}_{Nm+1})/N - 1 \to \log \lambda_{\max}, \quad \text{as} \quad N \to \infty,$$

where $\lambda_{\max}$ is the dominant eigenvalue of $\bar{V}$.

6. NUMERICAL RESULTS

Using the matrix defined by Eqs. (5.2)–(5.4), we have programmed a digital computer to calculate specific heat curves for the spin-$\frac{1}{2}$ chain in zero B-field. Considerations of computer time and storage space limited the treatment to cases where the interactions have range less than 8 lattice spacings: even so, 64×64 matrices were processed.

In order to test a conjecture made by Kac (see Sec. 7), we chose the mutual energy of two spins to be

$$E_{ij} = \begin{cases} -Js_is_j/|i-j|^p, & |i-j| \le n, \\ 0, & |i-j| > n, \end{cases}$$

where n is the range of the interaction.

The specific-heat curves are shown in Figs. (1)–(4) for various values of n and p.

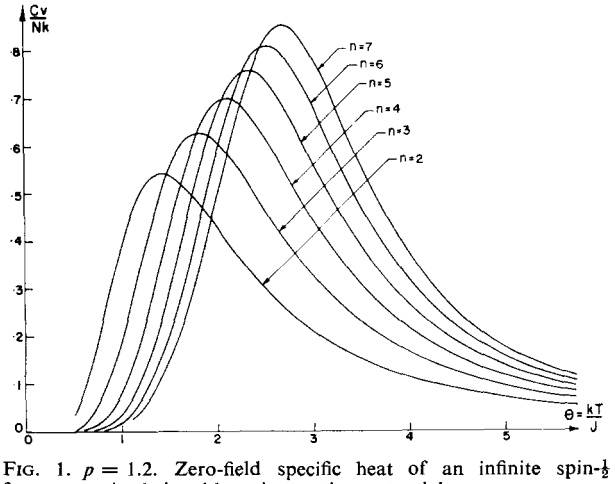

FIG. 1. $p = 1.2$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{1.2}, \quad |i-j| \le n.$$

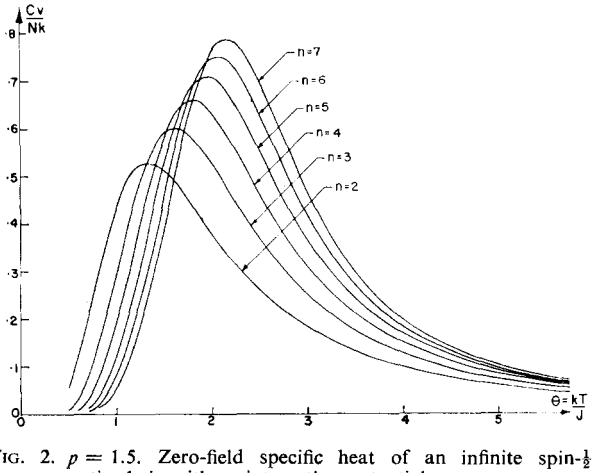

FIG. 2. $p = 1.5$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{1.5}, \quad |i-j| \le n.$$

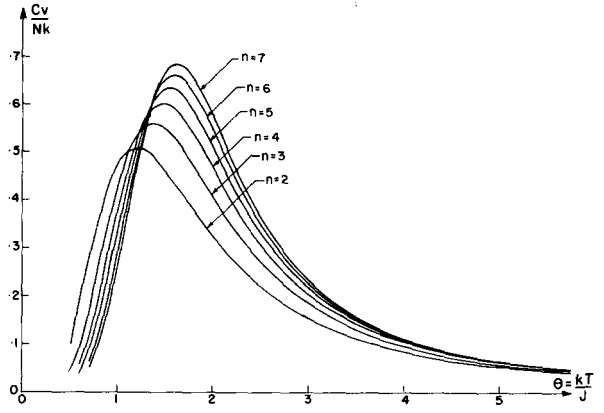

FIG. 3. $p = 2.0$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{2.0}, \quad |i-j| \leq n.$$

A direct method has been used elsewhere to calculate the partition function and specific heat for *finite* chains of length 6 and 7 with all spins interacting.[8] The results of the direct calculation do not differ greatly from those shown in Figs. (1)–(4). The infinite chain considered here naturally gives rise to slightly more sharply peaked curves, while the maxima occur at somewhat higher temperatures.

7. DISCUSSION

The one- and two-dimensional Ising models differ fundamentally in that no phase transition occurs in one dimension for any finite-ranged interaction,[9] while in two dimensions even a nearest-neighbor interaction results in a phase transition.[10] However it is known that in both one and two dimensions a potential of the form

$$H(s_1, \cdots, s_N) = -(J/N) \sum_{1 \leq i < j \leq N} s_i s_j, \quad N \to \infty,$$

leads to a finite discontinuity in the specific heat (the well-known "molecular field theory" type of phase transition). Domb[11] and Kac[12] have raised the question of phase transitions for a more physical infinite-ranged potential of the form

$$E_{ij} = -Js_i s_j/|i-j|^p.$$

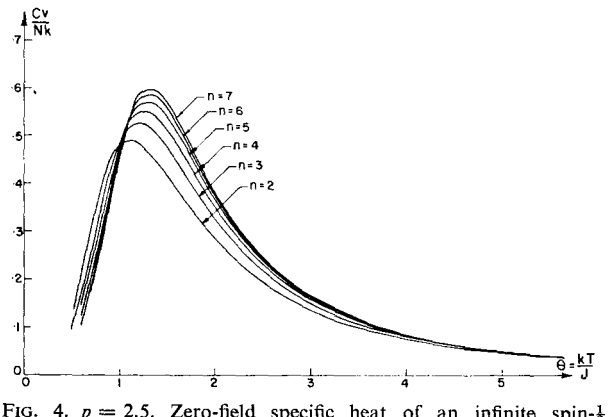

FIG. 4. $p = 2.5$. Zero-field specific heat of an infinite spin-$\frac{1}{2}$ ferromagnetic chain with an interaction potential

$$E_{ij} = -J/|i-j|^{2.5}, \quad |i-j| \leq n.$$

Kac conjectures that in one dimension a phase transition does occur when $1 < p \leq 2$, but not when $p > 2$.

Unfortunately the potentials treated in Sec. 6 do not have a long enough range to test Kac's conjecture conclusively. However for the case $p = 2.5$ [Fig. (4)] it seems clear that as the range (n) of the interaction increases the specific-heat plots are converging to a smooth curve with no discontinuity or divergence. For p between 1 and 2 the results are not inconsistent with a molecular-field type of transition but other kinds of behavior cannot be ruled out.

The curves do, however, permit an estimate to be made of the Curie temperature for an infinite-ranged potential (more strictly, a lower bound can be given for $\theta_{\max}$, the temperature at which the specific heat has its maximum value, finite or infinite; see Table I). The result quoted in Table I for $p = 2.0$ is

TABLE I. Estimates of the "Curie" temperature for an infinite-ranged interaction $1/r^p$.

p	$\theta_{\max}$
1.0	>3.1 (unphysical)
1.2	>2.7
1.5	>2.1
1.8	$\gtrsim 1.85$
2.0	$\gtrsim 1.63$
2.2	$\gtrsim 1.47$

in good agreement with a calculation by Joyce[13] who used series expansions to investigate the zero-field magnetic susceptibility of a chain with an infinite-ranged potential $J/|i-j|^2$. He obtained a Curie temperature of $\theta_c = 1.6_8$, compared with $\theta_{\max} \gtrsim 1.6_3$ as shown above.

[8] D. Rapaport (private communication).

[9] E. W. Montroll, J. Chem. Phys. **9**, 706 (1941). In particular, see p. 711. Montroll notes that the dominant eigenvalue of the matrix V must become degenerate if a phase transition is to occur. The theorem of Ref. 14 (see also the Appendix) rules out this degeneracy for a finite-ranged interaction.

[10] The first solution of the two-dimensional problem was given by L. Onsager, Phys. Rev. **65**, 117 (1944).

[11] C. Domb, in *Critical Phenomena, Proceedings of a Conference, Washington, D.C., 1965* (U.S. National Bureau of Standards, Washington, D.C., 1966); N.B.S. Misc. Publ. 273.

[12] M. Kac, *Brandeis Summer School Lectures, 1966* (to be published).

[13] G. S. Joyce, quoted by C. Domb (see Ref. 11, particularly p. 39).

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APPENDIX

Let

$$Q_N = \mathbf{U}^T V^N \mathbf{W} = \sum_{s=1}^{R} \sum_{s'=1}^{R} U_s (V^N)_{ss'} W_{s'}, \tag{A1}$$

where V is an $R \times R$ matrix with positive elements, and $\mathbf{U}$ and $\mathbf{W}$ are column vectors with positive elements.

Then (i) V has a nondegenerate eigenvalue λ_1 of largest modulus and $\lambda_1 > 0$ (this follows from a theorem of Frobenius[14]) and (ii) there exists a *positive* constant C such that

$$Q_N/\lambda_1^N \to C \quad \text{as} \quad N \to \infty.$$

(Since we are to take logarithms of this relation it is essential that $C \neq 0$.)

Proof of (ii): Any matrix V can be factorized in *Jordan canonical form*

$$V = P\Delta P^{-1}, \qquad V^N = P\Delta^N P^{-1}, \tag{A2}$$

where P is nonsingular and Δ is the direct sum of simple Jordan matrices D_i:

$$\Delta = \text{diag}\,(D_1, D_2, \cdots, D_M).$$

Corresponding to each *nondegenerate* eigenvalue λ the simple Jordan matrix is just the 1×1 matrix λ. However, to each *degenerate* eigenvalue λ_i there correspond one or more matrices D_i of the form

$$(D_i)_{\alpha\beta} = \lambda_i \delta_{\alpha\beta} + \delta_{\alpha+1,\beta}. \tag{A3}$$

(For matrices with complete eigenvector spaces the D_i are all 1×1 but for less well-behaved matrices the D_i are larger.)

We order the eigenvalues of V according to their modulus, $\lambda_1 > |\lambda_2| \geq |\lambda_3| \cdots \geq |\lambda_R|$. Since λ_1 is nondegenerate, D_1 is 1×1 and

$$\Delta = \text{diag}\,(\lambda_1, D_2, \cdots, D_M)$$

so that

$$\Delta^N/\lambda_1^N = \text{diag}\,(1, D_2^N/\lambda_1^N, \cdots, D_M^N/\lambda_1^N). \tag{A4}$$

[The basic aim is to show that all terms on the rhs of (A4) approach zero, except for the first term.]

From (A3) it follows by induction (or merely by inspection) that

$$(D_i^N)_{\alpha\beta} = \sum_{r=0}^{M_i - 1} \lambda_i^{N-r}\, {}^N C_r \delta_{\alpha+r,\beta}$$

where D_i is $M_i \times M_i$, i.e.,

$$(D_i^N)_{\alpha\beta} = \begin{cases} 0, & (\beta - \alpha) > N, \\ \lambda_i^{N-\beta+\alpha}\, {}^N C_{\beta-\alpha}, & N \geq (\beta - \alpha) \geq 0, \\ 0, & (\beta - \alpha) < 0. \end{cases}$$

Further routine manipulation shows that, for $N > 2\delta \equiv 2\,|\beta - \alpha|$,

$$|(D_i^N)_{\alpha\beta}/\lambda_1^N| \leq [\lambda_1^\delta\, |\lambda_2/\lambda_1|^{N/2-\delta}\, N^\delta]\, |\lambda_2/\lambda_1|^{N/2}, \quad \text{for} \quad i \geq 2,$$

where the term in square brackets is bounded (and in fact it $\to 0$) as $N \to \infty$.

Thus, for $i > 1$,

$$(D_i^N)_{\alpha\beta}/\lambda_1^N = O(p^N), \quad \text{as} \quad N \to \infty, \tag{A5}$$

where

$$p = |\lambda_2/\lambda_1|^{\frac{1}{2}} < 1.$$

(A4) and (A5) lead to the result

$$(\Delta^N)_{\alpha\beta}/\lambda_1^N = \delta_{\alpha 1}\delta_{1\beta} + O(p^N). \tag{A6}$$

This is the required "smallness condition" mentioned after Eq. (A4).

Substituting (A6) into (A2) we obtain

$$(V^N)_{\alpha\beta}/\lambda_1^N = P_{\alpha 1}(P^{-1})_{1\beta} + O(p^N), \tag{A7}$$

since a constant, finite, linear combination of $O(p^N)$ quantities is rigorously $O(p^N)$.

Now (A7) shows that

$$P_{\alpha 1}(P^{-1})_{1\beta} \geq 0; \tag{A8}$$

for V has positive elements and $\lambda_1 > 0$ so that $(V^N)_{\alpha\beta}/\lambda_1^N > 0$ for all finite N.

Combining (A1) and (A7),

$$Q_N/\lambda_1^N = \left[\sum_{\alpha,\beta} U_\alpha P_{\alpha 1}(P^{-1})_{1\beta} W_\beta\right] + O(p^N). \tag{A9}$$

Now the quantities $(P)_{\alpha 1}(P^{-1})_{1\beta}$ are nonnegative [by Eq. (A8)] and they cannot be zero for all α, β since this would make either P of P^{-1} singular, contrary to (A2). Hence from the positiveness of U_α and W_β, the quantity in square brackets in (A9) is positive, i.e.,

$$Q_N/\lambda_1^N \to C, \quad \text{as} \quad N \to \infty, \tag{A10}$$

where

$$C = \left[\sum_{\alpha,\beta} U_\alpha P_{\alpha 1}(P^{-1})_{1\beta} W_\beta\right] > 0. \qquad \text{Q.E.D.}$$

Taking logarithms of (A10) we find that

$$(\log Q_N)/N \to \log \lambda_1 \quad \text{as} \quad N \to \infty.$$

[14] S. B. Frobenius, Preuss. Akad. Wiss. 514 (1909).

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Comments on the Classical Theory of Magnetic Monopoles

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The classical theory of electromagnetism including magnetic monopoles is formulated in terms of harmonic functions. The fact that there is no consistent action-integral formulation of the field that yields both particle and field equations for both electric and magnetic charges is discussed in detail. It is seen that a consistent formulation can be developed through an action integral, but, in such a development, a monopole does not have what has been considered to be an appropriate interaction with either an electric charge or another monopole.

A number of analyses of the classical theory of magnetic monopoles has been presented.[1–4] The basic reason for an interest in such a classical theory is that, if magnetic monopoles exist in a quantum formulation of the electromagnetic field,[5–7] this formulation should have a demonstrable classical limit. A basic result of previous work on magnetic charge is that no action-integral formulation of electromagnetism exists from which one can derive both particle and field equations when both magnetic and electric charges are included, provided that magnetic charge is considered to be a source for a conventional magnetic field. In this paper we shall examine the classical action-integral formulation in detail and show that such a formulation can yield both particle and field equations, but only if one considers unexpected interactions between electric and magnetic charge and between magnetic charges. The essence of this paper is that we consider what happens if we insist upon a nonexact electromagnetic field (that is, a field whose tensor curl is nonzero) and also insist upon a consistent action-integral formulation of this field that yields both particle and field equations. The result is that magnetic charge does not have an appropriate behavior in the presence of electric charge, nor does it have the conventionally conceived interaction with a monopole field. Our work thus contrasts to that of Rosenbaum[4] who assumes the monopole is a source for a conventional magnetic field and shows that such an assumption is inconsistent with a classical action principle.

The work in this paper is motivated by the fact that to date the existence of monopoles has not been confirmed.[8] As long as such particles are absent it might be well to examine whether their absence is due, not to their nonexistence, but to assumptions of properties not in accord with their classical nature. We develop the theory of electric and magnetic charge in terms of Hodge's potential theory[9] and use the notation of differential forms of Flanders.[10]

In the subsequent development we shall generally consider that we are dealing with a four-dimensional manifold **M** with a signature of two. Let us consider the space of p-forms on **M** as an inner-product space through the product $\omega \wedge \vee {}^*\eta$ where ω and η are two p-forms, $*$ is the Hodge star operator, and $\wedge$ is the exterior-product symbol. It is a basic result of Hodge that if ω is any p-form on **M**, there is a $(p-1)$-form α, a $(p+1)$-form β, and a harmonic p-form γ such that

$$\omega = d\alpha - \delta\beta + \gamma, \tag{1}$$

where $d\alpha$ is the exterior derivative of α and $\delta\beta$ is ${}^*d\,{}^*\beta$ on **M**. We call γ harmonic if $d\gamma = \delta\gamma = 0$. It is clear that $(\delta d + d\delta)\gamma = 0$. The forms α, β, and γ can be proven to exist and furthermore they are unique.

Let us form

$${}^*\omega = \delta\,{}^*\alpha + d\,{}^*\beta + {}^*\gamma, \tag{2}$$

where we have used the relation that if μ is any p-form on M, ${}^{**}\mu = (-1)^{p+1}\mu$.

Equations (1) and (2) have been discussed by Cabbibo and Ferarri[1] and are completely equivalent to Eqs. (2.12) and (2.12*) of Rohrlich[3] except for the appearance of the free fields γ. Because of this fact we are led to associate the electromagnetic electric charge four-potential A_1 with the one-form α, the magnetic charge four-potential B_i with ${}^*\beta$, and a free-field solution of the electromagnetic field wave equation with γ. We associate a current density with the following two one-forms:

$$J_e = \delta\omega = \delta\, d\alpha, \tag{3}$$

$$J_m = {}^*d\omega = -{}^*d\delta\,\beta. \tag{4}$$

[1] N. Cabbibo and E. Ferarri, Nuovo Cimento **23**, 1147 (1962).
[2] P. A. M. Dirac, Phys. Rev. **74**, 817 (1948).
[3] F. Rohrlich, Phys. Rev. **150**, 1104 (1966).
[4] D. Rosenbaum, Phys. Rev. **147**, 891 (1966).
[5] P. A. M. Dirac, Proc. Roy. Soc. **A133**, 60 (1931).
[6] J. S. Schwinger, Phys. Rev. **144**, 1087 (1966).
[7] J. G. Taylor, Phys. Rev. Letters **18**, 713 (1967).
[8] It has been reported that H. H. Kolm [Phys. Today, No. 11, **20**, 69 (1967), "Search and Discovery"] has found some experimental evidence to support the existence of a monopole.
[9] W. V. D. Hodge, *Theory and Applications of Harmonic Integrals* (Cambridge University Press, Cambridge, Eng., 1952).
[10] H. Flanders, *Differential Forms* (Academic Press Inc., New York, 1963).

It is readily seen that $\delta J_e = \delta J_m = 0$, so that both currents are conserved. Let us consider a p-form ν and a $(p+1)$-form η. It can be shown that, if we choose an $(n-1)$-dimensional surface of **M** such that ν and η are zero over this surface (or assume **M** closed), then

$$d\nu \wedge {}^*\eta = \nu \wedge {}^*\delta\eta. \tag{5}$$

Let us note that, by (5),

$$\begin{aligned}\rho &= \omega \wedge {}^*\omega \\ &= (\alpha \wedge d\delta\, {}^*\alpha) + (\beta \wedge {}^*d\delta\, \beta) + (\gamma \wedge {}^*\gamma), \\ \sigma &= \omega \wedge \omega = 2\alpha \wedge \delta d\, {}^*\beta + \gamma \wedge \gamma.\end{aligned} \tag{6}$$

The quantities ρ and σ are four-forms and either one considered separately is suitable for the formation of an action integral that when varied with respect to α or ${}^*\beta$ yields the field equations of the electromagnetic field. If we take the sum or difference of ρ and η and form an action integral, variations with respect to α and β yield equations of the form

$${}^*d\delta\, \beta \pm \delta\, d\alpha = J_m \pm J_e. \tag{7}$$

Let us now set the currents equal to a constant times a velocity and consider a variation with respect to these velocities of the action-integral formulation for ρ and σ. The right-hand sides of Eqs. (6) contain the only terms of ρ and σ which cannot be reduced to a perfect differential and thus are the only nonzero terms involved in an action integral formed of ρ and σ since we have assumed **M** closed. If we write σ as an action integral in terms of particle velocities, we find

$$\sum \tfrac{1}{2} m_i^* \mathbf{v}_i \cdot \mathbf{v}_i + e_i^* \mathbf{A}_i \cdot \mathbf{v}_i + \sum_j \tfrac{1}{2} m_j \mathbf{u}_j \cdot \mathbf{u}_j + e_j \mathbf{B}_j \cdot \mathbf{u}_j, \tag{8}$$

where m_j, e_j, and $\mathbf{u}_j$ are the electric charge's mass, charge, and velocity, and m_i^*, e_i^*, and $\mathbf{v}_i$ are the corresponding quantities for the magnetic charges. The quantities A_i and B_j refer to the one-forms α and ${}^*\beta$ at the position of the jth electric and ith magnetic charges, respectively. The equations of motion for the magnetic and electric charges arise from a variation of the quantity (8) with respect to $\mathbf{v}_i$ and $\mathbf{u}_i$, respectively, and are given by

$$\begin{aligned} m_i^* (\dot{v}_i)^m + e_i^* (v_i)_n [\partial^n (A_i)^m - \partial^m (A_i)^n] &= 0, \\ m_j (\dot{u}_j)^m + e_j (u_j)_n [\partial^n (B_j)^m - \partial^m (B_j)^n] &= 0, \end{aligned} \tag{9}$$

where $\partial^n = \partial/\partial y_n$ and the superscripts on the field quantities refer to their four-space components. It is readily seen that neither of Eqs. (9) give an expected interaction between electric and magnetic charges, nor do they give any interactions at all between like (i.e., magnetic–magnetic or electric–electric) charges.

We would expect that the force of an electric charge in a magnetic monopole field would be given by $f^i = eP^{ijkl} u_j \partial_k B_l$, where P^{ijkl} is the four-dimensional Levi-Civita tensor density.

Let us now consider the interactions of a number of particles with an action integral formed of ρ alone. We see that the relevant terms in the particle Lagrangian are

$$\sum_i \tfrac{1}{2} m_j^* \mathbf{v}_i \cdot \mathbf{v}_i - e_i^* \mathbf{B}_i \cdot \mathbf{v}_i + \sum_j \tfrac{1}{2} m_j \mathbf{u}_j \cdot \mathbf{u}_j + e_j \mathbf{A}_j \cdot \mathbf{u}_j. \tag{10}$$

The minus signs on the terms $e_i^* \mathbf{B}_i \mathbf{v}_i$ arise because $\delta\beta \wedge {}^*\delta\beta = -(d\, {}^*\beta \wedge {}^*d\, {}^*\beta)$ on the manifold **M**. Variation of (10) with respect to $(v_i)_m$ yields

$$m_i^* (\dot{v}_i)_m - e_i^* [\partial_m (B_i)_n - \partial_n (B_i)_m](v_i)^n = 0. \tag{11}$$

This result shows that the interaction between stationarylike magnetic charges in a rest frame is attractive, but such a result is at complete variance with the forces arising from the divergence of the Maxwell stress tensor when monopoles with conventionally assumed properties are considered. The minus signs in (11) arise in an essential way from the action integral, the assumed velocity of the one-form β, and the metric properties of **M**, and are independent of the sign in Eq. (4). In addition we see that Eq. (10) yields only interactions between like charges, that is, magnetic–magnetic and electric–electric, but none between unlike charges. To include interactions between all charges, we are led to consider some linear combination of ρ and σ. If we use their sum or difference, since we must choose either the sum or the difference in order to obtain definite particle equations, we see from Eq. (7) that the fields are no longer appropriately specified. A monopole could give rise to an electric field and vice versa. We are thus led to the following action integral:

$$\mathfrak{L} = (\omega + i\, {}^*\omega) \wedge {}^*(\omega + i\, {}^*\omega). \tag{12}$$

This quantity when varied with respect to α or ${}^*\beta$ yields appropriate field equations.

We can further show that

$$\omega + i\, {}^*\omega = (d + i\, {}^*d)(\alpha + i\, {}^*\beta) = d_+ \alpha_+, \tag{13}$$

If we define $\omega_+ = d\alpha_+$ and, since $d_+ \alpha_+ \wedge {}^*d_+ \alpha_+ = 2\, d\alpha_+ \wedge {}^*d\alpha_+$, we see that

$$\begin{aligned}(\omega + i\, {}^*\omega) \wedge {}^*(\omega + i\, {}^*\omega) &= 2(\omega \wedge {}^*\omega + i\omega \wedge \omega) \\ &= 2\omega_+ \wedge {}^*\omega_+.\end{aligned} \tag{14}$$

It is of interest to note that by the last term in Eq. (13) the quantity in Eq. (12) can be considered to be the inner product of two-forms which are exact. A

reduction to a particle Lagrangian for one magnetic and one electric charge yields

$$\tfrac{1}{2}mv^2 + \tfrac{1}{2}m^* u^2 - e^* \mathbf{B}\cdot\mathbf{v} + e\mathbf{A}\cdot\mathbf{u} + ie^* \mathbf{A}\cdot\mathbf{v} + ie\mathbf{B}\cdot\mathbf{u}. \quad (15)$$

Variation of the quantity (13) with respect to $\mathbf{u}$ and $\mathbf{v}$ yields

$$mu_i + e(\partial_i A_j - \partial_j A_i)u^j + ie(\partial_i B_j - \partial_j B_i)u^j = 0,$$
$$m^* v_i - e^* (\partial_i B_j - \partial_j B_i)V^j + ie^* (\partial_i A_j - \partial_j A_i)v^j = 0. \quad (16)$$

If we consider the complex conjugate of Eq. (13) we would find

$$\omega - i\,{}^*\omega = (d - i\,{}^*d)(\alpha - i\,{}^*\beta) = d_-\,\alpha_- \quad (17)$$

and, if $\omega_- = d\alpha_-$,

$$(\omega - i\,{}^*\omega)\wedge {}^*(\omega - i\omega) = 2(\omega\wedge{}^*\omega - \omega\wedge\omega) = 2\omega_-\wedge{}^*\omega_-. \quad (18)$$

The quantity in (18) when varied with respect to α and $^*\beta$ yields appropriate field equations, and when varied suitably with respect to particle velocities yields Eqs. (16), except for a sign change on the last term in each equation. This sign change can be compensated for by the substitution $e^* \to -e^*$, so that nothing new has been achieved. It is interesting to note that the quantities displayed in (13) and (17) correspond to the tensors considered by Laporte and Uhlenbeck[11] in their work concerning a spinor formulation of electromagnetism.

In summary we have shown that if we consider a classical two-form field which admits of magnetic monopolies (i.e., such that $d\omega \neq 0$) and insist upon the existence of an action-integral formulation which yields both particle and field equations, we find that the interactions between monopoles and between monopoles and charges cannot be in accord with the customarily assumed properties of the monopoles. These interactions between monopoles and charges are displayed in Eqs. (16) and (10), and these equations are in turn the only significantly different equations permitted by the formalism. These results cannot help bring up the question as to whether the nonobservation of monopoles might arise from the fact that their anticipated and actual properties might be different.

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[11] O. Laporte and G. E. Uhlenbeck, Phys. Rev. 37, 1380 (1931).

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Note on Two Binomial Coefficient Identities of Rosenbaum

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This paper gives rapid proofs of two binomial coefficient identities found by Rosenbaum [J. Math. Phys. **8**, 1977 (1967)] who obtained the identities from rather involved considerations of commutation relations. The present proofs make use of the Vandermonde convolution, or addition, theorem and a well-known fact that the kth difference of a polynomial of degree $k-1$ is zero. In a sense the two special cases are not essentially new.

Put

$$A=\sum_{n=0}^{\alpha}(-1)^n\binom{n+\epsilon-1}{n}\binom{\epsilon}{\alpha-n} \tag{1}$$

and

$$B=\sum_{n=0}^{\alpha}(-1)^n\binom{n+\epsilon-1}{\alpha-1}\binom{\alpha}{n}. \tag{2}$$

Here, for all real or complex x and integers $n\geq 0$,

$$\binom{x}{n}=\frac{x(x-1)\cdots(x-n+1)}{n!},\quad \text{with}\quad \binom{x}{0}=1, \tag{3}$$

is a binomial coefficient and is a polynomial of degree n in x. Rosenbaum[1] recently found that $A=0$ for integers α, ϵ such that $\epsilon\geq\alpha\geq 2$, and $B=0$ for integers α, ϵ such that $\alpha\geq 1$, $\epsilon\geq 2$, and $\epsilon>\alpha$. We show here that both results are easy special cases of known binomial identities and in this sense are not new results at all. The techniques may be of interest to workers in physics unfamiliar with the vast older literature on binomial identities.

Our proofs make use of some familiar facts about binomial coefficients and finite differences. The reader may consult the excellent book by Schwatt[2] on operations with series, a standard book on finite differences,[3] an editorial note and related papers,[4] or various papers by the present author[5] for further information on these relations and more general ones.

The binomial coefficients satisfy the elegant addition theorem

$$\sum_{k=0}^{n}\binom{x}{k}\binom{y}{n-k}=\binom{x+y}{n}, \tag{4}$$

valid for all real (or complex) x and y, and any nonnegative integer n. This follows at once from the identity $(1+t)^x(1+t)^y=(1+t)^{x+y}$. The coefficients also have the property that

$$\binom{-x}{n}=(-1)^n\binom{x+n-1}{n} \tag{5}$$

for all real or complex x, and nonnegative integers n.

From relation (5) we find at once that

$$A=\sum_{n=0}^{\alpha}\binom{-\epsilon}{n}\binom{\epsilon}{\alpha-n}=\binom{0}{\alpha}$$

by (4) and, hence, the sum is zero for integers $\alpha>0$. What is more, it is also evident that $A=0$ for all real or complex ϵ, a fact not made evident by the commutation-relation proof of Rosenbaum. So much for A.

Let $f(x)$ be an arbitrary polynomial of degree m in x. Then it is a familiar fact from finite-difference theory that $\Delta^k f(x)=0$ for $k>m$, where we define $\Delta f(x)=f(x+1)-f(x)$ and $\Delta^{k+1}f(x)=\Delta\Delta^k f(x)$. What is more, it is well known and easily proved that

$$\Delta^k f(x)=\sum_{n=0}^{k}(-1)^{k-n}\binom{k}{n}f(x+n). \tag{6}$$

Thus we see that Rosenbaum's series B is merely $(-1)^\alpha\Delta^\alpha f(x)$, where

$$f(x)=\binom{x+\epsilon-1}{\alpha-1},$$

evaluated at $x=0$. Since $f(x)$ is a polynomial of degree $\alpha-1$ for $\alpha\geq 1$, it follows that the αth difference of this must be zero. Again, the result is true for all real or complex values of ϵ, which does not affect the application of our theorem.

The fact that the binomial coefficient $\binom{x}{n}$ is readily defined for arbitrary real or complex x seems to be overlooked in many applications and thereby proofs of identities become involved and cumbersome.

In closing we should like to point out a very general binomial identity found as early as the year 1793 and

[1] David M. Rosenbaum, J. Math. Phys. **8**, 1977 (1967).
[2] I. J. Schwatt, *Operations with Series* (The University of Pennsylvania Press, Philadelphia, Pa., 1924; reprinted by Chelsea Publ. Co., New York, 1962).
[3] C. Jordan, *Calculus of Finite Differences* (Chelsea Publ. Co., New York, 1950).
[4] *Editorial comment on r!*, Math. Mag. **39**, 157 (1966).
[5] H. W. Gould, Am. Math. Monthly **63**, 84 (1956); **64**, 409 (1957); Duke Math. J. **27**, 71 (1960); **28**, 193 (1961); **29**, 393 (1962); Math. Mag. **34**, 317 (1961).

still not widely known. A detailed history and many results concerning this may be found in a recent paper.[6]

The identity is due to Rothe and is as follows:

$$\sum_{k=0}^{n} \frac{x}{x+bk}\binom{x+bk}{k}\frac{y}{y+b(n-k)}\binom{y+b(n-k)}{n-k} = \frac{x+y}{x+y+bn}\binom{x+y+bn}{n} \quad (7)$$

and, with suitable attention, is valid for all real or complex x, y, and b, and all nonnegative integers n. The novel point about (7) is the parameter b which allows this formula to include not only the Vandermonde relation (4) but perhaps ninety percent of the common binomial identities. Relation (5) is particularly useful in manipulating binomial summations. It together with the symmetry $\binom{n}{k} = \binom{n}{n-k}$ and changes of summation variable suffices to reduce most all the known identities to some form of the Vandermonde or other theorem.

[6] H. W. Gould and J. Kaucký, J. Combinatorial Theory **1**, 233 (1966).

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Partially Alternate Derivation of a Result of Nelson

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The result of Nelson that the total Hamiltonian is semibounded for a self-interacting Boson field in two dimensions in a periodic box is derived by an alternate method. It is more elementary in so far as functional integration is not used.

In Ref. 1, Nelson has proved the semiboundedness of the Hamiltonian for a class of two-dimensional self-interacting Boson-field theories in a periodic spatial box. In Ref. 2, Glimm has detailed and extended the result of Ref. 1. We will give an alternate derivation of the results of Nelson avoiding the use of functional integration, central in Ref. 1. As will be seen, the idea of the proof, however, is not essentially different from that of Nelson and we draw on results of his paper. It is hoped that a new method of proof may lead to some new results or insights.

We consider a Hamiltonian of the form

$$H = H_0 + V, \quad (1)$$

where H_0 is the free Hamiltonian of a particle of mass $\mu_0 \neq 0$ expressed in terms of the neutral scalar field ϕ and its momentum conjugate π:

$$H_0 = \frac{1}{2}\int_0^1 dx : [(\nabla\phi)^2 + \mu_0^2\phi^2 + \pi^2]. \quad (2)$$

As is evident we are working in a periodic box of length 1. V is a polynomial function of the $\phi(x)$. We denote by H_0 and ${}^N V$ the parts of H_0 and V depending only on the creation and annihilation operators of the N lowest-energy modes of the free Hamiltonian. We always imagine we are working with ${}^N H_0$ and ${}^N V$, but derive inequalities independent of N.

Theorem: Assume for each $\alpha > 0$ that there is an M_α such that

$$\langle 0| \exp^{-\alpha {}^N V} |0\rangle \leq M_\alpha, \quad \text{all } N.$$

$|0\rangle$ denotes the vacuum of the free field. Then there is a B such that

$${}^N H_0 + {}^N V \geq B, \quad \text{for all } N.$$

Actually as will be seen it is not necessary to satisfy the condition above for all α, but only for some sufficiently large α that one can calculate. We refer to Refs. 1 or 2 for the result that the conditions of the theorem are satisfied for a large class of self-interactions. This much of Nelson's proof requires no functional integration.

We follow the notation of Ref. 2:

$$\phi(x) = \sum_k (2\omega_k)^{-\frac{1}{2}}(a_k + a_{-k}^*)e^{ikx} \quad (3)$$

[1] E. Nelson, "A Quarticinteraction in Two Dimensions" in *Mathematical Theory of Elementary Particles*, R. Goodman and I. Segal, Eds. (M.I.T. Press, Cambridge, Mass., 1965), pp. 69–73.
[2] J. Glimm, Commun. Math. Phys. **8**, 12 (1968).

still not widely known. A detailed history and many results concerning this may be found in a recent paper.[6]

The identity is due to Rothe and is as follows:

$$\sum_{k=0}^{n} \frac{x}{x+bk}\binom{x+bk}{k}\frac{y}{y+b(n-k)}\binom{y+b(n-k)}{n-k} = \frac{x+y}{x+y+bn}\binom{x+y+bn}{n} \quad (7)$$

and, with suitable attention, is valid for all real or complex x, y, and b, and all nonnegative integers n. The novel point about (7) is the parameter b which allows this formula to include not only the Vandermonde relation (4) but perhaps ninety percent of the common binomial identities. Relation (5) is particularly useful in manipulating binomial summations. It together with the symmetry $\binom{n}{k} = \binom{n}{n-k}$ and changes of summation variable suffices to reduce most all the known identities to some form of the Vandermonde or other theorem.

[6] H. W. Gould and J. Kaucký, J. Combinatorial Theory **1**, 233 (1966).

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Partially Alternate Derivation of a Result of Nelson

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The result of Nelson that the total Hamiltonian is semibounded for a self-interacting Boson field in two dimensions in a periodic box is derived by an alternate method. It is more elementary in so far as functional integration is not used.

In Ref. 1, Nelson has proved the semiboundedness of the Hamiltonian for a class of two-dimensional self-interacting Boson-field theories in a periodic spatial box. In Ref. 2, Glimm has detailed and extended the result of Ref. 1. We will give an alternate derivation of the results of Nelson avoiding the use of functional integration, central in Ref. 1. As will be seen, the idea of the proof, however, is not essentially different from that of Nelson and we draw on results of his paper. It is hoped that a new method of proof may lead to some new results or insights.

We consider a Hamiltonian of the form

$$H = H_0 + V, \quad (1)$$

where H_0 is the free Hamiltonian of a particle of mass $\mu_0 \neq 0$ expressed in terms of the neutral scalar field ϕ and its momentum conjugate π:

$$H_0 = \frac{1}{2}\int_0^1 dx : [(\nabla\phi)^2 + \mu_0^2\phi^2 + \pi^2]. \quad (2)$$

As is evident we are working in a periodic box of length 1. V is a polynomial function of the $\phi(x)$. We denote by H_0 and ${}^N V$ the parts of H_0 and V depending only on the creation and annihilation operators of the N lowest-energy modes of the free Hamiltonian. We always imagine we are working with ${}^N H_0$ and ${}^N V$, but derive inequalities independent of N.

Theorem: Assume for each $\alpha > 0$ that there is an M_α such that

$$\langle 0| \exp^{-\alpha {}^N V} |0\rangle \leq M_\alpha, \quad \text{all } N.$$

$|0\rangle$ denotes the vacuum of the free field. Then there is a B such that

$${}^N H_0 + {}^N V \geq B, \quad \text{for all } N.$$

Actually as will be seen it is not necessary to satisfy the condition above for all α, but only for some sufficiently large α that one can calculate. We refer to Refs. 1 or 2 for the result that the conditions of the theorem are satisfied for a large class of self-interactions. This much of Nelson's proof requires no functional integration.

We follow the notation of Ref. 2:

$$\phi(x) = \sum_k (2\omega_k)^{-\frac{1}{2}}(a_k + a_{-k}^*)e^{ikx} \quad (3)$$

[1] E. Nelson, "A Quarticinteraction in Two Dimensions" in *Mathematical Theory of Elementary Particles*, R. Goodman and I. Segal, Eds. (M.I.T. Press, Cambridge, Mass., 1965), pp. 69–73.
[2] J. Glimm, Commun. Math. Phys. **8**, 12 (1968).

and define

$$q_0 = \left(\frac{1}{2\omega_0}\right)^{\frac{1}{2}}(a_0 + a_0^*),$$

$$p_0 = -i\left(\frac{\omega_0}{2}\right)^{\frac{1}{2}}(a_0 - a_0^*),$$

$$q_{|k|} = \left(\frac{1}{4\omega_k}\right)^{\frac{1}{2}}(a_k + a_k^* + a_{-k} + a_{-k}^*),$$

$$q_{-|k|} = -i\left(\frac{1}{4\omega_k}\right)^{\frac{1}{2}}(-a_{|k|} + a_{|k|}^* + a_{-|k|} - a_{-|k|}^*), \quad (4)$$

$$p_{|k|} = -i\left(\frac{\omega_k}{4}\right)^{\frac{1}{2}}(a_k - a_k^* + a_{-k} - a_{-k}^*),$$

$$p_{-|k|} = \left(\frac{\omega_k}{4}\right)^{\frac{1}{2}}(a_{|k|} + a_{|k|}^* - a_{-|k|} - a_{-|k|}^*).$$

In terms of these variables,

$$H_0 = \sum_k \tfrac{1}{2}(p_k^2 + \omega_k^2 q_k^2 - \omega_k) = \sum_k H_k. \quad (5)$$

We represent these operators on the L^2 space of E^N with measure the product of the measures μ_k,

$$d\mu_k = (\omega_k/\pi)^{\frac{1}{2}} e^{-\omega_k q_k^2}\, dq_k \quad (6)$$

with q_k a multiplicative operator and

$$p_k = i(\partial/\partial q_k) - \omega_k q_k. \quad (7)$$

A complete set of eigenfunctions for H_k is given by

$$\phi_{kn}(q_k) = (2^n n!)^{-\frac{1}{2}} A_n[q_k(\omega_k)^{\frac{1}{2}}], \quad n = 0, 1, 2, \cdots, \quad (8)$$

with corresponding eigenvalues

$$E_{kn} = n\omega_k, \quad (9)$$

$A_n(x)$ is the nth Hermite polynomial.

The chief inequality we will exploit is the following numerical inequality for x, y real, $y \geq 0$:

$$xy \leq e^x + y \ln y. \quad (10)$$

The expectation value of the interaction V in a state with function F is given by

$$\langle F|\ V\ |F\rangle = \int d\mu\, |F|^2\, V. \quad (11)$$

We apply (10) with $x = rV$ and $y = r^{-1}|F|^2$ to derive the result

$$-\langle F|\ V\ |F\rangle \leq \int d\mu\, e^{-rV} + \frac{1}{r}\int d\mu\, |F|^2 \ln |F|^2 - \frac{1}{r}\ln r. \quad (12)$$

r is a numerical factor to be fixed later. Note that

$$\int d\mu\, e^{-rV} = \langle 0|\ e^{-rV}\ |0\rangle. \quad (13)$$

We intend to bound the second term on the right side of (12) by the expectation value of H_0 in the state F. We consider the following equation:

$$\int |F|^2 \ln |F|^2\, d\mu = \frac{2}{\lambda}\int F^* H_0 F\, d\mu + \frac{1}{\lambda}\frac{d}{dt}\int [(e^{-H_0 t}F)^*(e^{-H_0 t}F)]^{1+\lambda t}\, d\mu\big|_{t=0}, \quad (14)$$

which easily follows for functions F nice enough so that all the integrals exist and the differentiation may be moved inside the integral, a dense subspace in L^2. We do not discuss domain questions.

We rewrite (12) using (14):

$$-\langle F|\ V\ |F\rangle \leq \int d\mu\, e^{-rV} + \frac{2}{\lambda r}\langle F|\ H_0\ |F\rangle - \frac{1}{r}\ln r + \frac{1}{\lambda r}\frac{d}{dt}\int [(e^{-H_0 t}F)^*(e^{-H_0 t}F)]^{1+\lambda t}\, d\mu\big|_{t=0}. \quad (15)$$

The theorem we are after is established provided $\lambda r \geq 2$ and we can bound the last term in (15).

The remainder of the paper is devoted to a study of

$$\int [(e^{-H_0 t}F)^*(e^{-H_0 t}F)]^{1+\lambda t}\, d\mu = \int |e^{-H_0 t}F|^{2+2\lambda t}\, d\mu. \quad (16)$$

We consider, corresponding to any g in $L^2(\mu)$, its expression as a sum of products of the functions in (8):

$$g(q) = \sum_{i_1, i_2, \cdots, i_N} C_{i_1, i_2, \cdots, i_N} \prod_s [2^{i_s}(i_s!)]^{-1} e^{i_s} A_{i_s}[q_s(\omega_s)^{\frac{1}{2}}]. \quad (17)$$

(The q_s are merely the q_k in some order.) The $C_{i_1, i_2, \cdots, i_N}$ are now considered as functions on the discrete space whose points are the indices of the C's. To the point $(i_1, i_2, \cdots, i_N)$ is associated the point mass $\Pi_s e^{2i_s}$. With this measure, the transformation T that carries a set of C's into the corresponding function g as in (17) is norm preserving as a map from l^2 to L^2. We will later show that T is norm decreasing as a map from l^1 to L^4. Assuming this for a moment, we complete the proof of the theorem.

We apply the Riesz–Thorin convexity theorem to the transformation T obtaining

$$\int |e^{-H_0 t}F|^{2+2\lambda t}\, d\mu \leq \left(\sum_{i_1, i_2, \cdots, i_N} \prod_s e^{2i_s} |\exp[-\omega_{i_1, i_2, \cdots, i_N} t] \times C_{i_1, i_2, \cdots, i_N}|^{[2(1+\lambda t)/(1+3\lambda t)]}\right)^{[(1+3\lambda t)/2(1+\lambda t)]} \quad (18)$$

with

$$\omega_{i_1,i_2,\cdots,i_N} = \sum_s i_s \omega_s . \tag{19}$$

In the right-hand side of (18) we apply the Holder inequality to obtain an expression involving the weighted sum of the squares of the absolute values of the C's which is equal to one:

$$\int |e^{-H_0 t} F|^{2+2\lambda t} \, d\mu$$

$$\leq \left[\sum_{i_1,i_2,\cdots,i_N} \prod_s e^{2i_s} \exp\left(-\omega_{i_1,i_2,\cdots,i_N} \frac{2(1+\lambda t)}{2\lambda} \right) \right]^{2\lambda t}. \tag{20}$$

It follows that

$$\frac{d}{dt} \int |e^{-H_0 t} F|^{2+2\lambda t} \, d\mu \Big|_{t=0}$$

$$\leq 2\lambda \ln \left[\sum_{i_1,\cdots,i_N} \prod_s e^{2i_s} \exp\left(-\frac{1}{\lambda} \omega_{i_1,\cdots,i_N} \right) \right]. \tag{21}$$

If $\mu_0/\lambda > 2$, this gives an inequality with finite right-hand side in the limit $N \to \infty$. It is clear that the theorem is now reduced to establishing that T is norm decreasing from l^1 to L^4.

Lemma. Let S be the space of sequences $\{C_\gamma\}$ $\gamma = 0, 1, \cdots, N$ with measure at γ, $e^{2\gamma}$; and Y the space of functions on R^1 with measure

$$(1/\pi)^{\frac{1}{2}} e^{-x^2} \, dx; \tag{22}$$

and T the operator from S to Y given by

$$T(\{C_\gamma\}) = \sum_\gamma C_\gamma \frac{1}{[2^\gamma(\gamma!)]^{\frac{1}{2}}} e^\gamma A_\gamma(x) \tag{23}$$

with A_γ the γth Hermite polynomial; then, T is norm decreasing from l^1 to L^4.

It is easy to see that this lemma would follow from establishing that

$$\left| \left(\frac{1}{\pi}\right)^{\frac{1}{2}} e^{-a-b-c-d} \int_{-\infty}^{\infty} [2^{a+b+c+d}(a!)(b!)(c!)(d!)]^{-\frac{1}{2}} A_a(x) A_b(x) \times A_c(x) A_d(x) e^{-x^2} \, dx \right| \leq 1 \tag{24}$$

for all integers a, b, c, and $d \geq 0$.[3] We use the generating function

$$e^{-t^2+2tZ} = \sum \frac{t^N}{N!} A_N(Z) \tag{25}$$

to obtain

$$\frac{1}{(\pi)^{\frac{1}{2}}} \int_{-\infty}^{\infty} dx \, e^{-x^2} A_a(x) A_b(x) A_c(x) A_d(x)$$

$$= \frac{a!\, b!\, c!\, d!}{\frac{1}{2}(a+b+c+d)!} \cdot 2^{\frac{1}{2}(a+b+c+d)} \times (rs + rt + ru + st + su + tu)^{\frac{1}{2}(a+b+c+d)}_{\text{pick-a-power}}, \tag{26}$$

where pick-a-power means to find the coefficient of the monomial $r^a s^b t^c u^d$ in the expansion of the expression. Note that $a + b + c + d$ is even or the integral vanishes.

We make the crude estimate

$$(rs + rt + ru + st + su + tu)^{\frac{1}{2}(a+b+c+d)}_{\text{pick-a-power}} \leq 2^{\frac{1}{2}(-a-b-c-d)} \cdot (r + s + t + u)^{a+b+c+d}_{\text{pick-a-power}}. \tag{27}$$

Now,

$$(r + s + t + u)^{a+b+c+d}_{\text{pick-a-power}} = \frac{(a+b+c+d)!}{a!\, b!\, c!\, d!}. \tag{28}$$

Denoting the left-hand side of (24) by LHS and using (27) we obtain

$$\text{LHS} \leq e^{-a-b-c-d} \times \frac{(a+b+c+d)!}{(a!\, b!\, c!\, d!)^{\frac{1}{2}} \cdot [\frac{1}{2}(a+b+c+d)]!\, 2^{\frac{1}{2}(a+b+c+d)}}. \tag{29}$$

That the right-hand side of (29) is ≤ 1 we leave as any easy exercise.

[3] Actually, it is sufficient to let $a = b = c = d$.

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Dirac Formalism and Symmetry Problems in Quantum Mechanics. I. General Dirac Formalism*

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Dirac's bra and ket formalism is investigated and incorporated into a complete mathematical theory. First the axiomatic foundations of quantum mechanics and von Neumann's spectral theory of observables are reviewed and several inadequacies are pointed out. These defects then are remedied by extending the usual Hilbert space to a *rigged Hilbert space* as introduced by Gel'fand, i.e., a triplet $\Phi \subset \mathcal{H} \subset \Phi'$, where $\mathcal{H}$ is a Hilbert space, Φ a dense subspace of $\mathcal{H}$ provided with a new (finer) topology, Φ' the dual of Φ. It is shown that this mathematical structure, together with the Schwartz nuclear theorem, allows us to reproduce Dirac's formalism in a completely rigorous way, without losing its transparency; this makes the theory easier to handle. The temporal evolution of the system and the wave equation are considered. Finally the probabilistic interpretation and the physical aspects of the theory are discussed; Φ is identified with the set of all physically accessible states of the system, Φ' with the set of all possible experiments (apparatus) to which it can be subjected; this provides a direct connection with Feynman's formulation of quantum mechanics.

INTRODUCTION

For the needs of everyday calculations, for example, in atomic or nuclear physics, Schrödinger's language of wavefunctions is, in general, sufficient. Similarly, for the study of any particular process in quantum electrodynamics, Feynman's rules are a very powerful tool. But for more general problems, especially in the field of elementary particle physics or any situation where the occupation-number operator is essential, it becomes necessary, and also much simpler, to have recourse to Dirac's bra and ket formalism.[1] The latter has become therefore the standard presentation of quantum mechanics, owing to its remarkable elegance and simplicity.

However, it has been known for a long time that this formalism is not satisfactory from the mathematical point of view: it is not basically incorrect, but it is not well defined! Yet elementary quantum mechanics has been put on firm mathematical grounds by von Neumann[2] many years ago, and this approach has recently regained some popularity[3,4] among physicists in view of the achievements of axiomatic quantum field theory.[5] It has remained, however, very far from practical applications and effective use. On the other hand, the present state of quantum theory is rather fertile in difficulties, which have, in general, a highly mathematical character: Many problems in field theory have been solved by using more powerful mathematical tools, such as the theory of distributions or the theory of functions of several complex variables. We think that this procedure should be extended to a much bigger class of problems, which includes the study of symmetries; there also, a systematic use of more refined, and thus more efficient mathematics becomes increasingly necessary.[6] With this philosophy in mind, it becomes very natural to undertake a mathematical justification of Dirac's formalism. But we want in fact much more than an aesthetic satisfaction! Since this formalism in its usual form is already a very powerful as well as elegant tool, it is hoped that a refined version of it might be still more efficient and, if possible, be able to solve some of the difficulties that burden present-day elementary particle physics. There lies the heart of the problem!

The solution we propose is to replace the traditional Hilbert space structure by a richer one, namely, that of a *rigged Hilbert space*. This concept, introduced by Gel'fand *et al.*,[7] consists of a triplet of spaces $\Phi \subset \mathcal{H} \subset \Phi'$, where $\mathcal{H}$ is a Hilbert space, the usual space of states, Φ is a dense subspace of $\mathcal{H}$ provided with an additional, finer topology, and Φ' is the dual of Φ, i.e., the space of all continuous linear functionals

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[2] J. von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Julius Springer-Verlag, Berlin, 1932) (English transl.: *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton, N.J., 1955).

[3] G. W. Mackey, *Mathematical Foundations of Quantum Mechanics* (W. A. Benjamin, Inc., New York, 1963).

[4] A. R. Marlow, Ph.D. thesis (unpublished); J. Math. Phys. 6, 919 (1965).

[5] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics, and All That* (W. A. Benjamin, Inc., New York, 1964).

[6] M. Mayer, in *Proceedings of Seminar on Unified Theories of Elementary Particles*, H. Rechenberg, Ed. (München, 1965).

[7] I. M. Gel'fand, G. E. Schilow, and N. J. Wilenkin, *Verallgemeinerte Funktionen (Distributionen)* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1960) Bd. I–IV [English transl.: *Generalized Functions* (Academic Press Inc., New York, 1964)].

over Φ. This structure brings into the formalism the extremely powerful and well-developed theory of topological vector spaces,[8,9] in particular, a systematic use of distributions or generalized functions.[7,10] This proposition is not new; it was formulated first by Foias,[11] then by Maurin,[12] and recently, in a more explicit way, by Roberts in two remarkable papers.[13] All these works, however, are essentially of mathematical character, and several physical problems still need a solution, namely:

(1) To build a complete theory, starting from probabilistic axioms, and to see how rigged Hilbert spaces quite naturally emerge from the usual formalism, instead of being a pure mathematical *ad hoc* device.

(2) To interpret physically this construction; in particular, to define the role of the vectors of the spaces Φ and Φ' in the frame of the quantum theory of measurement.

(3) To work out specific examples in order to test the reliability of the formalism.

(4) To formulate the problem of symmetries in that context, and in particular, the difficulties arising from a systematic use of Lie algebras.

The study of these points is the aim of the present work. This first paper is concerned with the general Dirac formalism itself. Further ones will be devoted to the symmetry problem and to some examples, mainly systems of interacting particles (scattering theory).

The usual Dirac formalism is universally known and so are its difficulties. These essentially stem from the existence of unbounded observables and operators with a continuous spectrum; from this it follows that the ordinary Hilbert space theory is plagued with technical problems such as domains of definition of observables and the appearance of nonnormalizable eigenvectors. A radical remedy to the first difficulty would be to admit only bounded observables, as was first advocated by Segal,[14] but this spoils much of the simplicity of the theory; an impressive example is given by the canonical commutation relation $[q, p] = i\hbar$, which requires that at least one of the operators q, p be unbounded. Another solution, proposed by Kristensen *et al.*,[15] consists in keeping unbounded operators, but changing the space, more precisely changing its topology in such a way that these operators become continuous. This idea is the basic ingredient of Roberts's formalism,[13] which we try to incorporate in a complete physical theory. For that purpose we need to review in some detail the axiomatic approach to quantum theory[2–4] and to analyze the difficulties which prevent a rigorous formulation of Dirac's language in that frame.

The structure of the work is as follows. Section I deals mainly with axiomatics; the resulting structure of the space of states is discussed in terms of superselection rules and the concept of *labeled observables* introduced by Roberts.[13] In Sec. II we review briefly von Neumann's spectral decomposition with the help of direct integrals of Hilbert spaces, following Marlow,[4] and we point out the insufficiencies of this formalism. Section III contains a rapid survey of mathematical results concerning the spectral theory of observables in a rigged Hilbert space, and a discussion of their application to quantum mechanics. In Sec. IV we construct explicitly the general Dirac formalism, with particular emphasis on eigenvectors and eigenvalue equations, matrix elements of observables, and transformation theory. Section V is devoted to the temporal evolution of the system and the corresponding wave equation. In Sec. VI we present a physical (probabilistic) interpretation of the formalism, first as an adaptation of the usual interpretation and then a more speculative generalization. Section VII finally discusses the remaining open questions, as well as the domain of applicability of the formalism.

I. THE PROBABILISTIC FRAME OF QUANTUM MECHANICS

A. Axiomatics

The most fundamental aspect of quantum mechanics in its present interpretation is its probabilistic character. The description of a physical system requires two kinds of elements, the observables and the states of the system. Given, then, an observable A, a state α and a Borel[16] set Δ of the real axis, the aim of the theory is to evaluate the probability that a measurement of A in the state α shall give a result belonging to Δ.[3] Any axiomatization of the theory

[8] A. P. Robertson and W. J. Robertson, *Topological Vector Spaces* (Cambridge University Press, London, 1964).

[9] A. Pietsch, *Nukleare lokalkonvexe Räume* (Akademie Verlag, Berlin, 1965).

[10] L. Schwartz, *Théorie des distributions* (Hermann & Cie., Paris, 1957–1959), Vols. I, II.

[11] C. Foias, Acta Sci. Math. **20**, 117 (1959); Compt. Rend. **248**, 904, 1105 (1959); **255**, 247 (1962); Rev. Math. Pures Appl. Acad. Rep. Populaire Roumaine **7**, 241, 571 (1962).

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[14] I. E. Segal, *Mathematical Problems of Relativistic Physics* (American Mathematical Society, Providence, R.I., 1963).

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[16] P. R. Halmos, *Measure Theory* (D. Van Nostrand, Inc., Princeton, N.J., 1950).

will thus consist in giving a sufficient number of axioms for determining this probability. The possible schemes fall into two classes, depending upon whether the observables or the states are taken for the fundamental building blocks. The first choice seems easier[17] and has indeed enjoyed more popularity.

The decisive step in this direction was taken by Birkhoff and von Neumann[18] in their historic paper, introducing the calculus of propositions. Their method has recently regained actuality with the works of Finkelstein *et al.*,[19] Mackey,[3] Piron,[20] and Guenin.[21] In this approach the primary constituents of the theory are the *questions* or *propositions*, i.e., observables that have only 0 and 1 as possible values. Operations are defined on the set of these questions, thus giving it a lattice structure (the so-called *logic of the system*). The fundamental results can be summarized in the following theorem:

1. Any irreducible system of questions (i.e., a system where no nontrivial question is compatible with any other one) is isomorphic to the set of projection operators on all the closed subspaces of a Hilbert space.

2. Any system of questions is a direct union of irreducible systems.

The usual formulation of quantum mechanics is then a consequence of this result.

Let us consider first an irreducible system. *Observables* can be reconstructed from the questions; with the above theorem, this corresponds to the reconstruction of self-adjoint operators on the Hilbert space $\mathcal{H}$ from projection operators, as given by the spectral theorem.[22] The set of observables of an irreducible system is thus identified with the set of all self-adjoint operators on $\mathcal{H}$, compatible observables being represented by strongly commuting operators (i.e., all their spectral projection operators commute[23]); this will allow the simultaneous diagonalization of several observables (see Sec. II). The *states* of the system are defined as some linear functionals over the questions; by Gleason's theorem[24] this leads to the identification of a state with a *density operator*, and of a *pure state* with a unit ray of $\mathcal{H}$.

For a general system a similar analysis has been made by Guenin.[21] We shall consider here only the case where the system can be described by a single (separable, complex) Hilbert space $\mathcal{H}$; more general situations are possible, but they do not admit a simple physical interpretation in terms of superselection rules.[25] For this restricted case, the structure of the system is best characterized with von Neumann algebras,[26] as suggested by Jauch and Misra.[27] In this language, the system is defined by a von Neumann algebra $\mathcal{C}$ of operators on $\mathcal{H}$, with Abelian commutant: $\mathcal{Z} = \mathcal{C}' \subset \mathcal{C}$. Under von Neumann's central decomposition,[28] $\mathcal{C}$ is thus decomposed into irreducible constituents, with a corresponding decomposition of $\mathcal{H}$ into a direct integral:

$$\mathcal{H} = \int_Z^{\oplus} \mathcal{H}(z)\, d\mu(z), \tag{1}$$

where Z is the spectrum of the self-adjoint generator of $\mathcal{Z}$. The components $\mathcal{H}(z)$ are interpreted as superselection sectors[25]; this corresponds to the following identifications:

(i) The *observables* are the self-adjoint operators affiliated to $\mathcal{C}$ (i.e., their spectral projection operators belong to $\mathcal{C}$); they appear thus in (1) as the decomposable operators: $A \sim \{A(z)\}$, $A(z)$ affiliated to $\mathfrak{L}(\mathcal{H}(z))$[29];

(ii) The *essential observables*, which generate *supersymmetries*,[27] are those affiliated to $\mathcal{Z}$; they all commute (since $\mathcal{Z}$ is Abelian)[30]; they appear in (1) as the diagonal operators: $B \sim \{g(z)1(z)\}$, $g \in L^\infty(Z, \mu)$, $1(z)$ unit operator of $\mathcal{H}(z)$;

(iii) The *physically realizable pure states* of the system are those vectors f of $\mathcal{H}$ which have only one nonvanishing component $f(z_0)$, say.

This last restriction clearly leads to a difficulty of interpretation in the case of a continuous superselection rule, for the vector f has zero norm in $\mathcal{H}$ if

[17] See, for instance, the discussion of J. M. Jauch, Helv. Phys. Acta, **37**, 293 (1964).

[18] G. Birkhoff and J. von Neumann, Ann. Math. (N.Y.) **37**, 823 (1936).

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[24] A. Gleason, J. Ratl. Mech. Anal. **6**, 885 (1957).

[25] G. C. Wick, A. S. Wightman, and E. P. Wigner, Phys. Rev. **88**, 101 (1952); A. S. Wightman, Nuovo Cimento Suppl. **14**, 81 (1959).

[26] J. Dixmier, *Les Algèbres d'opérateurs dans l'espace hilbertien (Algèbres de von Neumann)* (Gauthier-Villars, Paris, 1957); M. A. Naïmark, *Normed Rings* (P. Noordhoff Ltd., Groningen, The Netherlands, 1964).

[27] J. M. Jauch, Helv. Phys. Acta **33**, 711 (1960); J. M. Jauch and B. Misra, *ibid.* **34**, 699 (1961).

[28] J. von Neumann, Ann. Math. (N.Y.) **50**, 401 (1949); also *Collected Works*, H. A. Taub, Ed. (Pergamon Press Ltd., London, 1961–1963), Vol. III.

[29] $\mathfrak{L}(\mathcal{K})$ denotes the set of all bounded linear operators on the space $\mathcal{K}$; similarly, $\mathfrak{L}(\mathcal{K}_1, \mathcal{K}_2)$ denotes the set of all continuous linear mappings from the space $\mathcal{K}_1$ into the space $\mathcal{K}_2$ (with $\mathcal{K}_1$, $\mathcal{K}_2$ two topological vector spaces).

[30] The hypothesis that all the supersymmetry operators commute, first made by Wightman,[25] has been shown by Galindo *et al.* [J. Math. Phys. **3**, 324 (1962)] to be equivalent to Jauch's condition[27] that the system shall have at least one complete system of commuting observables.

$\mu(\{z_0\}) = 0$! In order to avoid this trouble, we shall postulate that all superselection rules are *purely discrete*. This seems realistic: indeed all charges (electric, baryonic, muonic, $\cdots$), spin type, etc., are discrete; Bargmann's superconservation of total mass in a Galilei invariant theory[31] is always treated as a discrete superselection rule in practice (though the masses may take arbitrary values) and the gauge invariance of the BCS model of superconductivity does not imply a continuous superselection rule, as was claimed by Emch and Guenin[32]; every component $\mathcal{H}(\alpha)$ $(0 \leq \alpha \leq 2\pi)$ describes the *whole* system in the particular gauge α, so that the direct integral of all the $\mathcal{H}(\alpha)$ is *not* the space of states (see Sec. VII). We may thus suppose that the space $\mathcal{H}$ is a *direct sum* of coherent subspaces, in each of which the superposition principle is fully valid.

B. Choice of the Observables

Up to now we have supposed only that the system is characterized by the set of its observables, but we did not say anything about the choice of the particular observables: What makes the difference between two systems?

Let us consider first irreducible systems. Each of these is described by a separable Hilbert space $\mathcal{H}_i$ and the corresponding von Neumann algebra $\mathfrak{L}(\mathcal{H}_i)$; but all these Hilbert spaces are isomorphic, and so are the algebras $\mathfrak{L}(\mathcal{H}_i)$; they are, in fact, unitarily equivalent.[26] This would mean that all irreducible systems with any finite number of degrees of freedom are equivalent; physically, this is obviously wrong. Thus we must conclude that the description of a system by the von Neumann algebra of its observables is not complete.

In the general case a similar conclusion holds. To two different systems belong isomorphic Hilbert spaces $\mathcal{H}_1 \simeq \mathcal{H}_2$; their algebras must, of course, not be isomorphic; but once they are, they are even unitarily equivalent.[26] The structure of the system is, in fact, given entirely by the spectrum of the single generator of the Abelian von Neumann algebra $\mathcal{C}_i' = \mathcal{Z}_i$ corresponding to its supersymmetries: here again the description is not complete, for unitary equivalence does not imply physical equivalence!

These considerations clearly show that some important feature of the theory has been neglected. The origin of the trouble can be found in the ambiguous meaning of the word *observable*. This concept has indeed both a mathematical and a physical aspect, which have been confused so far. Mathematically, an observable is defined as a self-adjoint operator. Physically, an observable is, by definition, the quantity measured in some determined experiment. More precisely, the physical definition of an observable consists in giving either a prescription for measuring the quantity itself or a definite expression in terms of other measurable quantities. In the first case we shall speak of *labeled observables*, in the sense of Roberts[13]; a labeled observable is thus *a given self-adjoint operator together with a prescription as how to measure it physically*. In other words, this labeling procedure provides us with a kind of dictionary,[14] a one-to-one correspondence between some self-adjoint operators and some particular physical quantities, such as position, momentum, energy, angular momentum, etc. This correspondence really *defines* the system, up to a *physical* equivalence (which is also a unitary one, but the converse is not necessarily true).

The choice of such a family $\mathcal{O}_I = \{A_i, i \in I, I \text{ some index set}\}$ of labeled observables may in some respects be a matter of taste, but it is not completely arbitrary. First of all, the whole von Neumann algebra $\mathcal{O}$ of observables must be recovered from $\mathcal{O}_I$; for this we require that $\mathcal{O}_I' = \mathcal{O}'$ and thus $\mathcal{O}_I'' = \mathcal{O}'' = \mathcal{O}$ (i.e., nonlabeled observables appear as functions of labeled ones). Secondly, we must postulate that $\mathcal{O}_I$ contain at least one complete set of commuting observables (see Sec. II) and all the essential observables (supersymmetries) of the system. Thirdly, $\mathcal{O}_I$ must reflect the symmetry properties of the system in the following sense. Certain symmetries, like relativity, play such a fundamental role that no theory could be formulated at all without them. It is then clear that $\mathcal{O}_I$ must contain all the observables in terms of which the symmetry is defined—in particular, the conserved observables, if any. Otherwise the description of the system cannot satisfy the necessary symmetry requirements. In nonrelativistic quantum mechanics, for instance, the fundamental observables are those which refer to the physical properties of space–time and of inertia (through the variational principle), namely, q_i, p_i. In a similar way, a set of observables may be equivalent under the symmetry operations (such as q_1, q_2, q_3 under rotations). Again, $\mathcal{O}_I$ cannot contain one member of the set without the other ones; this would violate the symmetry.

In the sequel we shall present further arguments supporting the introduction of labeled observables, and see how they allow us to recover Dirac's formalism. To the question of which operators must be chosen as labeled observables, we hope to return in another publication.

[31] V. Bargmann, Ann. Math. (N.Y.) **59**, 1 (1954).
[32] G. Emch and M. Guenin, J. Math. Phys. **7**, 915 (1966).

II. VON NEUMANN'S SPECTRAL THEORY

A. Spectral Decompositions

In view of the results of the preceding section, we can now restrict our study to an irreducible system or, what amounts to the same, to a single coherent subspace. The analysis can be trivially extended to a general, reducible system with the help of Fubini's theorem[16] on successive integrations.

In Dirac's approach[1] an observable is a self-adjoint operator whose eigenvectors form a complete set. If its spectrum is purely discrete, this condition is always fulfilled; but it never is if part of the spectrum is continuous, since there is no eigenvector in $\mathcal{H}$ (i.e., a normalizable vector) corresponding to a point of the continuous spectrum. As a way out of this difficulty von Neumann[2] builds the whole quantum theory using only normalizable wave packets. This approach, of course, differs from that of Dirac in that it refuses to go out of $\mathcal{H}$. On the other hand, eigenfunctions (in the sense of differential equations) can be obtained very often for points of the continuous spectrum, and they may even be perfectly well-behaved functions, though not square integrable. A way to these extremely useful elements within Hilbert space theory can be found in direct integral decompositions of $\mathcal{H}$, introduced also by von Neumann[26,28] and systematically used by Marlow[4] in a recent work. We shall see that this formalism, though perfectly adapted for studying continuous spectra, is still not sufficient for justifying Dirac's. As an important step in this direction, however, it is of great interest.

The theory of direct integrals of Hilbert spaces and its use for the spectral decompositions of self-adjoint operators is well known,[7,26,28] and we shall mention here only the relevant results. Given a single self-adjoint operator A on $\mathcal{H}$, there exists a corresponding class of equivalent (spectral) measures on $\mathbf{R}$; with any element σ of this class, a unitary equivalence can be set up between $\mathcal{H}$ and a direct integral $\hat{\mathcal{H}}$, which diagonalizes A:

$$\mathcal{H} \to \hat{\mathcal{H}} = \int^{\oplus} \mathcal{H}(\lambda)\, d\sigma(\lambda),$$

$$\begin{aligned} f &\to \{f(\lambda)\}, \quad f \in \mathcal{H}, \quad f(\lambda) \in \mathcal{H}(\lambda), \\ Af &\to \{\lambda f(\lambda)\}, \quad f \in \text{domain of } A, \end{aligned} \tag{2}$$

$$\begin{aligned} (f, g)_{\mathcal{H}} &= \int (f(\lambda), g(\lambda))_\lambda \, d\sigma(\lambda) \\ &= \int \left[\sum_{n=1}^{\dim \mathcal{H}(\lambda)} \overline{f_n(\lambda)} g_n(\lambda) \right] d\sigma(\lambda), \end{aligned} \tag{3}$$

where the integrand is the scalar product in $\mathcal{H}(\lambda)$. If A is cyclic (i.e., has a nondegenerate spectrum), all the spaces $\mathcal{H}(\lambda)$ are one-dimensional and $\hat{\mathcal{H}} = L^2_\sigma$. This provides a *functional calculus*,[33] which is nothing else than the diagonalization of the Abelian von Neumann algebra $\mathfrak{A} = \{A\}''$; $\mathfrak{A}$ is the set of functions $u(A)$, $u \in L^\infty_\sigma$, i.e., bounded outside a σ-negligible subset of $\mathbf{R}$ (diagonal operators); $\mathfrak{A}'$ is the set of decomposable operators $B \sim \{B(\lambda)\}$, $B(\lambda) \in \mathfrak{L}(\mathcal{H}(\lambda))$, and $\mathfrak{A} \subseteq \mathfrak{A}'$. If A is cyclic $\{\dim \mathcal{H}(\lambda) = 1$ for any $\lambda\}$, $\mathfrak{A} = \mathfrak{A}'$ (maximal Abelian).

The same analysis can be made for a finite or countably infinite family of strongly commuting self-adjoint operators $A_1, A_2, \cdots$ (all spectral projections commute)[33]; they generate an Abelian von Neumann algebra $\mathfrak{A} = \{A_1, A_2, \cdots\}''$, which, in turn, is generated by one single bounded self-adjoint operator A, $\mathfrak{A} = \{A\}''$, according to von Neumann's theorem.[26] $\mathfrak{A}$ is maximal Abelian (A cyclic) whenever $\{A_1, A_2, \cdots\}$ is a "complete set of commuting observables."[1]

The physical interpretation of these decompositions is obvious. A is represented in the component $\mathcal{H}(\lambda)$ by the multiplication operator λ; $\mathcal{H}(\lambda)$ must then be interpreted as an eigenspace corresponding to the eigenvalue λ. These eigenspaces are even orthogonal in the sense of Parseval's relation:

$$\|f\|^2 = \int \|f(\lambda)\|^2_\lambda \, d\sigma(\lambda). \tag{4}$$

A similar interpretation holds for the operators $A_1, A_2, \cdots$. But the trouble comes from the fact that $\mathcal{H}(\lambda)$ is *not* a subspace of $\mathcal{H}$ if λ is a point of σ-measure zero, because any element f of $\mathcal{H}$, whose only non-vanishing component is $f(\lambda)$, has zero norm in $\mathcal{H}$. Thus we cannot treat all eigenvectors, the discrete and the continuous ones, on the same footing; but this is precisely the essence of Dirac's formalism, which gives it its superiority from the practical point of view.

Let us now introduce[4] a basis $\{|\lambda, n),\ n = 1, 2, \cdots, \dim \mathcal{H}(\lambda)\}$ in $\mathcal{H}(\lambda)$ [the notation $|.)$ instead of $|.\rangle$ shall remind us that $|f(\lambda)), |\lambda, n) \notin \mathcal{H}$]. In Dirac's notation we find that

$$(f(\lambda) \mid g(\lambda))_\lambda = \sum_n (f(\lambda) \mid \lambda, n)(\lambda, n \mid g(\lambda)).$$

Now Marlow writes

$$f_n(\lambda) \equiv (\lambda, n \mid f(\lambda)) = (\lambda, n \mid f\rangle, \tag{5}$$

such that

$$\langle f \mid g\rangle = \int \sum_n \langle f \mid \lambda, n)(\lambda, n \mid g\rangle \, d\sigma(\lambda).$$

But this relation is not equivalent to the similar one of Dirac because $(\lambda, n \mid f\rangle$ *does not represent the scalar*

[33] J. M. Jauch and B. Misra, Helv. Phys. Acta **38** (1965).

product of two elements of $\mathcal{H}$; it is a symbolic expression representing the scalar product $(\lambda, n \mid f(\lambda))$ *in* $\mathcal{H}(\lambda)$! There is for instance no possibility at all for inserting between $(\lambda, n|$ and $|f\rangle$ the identity operator *of* $\mathcal{H}$ in its usual form ("complete set of states"):

$$I = \int \sum_n |\lambda, n)(\lambda, n| \, d\sigma(\lambda)$$
$$= \int I(\lambda) \, d\sigma(\lambda),$$

where $I(\lambda)$ is the identity operator in $\mathcal{H}(\lambda)$. We see here that this formalism, although presenting a considerable improvement over the usual one, still suffers from insufficiencies, which we shall now analyze.

B. Difficulties of this Formalism

A first difficulty, already mentioned above, is due to the fact that $\mathcal{H}(\lambda)$ is not a subspace of $\mathcal{H}$ if λ belongs to the continuous part of the spectrum. Therefore such eigenvectors cannot be interpreted as pure states of the system. But then the question arises: What is their physical interpretation at all? Furthermore, the connection between $f \in \mathcal{H}$ and its components is rather loose (measure theoretical); there is no straightforward generalization of the projection operator $f \to f(n)$ of the discrete case. One possibility would be to consider $f_n(\lambda)$ as the value which some linear functional takes at the element f. This is suggested by Marlow's notation $f_n(\lambda) = (\lambda, n \mid f\rangle$. In other words, $(\lambda, n|$ should be considered as a *distribution*.[7,10] But there appears now another major difficulty, for the functional $f \to f_n(\lambda)$ is *not continuous* under the topology of $\mathcal{H}$, if the set $\{\lambda\}$ is of σ-measure zero!

An analogous difficulty appears if one tries to represent *nondiagonal operators*. Let A be an observable, which, for simplicity, we assume to be cyclic, and $\{\xi\}$ a representation in which A is not diagonal. Given $f \sim \{f(\xi)\}$, $g = Af \sim \{g(\xi)\}$, Marlow[4] remarks that the function $g(\xi)$ is a linear functional of the function $f(\xi)$ and he writes this property in the following way[34]:

$$g(\xi) \equiv (\xi \mid g\rangle = \int (\xi| \, A \, |\xi') f(\xi') \, d\mu(\xi').$$

This relation is meaningful if A is an integral operator in the $\{\xi\}$ representation, of Hilbert–Schmidt type say, with the kernel $A(\xi, \xi') \equiv (\xi| \, A \, |\xi')$. But this is by no means always true! Here also we cannot use the theory of distributions, for the functional $g[f]$ is not continuous if A is unbounded. In the same way Marlow uses the following integral representation for a matrix element of $A(h, f \in \mathcal{H})$:

$$\langle h| \, A \, |f\rangle = \iint (\xi| \, A \, |\xi') h(\overline{\xi}) f(\xi') \, d\mu(\xi) \, d\mu(\xi').$$

But here again A can be interpreted as a *kernel* in the sense of Schwartz[7,10] and have such a representation only if the left-hand side is a *separately continuous* bilinear (or Hermitian) functional of h and f. To overcome this difficulty, it will be necessary to make the operator A continuous by restricting it to an invariant dense domain in which a suitable new topology is defined (one finer than that of $\mathcal{H}$). But, of course, this will not be possible for all observables simultaneously, if only because of the requirement of the common dense domain! Here again we are faced with the problem of selecting a family of labeled observables.

A further difficulty connected with the von Neumann–Marlow formalism stems from the change of a representation. We saw that fixing a representation is equivalent to choosing a particular maximal Abelian von Neumann subalgebra of $\mathfrak{L}(\mathcal{H})$. But it is known[35] that $\mathfrak{L}(\mathcal{H})$ contains maximal Abelian subalgebras which are not unitarily equivalent to each other. Moreover, each of them may be generated by a single operator, so that the usual notion of *dimension* does not apply to such a subalgebra. Yet it is used implicitly, as the number of degrees of freedom of the system. An answer to this puzzle may be given as follows. The number of degrees of freedom is a purely classical concept, which can be transferred to quantum mechanics through canonical quantization.[14] This procedure uses the correspondence principle for identifying a classical dynamical variable with a self-adjoint operator. [Reference to classical mechanics cannot be avoided, for a measurement apparatus is, in general, a classical (macroscopic) object!] Of course, not all quantum observables can be obtained in this way, but it must be emphasized that neither is this applicable to *all* classical dynamical variables,[36] if one wishes to maintain correspondence between the commutator and Poisson bracket.[37] A choice has to be made among the dynamical variables; this is equivalent to the labeling of observables which we have already met several times. Thus the only admissible maximal Abelian von Neumann subalgebras of $\mathfrak{L}(\mathcal{H})$ are those generated by labeled observables

[34] A similar relation can be written with two different representations $\{\xi\}$ and $\{\lambda\}$.

[35] J. Dixmier, Ann. Math. (N.Y.) **59**, 279 (1954).

[36] Even in classical mechanics, not all reasonable (e.g., twice differentiable) functions of q_i, p_i can be dynamical variables; a Hamiltonian, for instance, can, in general, be at most a *quadratic form* in the canonical momenta p_i; otherwise, one runs into serious difficulties.

[37] R. Arens and D. Babbitt, J. Math. Phys. **6**, 1071 (1965).

(the generator of such an algebra has, in general, no obvious physical meaning); for these, the number of operators can play the role of a dimension number; it is related to the number of degrees of freedom of the corresponding classical system (this one exists at least partially). Given two such physically meaningful representations $\{\lambda^{(i)}\}$ and $\{\lambda^{(j)}\}$, with corresponding spectral measures σ_i and σ_j, the transformation from the one to the other is described by a unitary equivalence between $L^2_{\sigma_i}$ and $L^2_{\sigma_j}$, and this causes the same difficulty as the representation of nondiagonal operators did—for instance, Dirac's relation

$$|\lambda^{(i)}\rangle = \int |\lambda^{(j)}\rangle \langle \lambda^{(j)} \mid \lambda^{(i)}\rangle \, d\sigma_j(\lambda^{(j)})$$

has no meaning here, since $|\lambda^{(i)}\rangle$ and $|\lambda^{(j)}\rangle$ do not belong to $\mathcal{H}$, and their scalar product is not defined. Of course this unitary equivalence between Hilbert spaces does not imply that the corresponding maximal Abelian algebras $\mathfrak{A}^{(i)}$ and $\mathfrak{A}^{(j)}$ will be unitarily equivalent. If they are, the change of representation becomes rather trivial.[38]

In conclusion, we may say that this formalism gives a correct treatment of continuous spectra, but that there remain difficulties due to the unbounded character of observables and to the necessity of choosing a family of privileged (labeled) observables. In the following sections we shall try to remedy these defects.

III. MATHEMATICAL ASPECTS OF THE PROBLEM

A. Preliminaries

The spectral theory of observables is part of a much larger mathematical problem, namely, the spectral theory of symmetric and normal operators in Hilbert space and, in particular, the problem of differential and partial differential operators, their eigenfunctions, and the expansion of arbitrary functions in terms of these eigenfunctions. Two main directions (both leading out of $\mathcal{H}$) have been followed.

1. Use of Direct Integral Decompositions

This method arose from the "Reduction Theory" of von Neumann[28] and was developed further by authors like Mautner, Browder, Gårding, etc. (see the references in Gel'fand's book[7]); we have outlined it in Sec. II and pointed out its inconveniences.

2. Use of Supplementary Topological Structures in $\mathcal{H}$ (Mainly Nuclear)

This second method, first proposed by Gel'fand and Kostiuchenko, was developed mostly by Russian authors[7] (Gel'fand, Chilov, Vilenkin, Berezanski, Katz, Maurin, etc.). The idea is to build a mathematical structure that remedies the defects analyzed above:

(i) The functional $f \to f(\lambda)$, arising in the direct integral decomposition of $\mathcal{H}$ with respect to A, can be made continuous on a subspace $\Phi \subset \mathcal{H}$ endowed with a suitable, finer, topology; we shall write $\phi(\lambda) = \langle \xi_\lambda, \phi \rangle$ for $\phi \in \Phi$, $\xi_\lambda \in \Phi'$, the strong dual of Φ (i.e., the space of continuous linear functionals over Φ, provided with the strong topology).

(ii) If Φ is dense in $\mathcal{H}$, and if the injection $\Phi \to \mathcal{H}$ is continuous, we can embed $\mathcal{H}$ (densely) in Φ'; the result is then the following triplet structure:

$$\Phi \subset \mathcal{H} \subset \Phi'. \tag{6}$$

If, moreover, the operator A leaves Φ invariant and is continuous under its topology, duality between Φ, Φ' allows us to define an extension A' which is a continuous operator on Φ':

$$\langle A'\xi, \phi \rangle \equiv \langle \xi, A\phi \rangle, \quad \phi \in \Phi, \quad \xi \in \Phi' \tag{7}$$

and the functionals ξ_λ defined in (i) above are eigenfunctionals of A', i.e.,

$$\langle A'\xi_\lambda, \phi \rangle \equiv \langle \xi_\lambda, A\phi \rangle = \lambda \langle \xi_\lambda, \phi \rangle, \quad \forall \phi \in \Phi, \tag{8}$$

or, for short,

$$A'\xi_\lambda = \lambda \xi_\lambda.$$

This method has been studied in great detail by Gel'fand *et al.*,[7] Foias,[11] Maurin,[12] and recently by Roberts.[13] We shall follow it (except for some minor modifications) and see how it enables us to reproduce Dirac's formalism. The mathematical problem, then, is the following: Given an observable A, to construct a space Φ endowed with the following properties:

(i) Φ can be identified with a dense subspace of $\mathcal{H}$, stable under A, and its topology must be such that A is continuous under it;

(ii) the embedding $\Phi \to \mathcal{H}$ is continuous, so that a triplet (6) can be built and A can be extended to A';

(iii) Φ' contains a complete orthonormal system of eigenfunctionals of A'.

Here *complete* means that any element of Φ admits an expansion in eigenfunctionals which is unique, and *orthonormal* means that this expansion satisfies a Parseval relation (there is no scalar product in Φ'!). Finally, this construction must first be applied to a whole family of compatible observables, then also to noncompatible observables.

It must be emphasized that the problem has two very different aspects.

[38] J. M. Jauch and J.-P. Marchand, Helv. Phys. Acta **39**, 325 (1966).

a. Topological Properties of Φ: Φ must be a stable subspace of the domain of all operators to be made continuous; its topology will depend on their number and their (un)bounded character. It can be a norm topology ($\rightarrow$ Banach space), a metrizable topology ($\rightarrow$ Fréchet space), or even a nonmetrizable topology (i.e., with a noncountable base of neighborhoods).

b. Properties of the Embedding Mapping $\tau: \Phi \rightarrow \mathcal{H}$: It must allow the existence of the required spectral decompositions.

B. Survey of Mathematical Results

The problem just described has been studied already in several works, which we shall review here briefly.

1. The Solution of Gel'fand–Chilov[39]

These authors extend the original idea of Gel'fand–Kostiuchenko, based on differentiability properties of functionals of bounded variation over nuclear topological vector spaces. Their method, although elegant, is not very useful for practical applications. This approach is very close to that of von Neumann[2] and Marlow.[4]

2. The Solution of Foias[11]

Instead of direct integrals of Hilbert spaces, this author uses continuous linear mappings from Φ into $\Phi^{\times}$, the space of continuous antilinear functionals over Φ, and he defines the concept of an integral decomposition of Φ in terms of *eigenoperators* of A. This method has been studied systematically by Roberts.[13]

3. The Solution of Hirschfeld[40]

This is by far the simplest method; it uses only the spectral theorem in $\mathcal{H}$.[22] In the case of a single bounded operator A, Φ is the Banach space (thus *not* nuclear) of continuous functions on the spectrum of A. However, the extension of this method to unbounded operators does not seem straightforward in its present form; for this reason we are forced to abandon it, at least provisionally.

4. The Solution of Maurin[12] *and of Gel'fand–Vilenkin*[41]

This last solution combines in fact the two different approaches outlined at the beginning of this section. The idea is to build a triplet $\Phi \subset \mathcal{H} \subset \Phi'$, to decompose $\mathcal{H}$ into a direct integral, and then to embed each component continuously into Φ'. This method has the advantage of using explicitly direct integral decompositions of $\mathcal{H}$; as we have seen above (Sec. II), this is a very convenient language for spectral theory of operators in a Hilbert space; furthermore, it appears automatically in the study of symmetry groups (or algebras) through the decomposition of a representation into its irreducible constituents (cf. a forthcoming article). For these reasons we shall adopt this approach in the following. But we note that it is completely equivalent to the method of Foias. Therefore we shall be justified in borrowing several elements also from the latter.

Before we pass to the construction of Dirac's formalism, we shall state the mathematical results of the Maurin–Gel'fand–Vilenkin analysis. The key of their method is the following fundamental lemma, due to Gårding[12] (for further details, see also Roberts[13]):

Lemma: Let Φ be a locally convex topological vector space[8,42] with a *nuclear* embedding into a Hilbert space, $\Phi \rightarrow \mathcal{H}$; let

$$\mathcal{H} \rightarrow \hat{\mathcal{H}} = \int^{\oplus} \mathcal{H}(\lambda)\, d\mu(\lambda)$$

be an isometric mapping of $\mathcal{H}$ onto a direct integral (thus the embedding $\Phi \rightarrow \mathcal{H}$ is nuclear too); then the mapping

$$\tau_\lambda: \phi \rightarrow \phi(\lambda), \quad \phi \in \Phi, \quad \phi(\lambda) \in \mathcal{H}(\lambda)$$

is continuous and nuclear for every λ except on a fixed set Λ_0 of μ-measure zero, independent of ϕ.

The mapping τ_λ being nuclear, for any $\phi \in \Phi$ we may write

$$\tau_\lambda \phi = \phi(\lambda) = \sum_n \langle \phi'_n(\lambda), \phi \rangle h_n(\lambda),$$

with $\phi'_n(\lambda) \in \Phi'$ and a basis

$$\{h_n(\lambda),\ n = 1, 2, \cdots, \dim \mathcal{H}(\lambda)\}$$

of $\mathcal{H}(\lambda)$. This relation is valid for any λ if τ_λ is put equal to zero on the exceptional set Λ_0. Moreover, the dual mapping $\tau'_\lambda: \mathcal{H}(\lambda) \rightarrow \Phi'$ is continuous and allows us to identify each vector ξ of $\mathcal{H}(\lambda)$ with a functional $\tilde{\xi}$ of Φ' through the following equalities ($\phi \in \Phi$):

$$\langle \tilde{\xi}, \phi \rangle = (\xi, \phi(\lambda))_\lambda = (\xi, \tau_\lambda \phi)_\lambda = \langle \tau'_\lambda \xi, \phi \rangle.$$

With help of this lemma the spectral theorem of

[39] Reference 7, Vol. III.

[40] R. A. Hirschfeld, Indag. Math. **27**, 513 (1965) and private communication.

[41] Reference 7, Vol. IV. The spectral theorem, proved somewhat loosely in this volume, has been corrected by Roberts[13] and Gould [J. London Math. Soc. **43**, 745 (1968)].

[42] F. Treves, *Topological Vector Spaces, Distributions and Kernels* (Academic Press Inc., New York, 1967).

Maurin–Gel'fand–Vilenkin may now be stated as follows:

Theorem: Let A be a self-adjoint operator in $\mathcal{H}$; let $\mathcal{H} \to \hat{\mathcal{H}} = \int^{\oplus} \mathcal{H}(\lambda)\, d\mu(\lambda)$, the corresponding integral decomposition; and let Φ be as in the lemma.

Then:

1. The functionals $\phi'_n(\lambda)$ defined by the lemma form a complete orthonormal system ($\phi, \psi \in \Phi$):

$$(\phi, \psi) = \int (\phi(\lambda), \psi(\lambda))_\lambda \, d\mu(\lambda)$$
$$= \int \sum_{n=1}^{\dim \mathcal{H}(\lambda)} \overline{\langle \phi'_n(\lambda), \phi \rangle} \langle \phi'_n(\lambda), \psi \rangle \, d\mu(\lambda).$$

2. If A leaves Φ invariant and is continuous under the topology of Φ, $\phi'_n(\lambda)$ is for every λ and every n an eigenfunctional of A', the extension of A to Φ':

$$A'\phi'_n(\lambda) = \lambda \phi'_n(\lambda), \quad n = 1, 2 \cdots \dim \mathcal{H}(\lambda).$$

3. The same results hold true for a countable family of strongly commuting operators.

This spectral theorem satisfies all the conditions of Dirac. Moreover, the operator $\chi_\lambda = \tau'_\lambda \tau_\lambda$, which is a nuclear operator mapping Φ into Φ', acts as a projection operator onto the eigensubspace $\Phi'_\lambda \subset \Phi'$, corresponding to the eigenvalue λ. But it must be noted that the operator A', the extension of A to Φ', may very well have eigenvalues which do not belong to the Hilbert space spectrum of A (this property has been emphasized by Roberts[13]; it stems from the mere fact that A' has a larger domain of definition than A). However, these supplementary eigenvalues are deprived of any physical significance, for probabilities are defined in $\mathcal{H}$ only. Accordingly, the spectral decomposition of $\mathcal{H}$ selects precisely those eigenvalues of A' which form the Hilbert space spectrum of A. (This partly justifies the explicit use of direct integrals.) For this reason, we shall discard these nonphysical eigenvalues throughout the rest of the work.

C. Physical Remarks

We know from Secs. I and II that a physical system is defined by a family of *labeled observables*, represented by self-adjoint operators. Now we must build a space Φ such that the general spectral theorem applies to these observables. Let us consider first a family of commuting operators. The theorem requires that Φ shall be contained in the domain of each member of the family, that it be stable under all of them, and that it be dense in $\mathcal{H}$. In other words, the family of operators must have a *common dense invariant domain* $\mathfrak{D}$ in $\mathcal{H}$.[42a] Then the space Φ is obtained simply by introducing into $\mathfrak{D}$ a suitable new topology and completing it under this topology. Such (nuclear) topologies have been explicitly constructed by Foias[11] and Maurin.[12] But we need more; any observable, and, in particular, any labeled observable, can belong to a complete system of commuting observables. Thus, if we want the space Φ to be characteristic of the whole system and not only of a particular representation, we must require that the *same* space Φ shall work for *all* labeled observables; this will enable us to represent nondiagonal operators also, to formulate a transformation theory, and to give a reasonable physical interpretation of the formalism. These considerations, together with the results of Sec. I, may now be collected in the following definition[13]:

"An *irreducible physical system* is determined by an irreducible family $\mathcal{O}_I$ of (labeled) self-adjoint operators in a complex separable Hilbert space $\mathcal{H}$, with a common invariant dense domain $\mathfrak{D}$ and containing at least one complete Abelian system."

The irreducibility condition ensures that the family $\mathcal{O}_I$ is sufficient to generate the von Neumann algebra of all (bounded) observables:

$$\mathcal{O}'_I = \mathcal{O}' = \{\alpha 1\}; \quad \mathcal{O}''_I = \mathcal{O}'' = \mathcal{O} = \mathfrak{L}(\mathcal{H}).$$

It also entails the existence of at least one maximal Abelian von Neumann subalgebra,[30] but we must require, in addition, that this algebra be generated by *labeled* observables (see Sec. II). From the existence of the domain $\mathfrak{D}$, it follows that the restriction $\mathcal{O}_I^0$ of $\mathcal{O}_I$ to $\mathfrak{D}$ generates an algebra of operators with a unit (the restriction to $\mathfrak{D}$ of the identity operator of $\mathcal{H}$); sums and products of its elements can be performed without consideration of domains (which causes much trouble in $\mathcal{H}$); this point was emphasized by Roberts.[13]

Having now the domain $\mathfrak{D}$ at our disposal, we must endow it with a suitable topology. The minimal conditions are the following:

1. All operators of $\mathcal{O}_I$ shall be continuous on Φ; therefore the topology shall be finer than the one induced by $\mathcal{H}$;

2. The embedding $\Phi \to \mathcal{H}$ shall be a nuclear mapping.

We shall see below, however, that it is very useful to replace 2 by the stronger condition:

2′. Φ shall be a nuclear space, and the embedding $\Phi \to \mathcal{H}$ shall be continuous.

[42a] Such a domain $\mathfrak{D}$ always exists for a family of *commuting* observables, but this is no longer true in the general case.

Roberts[13] has given a general and canonical solution to this problem, simply by requiring the *coarsest topology* satisfying condition 1 (which is, of course, the most economical solution); but he has then to check explicitly that this topology is nuclear (it is so indeed in most elementary situations). Nevertheless, this canonical solution is not necessarily the best one for practical purposes; much benefit can be gained by taking for Φ a well-known "test-function" space,[7,9,10] such as $\mathcal{D}(\mathbf{R}^n)$, $\mathcal{D}(\Omega)$ (Ω open set of $\mathbf{R}^n$ or C^∞ manifold), $\mathcal{S}$, $K(M_p)$, etc., because the general form of a continuous functional over any of those spaces is known. Of course, for a justification of the abstract formalism, the bare existence of at least one space Φ is sufficient, but for studying practical problems, one must choose a concrete realization of Φ as a space of functions, just as one usually does with $\mathcal{H}$. Since the aim of the present formalism is the simplification of the theory, we prefer to take Φ as simple as possible, and this excludes any canonical and abstract solution, however elegant it may be. At the same time, the structure of Φ shall reflect, as much as possible, the characteristics of the system. This principle is central in our analysis and it will guide us throughout this work. In particular, it is essential to take care of the *symmetry properties* of the system from the start, by requiring that Φ be invariant under all symmetry operations. This will ensure consistency of the theory and also makes it simpler. We shall come back to this point in a forthcoming article.

IV. DIRAC FORMALISM FOR AN IRREDUCIBLE QUANTUM SYSTEM

A. Construction of the Triplet Space and Notations

Let $\{A_j, j \in I\}$ be a family of labeled observables characterizing an irreducible physical system as described in Sec. III. In the corresponding domain $\mathcal{D}$, we define a nuclear topology with all required properties. We then obtain the triplet

$$\Phi \subset \mathcal{H} \subset \Phi', \tag{6}$$

where Φ is complete and nuclear, thus reflexive[7] ($\Phi'' = \Phi$) and dense in $\mathcal{H}$; the injection mapping $\tau: \Phi \to \mathcal{H}$ is continuous, and so is the dual mapping $\tau': \mathcal{H} \to \Phi'$, which maps $\mathcal{H}$ on a dense subspace of Φ' (dense in the sense of sequential convergence[11]). If the family $\{A_j\}$ is countable, Φ can be taken to be a nuclear Fréchet space[13]; that is, Φ is the projective limit[8] ("intersection" in the language of Gel'fand *et al.*[7]) of a decreasing sequence of Hilbert spaces Φ_n corresponding to an increasing sequence of nondegenerate scalar products, Φ_n being the completion of Φ with respect to the scalar product $(\cdot, \cdot)_n$ (or the corresponding norm $\|\cdot\|_n$). Similarly, Φ' is the inductive limit[8] ("union") of the respective dual spaces Φ_n'. In other words, the triplet (6) is a *rigged Hilbert space*, in the sense of Gel'fand *et al.*,[41] whose structure can be represented as follows:

$$\begin{aligned}\Phi &= \operatorname*{lim\,proj}_{n=1,2\cdots} \Phi_n \subseteq \cdots \subseteq \Phi_2 \subseteq \Phi_1 \subseteq \Phi_0 \\ &\equiv \mathcal{H} \subseteq \Phi_1' \subseteq \Phi_2' \subseteq \cdots \subseteq \Phi' = \operatorname*{lim\,ind}_{n=1,2\cdots} \Phi_n'. \end{aligned} \tag{9}$$

In this scheme we use the following definitions: *ket vectors*, the elements of Φ, denoted $|\phi\rangle$, $|\psi\rangle, \cdots$; *normalizable vectors*, the elements of $\mathcal{H}$, denoted f, $g, \cdots$, with the scalar product $(f \mid g)$; *bra vectors*, the elements of Φ', denoted $\langle\phi'|$, $\langle\psi'| \cdots$. Thus we recover Dirac's language, except that we have now many more bras than kets (Roberts[13] interchanges Φ and Φ' in this interpretation; this is, of course, a matter of taste, but our convention coincides with Dirac's, who calls "representation" a complete set of *eigenbras*). The injection $\tau'\tau$ from Φ into Φ' is called γ; it is an *antilinear* operator:

$$\phi' = \gamma\phi, \quad \text{i.e.,} \quad \langle\phi'| = \gamma\,|\phi\rangle, \quad \phi \in \Phi, \quad \phi' \in \Phi'.$$

If $\langle\cdot \mid \cdot\rangle$ denotes the bilinear form expressing the duality between Φ and Φ', we normalize it in such a way that the following relation holds for any ϕ, $\psi \in \Phi$:

$$\langle\psi' \mid \phi\rangle = \langle\gamma\psi \mid \phi\rangle = (\psi \mid \phi). \tag{10}$$

Finally, given a continuous linear operator A from Φ into Φ, we define the following: A' as its adjoint, a continuous linear operator from Φ' into Φ'; $\hat{A} = \gamma A$ as its continuous extension to $\mathfrak{L}^\times(\Phi, \Phi')$, the space of continuous antilinear mappings from Φ into Φ'; also by A we denote its self-adjoint extension to $\mathcal{H}$ when it exists. (We do not need a new symbol, since the form of the parentheses tells whether A acts in Φ or in $\mathcal{H}$.) Then, for any ϕ, $\psi \in \Phi$, we can write

$$(\psi|\, A\,|\phi) = \langle\psi' \mid A\phi\rangle = \langle A'\psi' \mid \phi\rangle. \tag{11}$$

Note that adjunction is an antilinear operation:

$$(\lambda A)' = \bar{\lambda} A' \quad \text{and} \quad \widehat{(\lambda A)} = \bar{\lambda}\hat{A}$$

(λ any complex number).

B. Choice of a Representation

Let us consider now a complete system of compatible *labeled* observables $\{D_j, j = 1, 2 \cdots\}$; such a system exists by hypothesis. This system $\{D_j\}$ induces an integral decomposition of $\mathcal{H}$ into one-dimensional spaces $\mathcal{H}(\lambda)$ (λ denotes the set $\lambda_1, \lambda_2 \cdots$ of eigenvalues

of D_1, $D_2 \cdots$), as in Sec. II:

$$\mathcal{H} = \int^{\oplus} \mathcal{H}(\lambda)\, d\mu(\lambda),$$

$$(f \mid g) = \int \overline{f(\lambda)} g(\lambda)\, d\mu(\lambda),$$

$$D_j f \sim \{\lambda_j f(\lambda)\}, \quad j = 1, 2 \cdots, \quad f \in \text{domain of } D_j.$$

This decomposition of $\mathcal{H}$, in turn, induces an integral decomposition of Φ by nuclear operators χ_λ from $\mathfrak{L}^\times(\Phi, \Phi')$, which are eigenoperators[11,13] of D_j:

$$(\phi \mid \psi) = \int \langle \chi_\lambda \phi \mid \psi \rangle\, d\mu(\lambda), \quad \phi, \psi \in \Phi$$

with

$$\langle \chi_\lambda \phi \mid \psi \rangle = \overline{\langle \lambda \mid \phi \rangle} \langle \lambda \mid \psi \rangle,$$
$$\langle \lambda \mid \phi \rangle = \phi(\lambda), \tag{12}$$

where $\langle \lambda | \in \Phi'$ is a simultaneous eigenfunctional of all the D_j', $j = 1, 2 \cdots$:

$$\langle \lambda |\, D_j' \equiv \langle D_j \lambda | = \lambda_j \langle \lambda |, \qquad = 1, 2 \cdots.$$

Following Schwartz[10] and Gel'fand *et al.*,[7] we shall denote in this $\{\lambda\}$ representation the elements of Φ' as functions of λ, whether they are true functions or only generalized functions (e.g., distributions)

$$\langle \xi' \mid \phi \rangle = \int \xi'(\lambda) \phi(\lambda)\, d\mu(\lambda), \quad \xi' \in \Phi', \quad \phi \in \Phi,$$

in the same way as we have for $\phi, \psi \in \Phi$:

$$\langle \psi' \mid \phi \rangle = (\psi \mid \phi) = \int \overline{\psi(\lambda)} \phi(\lambda)\, d\mu(\lambda).$$

In particular,

$$\lambda_0(\lambda) = \delta_{\lambda_0}(\lambda) = \delta(\lambda - \lambda_0)$$

(with respect to the measure μ).

Similarly the *kernels*, i.e., elements of $(\Phi \hat{\otimes} \Phi)'$,[42b] the dual of the *projective* tensor product,[9,42] will be represented as integral operators:

$$\langle F \mid \phi \otimes \psi \rangle = \iint F(\lambda, \lambda') \phi(\lambda) \psi(\lambda')\, d\mu(\lambda)\, d\mu(\lambda'),$$
$$F \in (\Phi \hat{\otimes} \Phi)', \ \phi, \psi \in \Phi.$$

C. Eigenvalue Equations

In virtue of the general spectral theorem (Sec. IIIB), every labeled observable—and, more generally, any member of the algebra generated by labeled observables—admits in Φ' a complete orthonormal system of eigenfunctionals. Let A be such an observable; it also induces a direct integral decomposition of $\mathcal{H}$, which reads as follows:

$$\mathcal{H} = \int_{Sp A}^{\oplus} \mathcal{H}(\xi)\, d\nu(\xi),$$

$$(f \mid g) = \int (f(\xi) \mid g(\xi))_\xi\, d\nu(\xi),$$

$$= \int \sum_m \overline{f_m(\xi)}\, g_m(\xi)\, d\nu(\xi), \tag{13}$$

and similarly for the elements of Φ, with the further properties

$$\phi_m(\xi) = \langle \xi, m \mid \phi \rangle, \quad \phi \in \Phi, \quad \langle \xi, m | \in \Phi', \quad m = 1, 2 \cdots \dim \mathcal{H}(\xi),$$
$$\langle \xi, m |\, A' = \xi \langle \xi, m |, \tag{14}$$
$$\langle \chi_\xi \phi \mid \psi \rangle = (\phi(\xi) \mid \psi(\xi))_\xi, \quad \phi, \psi \in \Phi,$$
$$= \sum_{m=1}^{\dim \mathcal{H}(\xi)} \overline{\langle \xi, m \mid \phi \rangle} \langle \xi, m \mid \psi \rangle.$$

The orthonormality is given by the Parseval equality

$$\|\phi\|^2 = \int \sum_m |\langle \xi, m \mid \phi \rangle|^2\, d\nu(\xi). \tag{15}$$

These abstract relations can be realized in any given representation, say $\{\lambda\}$. With the convention stated above, the functional $\langle \xi, m|$ is now represented by a generalized function $\xi_m(\lambda)$, so that (14) can be written in the usual form:

$$A' \xi_m(\lambda) = \xi \xi_m(\lambda), \quad m = 1, 2 \cdots \dim \mathcal{H}(\xi). \tag{16}$$

We thus obtain an *eigenvalue equation in Φ', not in $\mathcal{H}$*. This allows us to use the theory of differential and partial differential equations with its full power; indeed, many eigenvalue equations of this type admit solutions which are not true functions, but only distributions: these could not be accepted in the usual theory, at least not without a supplementary apparatus by which the theory loses its simplicity and transparency. Here, however, they can. But, of course, A' is not necessarily a (partial) differential operator in any representation! This also makes more precise the nature of the nonnormalizable solutions of the eigenvalue equations of elementary quantum mechanics: they should be interpreted simply as elements of the corresponding Φ'. It must be noticed, however, that the eigenvalue equation alone, if not looked at from the point of view of the spectral decomposition, may lead to extra solutions which do not correspond to points of the Hilbert-space spectrum (see Sec. IIIB). These, of course, must be rejected!

[42b] Strictly speaking, this definition is valid only for a Fréchet space. In the general case, a kernel must be defined as follows. The elements of Φ are usually C^∞ functions on some C^∞ manifold, Ω say: $\Phi \equiv \Phi(\Omega)$. Then a *kernel over* $\Phi(\Omega)$ is an element of $\Phi'(\Omega \times \Omega)$, and this space may be strictly larger than $(\Phi(\Omega) \hat{\otimes} \Phi(\Omega'))$ if Φ is not Fréchet.

D. Matrix Elements of an Operator

First we remark that Φ and $\bar{\Phi}$, its complex conjugate space,[13] have the same topological properties; for instance, $\bar{\Phi}$ is nuclear whenever Φ is. Moreover, the following identity holds:

$$\mathfrak{L}^{\times}(\Phi, \Phi') = \mathfrak{L}(\bar{\Phi}, \Phi'),$$

which says that a Hermitian form in ϕ, ψ can be considered as bilinear in $\bar{\phi}$, ψ. We shall now suppose that Φ is a Fréchet space (metrizable topology). This is sufficient for all practical applications (systems defined by a countable set of labeled observables), except for field theory. The general case will be studied elsewhere.

Being both nuclear and Fréchet, Φ satisfies a refined version of Schwartz's *nuclear theorem* (*kernel theorem*). We shall use it under the two following forms.[43]

(a) Any continuous, antilinear mapping from Φ into Φ' defines a Hermitian kernel over Φ and vice versa:

$$\mathfrak{L}^{\times}(\Phi, \Phi') = (\bar{\Phi} \hat{\otimes} \Phi)'$$

both algebraically and topologically.

(b) For any bilinear form $b(\phi, h)$, $\phi \in \Phi$, $h \in \mathcal{H}$, separately continuous over $\Phi \times \mathcal{H}$, there exists a norm $\|\cdot\|_n$ over Φ and a Hilbert–Schmidt operator B from Φ_n into $\mathcal{H}'$ such that $b(\phi, h) = (B\phi \mid h)$.

It is now straightforward to apply this theorem to observables of the following classes (which do overlap):

1. *Labeled Observables or Elements of the Algebra That They Generate*

These are continuous operators from Φ to Φ; with the form (a) of the theorem, we have for any $\phi, \psi \in \Phi$, in the $\{\lambda\}$ representation,

$$(\phi| B |\psi) = \langle \hat{B}\phi \mid \psi \rangle = \iint B(\lambda, \lambda')\overline{\phi(\lambda)}\psi(\lambda')\, d\mu(\lambda)\, d\mu(\lambda').$$

2. *Bounded Observables*

That means continuous operators from $\mathcal{H}$ to $\mathcal{H}$; the form (b) gives for any $\phi \in \Phi$, $h \in \mathcal{H}$,

$$(\phi| B |h) = \iint B(\lambda, \lambda')\overline{\phi(\lambda)}h(\lambda')\, d\mu(\lambda)\, d\mu(\lambda').$$

3. *Continuous Observables*

That is, more generally, continuous operators from Φ to $\mathcal{H}$, thus from Φ into Φ' (this class contains the two other ones):

$$(\hat{B}\phi \mid \psi) = \iint B(\lambda, \lambda')\overline{\phi(\lambda)}\psi(\lambda')\, d\mu(\lambda)\, d\mu(\lambda').$$

For any continuous observable B, in particular, for a labeled or bounded observable, we can give in this way a meaning to the *matrix elements* $\langle\lambda| B |\lambda'\rangle$ of Dirac's formalism: they appear here as the "values" $B(\lambda, \lambda')$ of the corresponding kernel, written in the $\{\lambda\}$ representation. But such an interpretation *is not possible* for observables which are not continuous from Φ into $\mathcal{H}$. Moreover, if A and B belong to the algebra generated by labeled observables, their product does so too (by definition) and the same is true for the corresponding kernels; in the $\{\lambda\}$ representation this gives (exactly as with integral operators)

$$(AB)(\lambda, \lambda') = \int A(\lambda, \lambda'')B(\lambda'', \lambda')\, d\mu(\lambda''). \tag{17}$$

Among the kernels obtained by application of the nuclear theorem, those which correspond to decomposable operators (observables commuting with the D_j's) admit an integral decomposition of the following form:

$$B = \int B_\lambda\, d\mu(\lambda);$$

or, more precisely,

$$(\phi| B |\psi) = \langle \hat{B}\phi \mid \psi \rangle = \int \langle \hat{B}_\lambda \phi \mid \psi \rangle\, d\mu(\lambda), \quad \phi, \psi \in \Phi,$$

where $\hat{B}_\lambda$ is an eigenkernel[12] of the D_j's, i.e.,

$$D_j'\hat{B}_\lambda = \hat{B}_\lambda D_j = b(\lambda)\hat{D}_j, \quad j = 1, 2 \cdots$$

$$\{b(\lambda) = \text{scalar function}\}.$$

In particular, the operator γ itself decomposes into the eigenkernels χ_j introduced above,[11]

$$\gamma = \int \chi_\lambda\, d\mu(\lambda). \tag{18}$$

In the $\{\xi\}$ representation, this becomes

$$\delta^{\times}(\xi - \xi') = \int \chi_\lambda(\xi, \xi')\, d\mu(\lambda), \tag{19}$$

where, by definition,

$$\int \delta^{\times}(\xi - \xi')\phi(\xi)\psi(\xi')\, d\nu(\xi)\, d\nu(\xi') = \int \overline{\phi(\xi)}\psi(\xi)\, d\nu(\xi).$$

[This relation is just Eq. (10) written in the $\{\xi\}$ representation.] Relations (18)–(19) coincide with the so called *closure relation*,[1] which expresses the completeness of the system of eigenvectors.

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[43] The form (a) stems from the original form of Schwartz [see Ref. 42 and also L. Gårding and J. L. Lions, Nuovo Cimento Suppl. **14**, 9 (1959)]. The form (b) is the analog of the theorem given by Gel'fand and Vilenkin.[41] These authors prove it for the case of countably-Hilbert spaces, but it is well-known that every nuclear Fréchet space is countably-Hilbert.[41] If we do not suppose that $\Phi \equiv \Phi(\Omega)$[42b] is Fréchet, the nuclear theorem reads:

$$(\Phi \hat{\otimes} \Phi)' \subseteq \Phi'(\Omega \times \Omega) = \mathfrak{L}(\Phi, \Phi').$$

If Φ is Fréchet, the three spaces coincide.

E. Transformation Theory

Given two representations $\{\lambda\}$ and $\{\xi\}$, we have ($\phi, \psi \in \Phi$):

$$\overline{\phi(\lambda)}\psi(\lambda) = \langle \chi_\lambda \phi \mid \psi \rangle = \int \chi_\lambda(\xi, \xi')\overline{\phi(\xi)}\psi(\xi')\, d\nu(\xi)\, d\nu(\xi').$$

Similarly,

$$\phi(\lambda) \equiv \langle \lambda \mid \phi \rangle = \int \lambda(\xi)\phi(\xi)\, d\nu(\xi).$$

Of course, $\lambda(\xi)$ may be only a generalized function. If it is a true function, one can prove the usual identity

$$\lambda(\xi) = \overline{\xi(\lambda)}. \tag{20}$$

But it must be emphasized that (20) does not come from the Hermiticity property of a scalar product $\langle \lambda \mid \xi \rangle$, because no such scalar product exists; this is why Eq. (20) does *not* always have a meaning.

To sum up: we have reproduced the main features of Dirac's formalism by using a nuclear space Φ together with the convention that the generalized functions are written exactly as true functions, and Schwartz kernels as true integral operators. All of this becomes particularly simple in the case of the $\{x\}$ and $\{p\}$ representations: the spectral measure reduces to Lebesgue measure and we recover the usual theory of distributions over $\mathbf{R}^n$. For instance,

$$p(x) = e^{-ipx},$$

$$\delta(x - y) = \int e^{ip(x-y)}\, dp.$$

This last relation expresses the completeness property (19) of the eigenfunctionals of p (apart from complex conjugation). It may be useful to point out here that the three different meanings of the usual δ functions are all reproduced:

1. $\delta(x - x')$ is the matrix element of the unit operator in the $\{x\}$ representation, represented here (apart from a complex conjugation) by γ and its corresponding kernel (18)–(19);
2. $\delta(x - x')$ is the eigenfunction of the operator x, represented here by the eigenfunctional $\langle x' |$ in the $\{x\}$ representation (see Sec. IVB);
3. $\delta(x - x')$ appears as the normalization factor (scalar product) of the eigenfunctions of x; this is equivalent to the Parseval identity (15).

Note: We have considered an irreducible system only. The generalization to the case of discrete superselection rules $\mathcal{H} = \oplus_n \mathcal{H}_n$ is obvious: For each n, we take $\Phi_n \subset \mathcal{H}_n \subset \Phi'_n$ and then construct a big (nuclear) space Φ with all the Φ_n, e.g., as a topological direct sum or a topological product.[8] In the case of continuous superselection rules, we can obtain an integral decomposition of *the three spaces* Φ, $\mathcal{H}$, and Φ' by requiring that the essential observables be *natural operators of* Φ, in the sense of Foias,[11] i.e., operators which are Hermitian with respect to *all* the countable scalar products $(\cdot, \cdot)_n$ of Φ. However, this case seems to have an academic interest only (cf. Sec. I) so that we shall not go into further details.

V. THE TEMPORAL EVOLUTION AND THE WAVE EQUATION

Up to now we have described the system at a fixed time t_0 only; we must now consider its evolution in time. Let us start in the Schrödinger picture with the evolution equation[1]

$$f_t = U(t, t_0)f_{t_0}, \quad f_{t_0} \in \mathcal{H},$$

where $U(t, t_0)$ is postulated to be a unitary operator, with the group property

$$U(t_2, t_1)U(t_1, t_0) = U(t_2, t_0), \qquad U(t_0, t_0) = 1. \tag{21}$$

In the case of an isolated system, $U(t_1, t_0)$ depends on the difference $(t_1 - t_0)$ only, so that the operators $V(t) \equiv U(t, 0)$ constitute a one-parameter group of unitary operators, which can be made continuous by a suitable choice of phases.[3,25] Stone's theorem[21] then says that this one-parameter group has a *self-adjoint* infinitesimal generator H:

$$V(t) = \exp(-iHt), \qquad i(\partial/\partial t)V(t) = HV(t).$$

Identifying H with the total Hamiltonian as usual, we get the time-dependent Schrödinger equation:

$$i(\partial/\partial t)f_t = Hf_t. \tag{22}$$

In the general case of a nonisolated system, one has to *postulate* the existence and the self-adjointness of an operator $H(t)$ such that

$$i(\partial/\partial t)U(t_1, t_0) = H(t)U(t_1, t_0).$$

(This appears as a *presymmetry* in the sense of Ekstein.[44]) Again supposing that this $H(t)$ represents the total energy, we recover Schrödinger's equation:

$$i(\partial/\partial t)f_t = H(t)f_t. \tag{23}$$

Let us come back to our formalism now. We stick to the principle stated in Sec. IIIC, namely, the space Φ itself must characterize the system as much as

[44] H. Ekstein, Phys. Rev. **153**, 1397 (1967).

possible. In the present case, this means that Φ shall describe the whole history of the system, not only its behavior at a fixed time t_0. This leads to the following:

Postulate: If Φ characterizes the system at time t_0, it is required that

$$U(t, t_0)\Phi = \Phi \quad \text{for any } t.$$

This requirement looks very reasonable, for it ensures that the triplet space $\Phi \subset \mathcal{H} \subset \Phi'$ describes the system in an intrinsic way. But, with the physical interpretation we shall present in the next section, the postulate will appear as an essential consistency condition of the theory[45] (cf. Sec. IIIC).

As an immediate consequence, we have $H(t)\Phi \subseteq \Phi$ for any t; what leads us to include the total Hamiltonian among the labeled observables [continuity of $H(t)$ under the topology of Φ will be achieved in the explicit construction (cf. a forthcoming article); here it is postulated]. From this it follows that Schrödinger's equation [(22) or (23)] is valid in Φ, and thus in Φ'. But it must be emphasized that this concerns the *time-dependent equation* only, since the (time-independent) eigenvalue equation of the Hamiltonian admits in the continuous case solutions in Φ' only. As a trivial example, consider a nonrelativistic free particle: the eigenfunctional corresponding to momentum p is the planewave $\exp(i\mathbf{p}\cdot\mathbf{x})$, which belongs to $\Phi' \equiv \mathcal{S}'$,[13] whereas the time-dependent equation admits solutions of the type

$$f(\mathbf{x}, t) = \int d\mathbf{p}\tilde{f}(\mathbf{p}) \exp(i\mathbf{p}\cdot\mathbf{x} - ip^2t/2m),$$

which can also belong to $\Phi \equiv \mathcal{S}$ or $\mathcal{H} \equiv L^2$, according to the properties of $\tilde{f}(\mathbf{p})$.

The same postulate also ensures that the description of the system by the space Φ is valid in the Heisenberg picture, too, the transition being effected precisely by the time evolution operator. Similarly, it allows Dirac's construction[1] of the *quantum-action function* in order to justify the classical limit of the theory. Indeed, the operator $U(t_1, t_0)$, which belongs to $\mathfrak{L}(\Phi, \Phi)$, may be identified with a kernel:

$$\langle q|\, U(t_1, t_0)\, |q'\rangle_{\text{Dirac}} \equiv [U(t_1, t_0)](q, q').$$

The group property (21) then allows us to write the product of these kernels:

$$[U(t, t')](q, q') = \int\int \cdots \int [U(t, t_1)](q, q_1)[U(t_1, t_2)] \times (q_1, q_2) \cdots [U(t_m, t')](q_m, q')\, d\mu(q_1) \cdots d\mu(q_m).$$

[45] The same postulate will be extended later to any symmetry group.

VI. PROBABILISTIC INTERPRETATION

A. Reformulation of the Usual Interpretation

We have given a precise mathematical meaning to Dirac's formalism, but at the price of introducing the new elements Φ, Φ', and we must now investigate their physical significance. Let us start with the general probabilistic interpretation outlined in Sec. I. Given a question Q and a state h, the probability of getting a positive answer for that state is given by the expectation value of the corresponding projection operator Q^E:

$$\text{Prob}\,(Q, h) = (h, Q^E h).$$

Now let A be an observable, $\{\lambda\}$ a representation in which A is diagonal, E_Δ^A the projection operator on the subset Δ of the spectrum of A. We have

$$(h, E_\Delta^A h) = \int_\Delta d(h, E_\lambda^A h) = \int_\Delta |h(\lambda)|^2\, d\mu(\lambda),$$

i.e., the probability that A shall have, in the state h, a value between λ and $\lambda + d\lambda$ is given by $|h(\lambda)|^2\, d\mu(\lambda)$, where $d\mu(\lambda) = \mu(\lambda, \lambda + d\lambda)$. In Dirac's language this quantity reads $|\langle\lambda \mid h\rangle|^2\, d\lambda$ and leads to the concept of a *transition probability amplitude*, represented by the scalar product $\langle\lambda \mid h\rangle$.

Now, if λ is a point of the continuous spectrum of A, $\langle\lambda|$ belongs only to Φ', and Dirac's interpretation is not possible anymore unless $h \in \mathcal{H}$ is an element of Φ (precisely $h = \tau\phi$, with $\phi \in \Phi$); in this case, we indeed have

$$\phi(\lambda) = \langle\lambda \mid \phi\rangle.$$

For such a pair λ, ϕ we can thus write a probability amplitude. For interpreting it physically, we shall follow the analogy of Feynman's theory of path integrals.[46] His argument may be outlined (somewhat naively) as follows. Let the history of the system be represented by some path in space–time, and consider for some fixed time t two portions of this history corresponding to regions R' ($t' < t$) and R'' ($t'' > t$), respectively; then the transition probability amplitude from R' to R'' is given by

$$\text{Ampl}\,(R', R'') = \int \overline{\chi(x, t)}\psi(x, t)\, dx = \langle\chi \mid \psi\rangle.$$

In this expression $\psi(x, t)$ is a wavefunction describing the history of the system up to time t, i.e., the *prepared*

[46] R. P. Feynman, Rev. Mod. Phys. **20**, 267 (1948).

system at time t; $\chi(x, t)$ is a wavefunction describing the future of the system, that is, the possible experiments to which it can be subjected at times later than t. Moreover, both wavefunctions satisfy a Schrödinger evolution equation. If one identifies such an experiment (question) with the (unique) state in which it gives a positive answer with certitude, then $\chi(x, t)$ represents a state in which the system may jump, and we come back to the usual interpretation of the probability amplitude (scalar product in $\mathcal{H}$).[1]

The class of states χ is normally assumed to be identical with the class of states ψ, but this requires χ to be normalizable. If we drop this restriction, we have a situation (already mentioned by Feynman[46] in a footnote) in which the two classes are not identical anymore: to some experiments correspond "idealized" states χ, in which the system cannot be, i.e., states which cannot be prepared. With this idea in mind, we shall now give the following interpretation to the "triplet" formalism: Φ represents the class of physical states which can be prepared; the preparation of the system must then be described by a kind of projection on Φ; on the other hand, Φ' represents all the potential experiments which can be performed on the system or, equivalently, the possible measurement instruments. The corresponding states may be nonphysical or idealized, i.e., represented by an unnormalizable vector. This interpretation is quite intuitive, for the concept of functional is very close to that of experiment. A measurement on the system can be defined as an operation which associates a *number* to each state of the system, i.e., a functional! Take for instance the eigenfunctional $\langle\lambda_0|$ of A; it corresponds to the question, "What is the probability that A takes the value λ_0 in a given state?" More precisely:

1. If λ_0 belongs to the discrete spectrum, there exists a true state in which the answer is 1: $(\lambda_0 \mid \lambda_0) = 1$.

2. If λ_0 belongs to the continuous spectrum, no such state exists, but $\langle\lambda_0|$ can give a relative probability[1] for any two physical states $\phi_1, \phi_2 \in \Phi$ (see below).

With this interpretation, it is *essential* that Φ and Φ' be stable during the time evolution: a physically accessible state must remain such throughout its time evolution if it does not suffer any external perturbation; this means that the evolution equation needs to be valid in both Φ and Φ', which results from the basic postulate of Sec. V.

We want to emphasize that this extended interpretation is not incompatible with *time reversal invariance*. Indeed, this law compares a process like

physical state $I \rightarrow$ experiment $B \rightarrow$ physical state II

with the time reversed process

$$\text{physical state } I \leftarrow \begin{matrix}\text{time reversed} \\ \text{experiment } B^T\end{matrix} \leftarrow \text{physical state II}.$$

If we take for the physical states I and II two elements of Φ, the usual discussion remains entirely valid and no difficulty arises.

B. A Possible Generalization

The interpretation offered here is simply an adaptation of the conventional one, based on the concept of probability amplitude. But the structure itself of the mathematical construction suggests a possible generalization, along the lines of Grossmann.[47] We shall only sketch it briefly, for several problems remain open.

To the triplet (6) correspond the following inclusions, both algebraic and topological[29]:

$$\mathfrak{L}(\Phi', \Phi) \subset \mathfrak{L}(\mathcal{H}, \mathcal{H}) \subset \mathfrak{L}(\Phi, \Phi'). \tag{24}$$

N.B. We forget here for a while that certain operators are antilinear; this will be taken into account in the probabilities below.

In particular, $\mathfrak{L}(\mathcal{H}, \mathcal{H})$ contains projection operators representing questions (Sec. I). Since they are a special class of observables, we shall call them *observable questions*. But relation (24) suggests to us to introduce two other types of questions belonging to $\mathfrak{L}(\Phi', \Phi)$ and $\mathfrak{L}(\Phi, \Phi')$, which we shall call *universal questions* and *generalized questions*, respectively. For these three types probabilities can be defined as follows:

1. Observable Question

Projection operator P, applicable to any normalizable vector $h \in \mathcal{H}$; the usual probabilistic interpretation is given by the two rules:

(a) The relative probability of positive answer to the observable questions P_1, P_2 in the state h is given by

$$\text{Rel Prob}\,(P_1, P_2; h) = \frac{(h|\, P_1\, |h)}{(h|\, P_2\, |h)}. \tag{25}$$

(b) The observable question P projects the system into the state $P\mathcal{H}$; in particular, the elementary question $P_g = |g)\,(g|$ projects the system into the pure state g.

2. Universal Question

Operator Π from $\mathfrak{L}^\times(\Phi', \Phi)$ such that $P = \tau\Pi\tau'$ is a projection operator of $\mathcal{H}$; it is applicable to any

[47] A. Grossmann, J. Math. Phys. **5**, 1025 (1964).

idealized state, i.e., any bra vector $\phi' \in \Phi'$. The probabilistic rules are the following:

(a)

$$\text{Rel Prob}\,(\Pi_1, \Pi_2; \phi') = \frac{\langle \phi' \mid \Pi_1 \phi' \rangle}{\langle \phi' \mid \Pi_2 \phi' \rangle}. \qquad (26)$$

If ϕ' is normalizable, $\phi' = \tau' h$ and $\langle \phi' \mid \Pi_j \phi' \rangle = (h| P_j |h)$; that gives again the standard formula (25).

(b) The universal question Π projects the sytem into the state $\Pi\Phi' \subseteq \Phi$; in particular, the elementary universal question Π_ϕ defined by

$$\Pi_\phi \phi' = \overline{\langle \phi' \mid \phi \rangle}\, |\phi\rangle \; (\forall \phi' \in \Phi')$$

projects the system into the state $\phi \in \Phi$. Equation (26) then gives

$$\text{Rel Prob}\,(\Pi_{\phi_1}, \Pi_{\phi_2}; \phi') = \left| \frac{\langle \phi' \mid \phi_1 \rangle}{\langle \phi' \mid \phi_2 \rangle} \right|^2.$$

With $\langle \phi' | = \langle \lambda |$, for instance, we get $|\phi_1(\lambda)/\phi_2(\lambda)|^2$, which is obviously the relative probability of finding a λ component [i.e., a positive answer to the question associated with $\langle \lambda |$) in the states ϕ_1, ϕ_2.]

3. *Generalized Question*

Operator π from $\mathfrak{L}^\times(\Phi, \Phi')$, applicable to any ket vector $\phi \in \Phi$ (physical state); the probabilistic rules go as follows:

(a)

$$\text{Rel Prob}\,(\pi_1, \pi_2; \phi) = \frac{\langle \pi_1 \phi \mid \phi \rangle}{\langle \pi_2 \phi \mid \phi \rangle}. \qquad (27)$$

If there exists a projection operator P such that $\pi = \tau' P \tau$, π becomes observable and we recover (25) again.

(b) The generalized question π projects the system into the idealized state $\pi\Phi \subseteq \Phi'$; the elementary generalized question $\pi_{\phi'}$, defined by $\pi_{\phi'} |\phi\rangle = \overline{\langle \phi' \mid \phi \rangle}\, \langle \phi' |$, $\forall \phi \in \Phi$, projects the system onto $\phi' \in \Phi'$, so that

$$\text{Rel Prob}\,(\pi_{\phi_1'}, \pi_{\phi_2'}; \phi) = \left| \frac{\langle \phi_1' \mid \phi \rangle}{\langle \phi_2' \mid \phi \rangle} \right|^2.$$

With $\langle \phi_1' | = \langle \lambda_1 |$, $\langle \phi_2' | = \langle \lambda_2 |$, we get $|\phi(\lambda_1)/\phi(\lambda_2)|^2$; i.e. the relative probability of positive answer to the questions associated with $\langle \lambda_1 |$, $\langle \lambda_2 |$.

We have seen above a possible interpretation of the probability amplitude $\langle \xi' \mid \phi \rangle$, where the vector ϕ represents the state of the *prepared* system; this suggests to us to describe the *preparation of the system* by a universal question, in the same way as it is usually done by an ordinary projection operator. On the other hand, we don't see at present an obvious physical interpretation for generalized questions (except for the operators χ_λ introduced in Sec. IV, which act as projection operators onto the eigenspaces in Φ'); they are not even completely defined, since we lack a criterion to distinguish a nonelementary generalized question from an ordinary operator of $\mathfrak{L}^\times(\Phi, \Phi')$. Another open question is the following: How can Gleason's theorem,[24] and thus the density operator, be generalized to the new classes of questions? This last problem is certainly nontrivial, since Gleason's theorem is intimately connected with the properties of von Neumann algebras (definition of a trace), which are typical of Hilbert space!

VII. CONCLUSIONS

The formalism which we have built in the spirit of Gel'fand, Foias, Roberts, and others provides a reasonable and satisfactory formulation of Dirac's language. But the problem can by no means be considered as closed: the present work is a starting point rather than a definitive achievement. Indeed, many open questions remain—mainly of physical character. A first problem is the uniqueness of the space Φ. We have required several times that it should characterize the system as completely as possible—in particular, that it should be invariant under all the symmetry operations of the system—and the interpretation given above implicitly supposes a unique Φ. But we have seen also that practical reliability of the formalism requires the existence of a sufficiently well-known space Φ, which does not necessarily coincide with the canonical solution of Roberts.[13] Our guess is that all the admissible spaces (that is, spaces invariant under all the labeled observables and making them continuous, and the same for all the symmetry operators of the system) will be physically equivalent, in the sense that choosing one or another of them will not bring any *observable* difference; this is rather reasonable, but, of course, it requires a proof! Also, the probabilistic interpretation deserves further study: the whole theory of quantum measurement should be rewritten in this new context; this would provide (probably) an answer to the preceding question, too.

What is the domain of applicability of this formalism? For a *finite nonrelativistic system* (finite number of degrees of freedom), it works easily, since one deals only with a finite number of labeled observables. The most interesting case is, of course, a system of interacting particles, i.e., scattering theory; this problem will be studied in a further article. A *finite relativistic system* can be treated in exactly the same way; it presents, however, consistency difficulties

which have nothing to do with spectral theory of observables. But, of course, *infinite systems*, both relativistic and nonrelativistic, are much more interesting; here the need of a new language is most pressing. For applications of the present formalism, it is useful to distinguish three kinds of infinite systems.

A. System with a Unique Normalizable Vacuum

This is the type of system studied in axiomatic field theory.[5] It has been shown by Maurin[48] (see also Roberts[13]) that the Wightman–Borchers[5,49] formulation is essentially equivalent to a "triplet" formalism, but the physical idea is very different: $\mathcal{H}$ is determined there by a particular (Wightman) functional over a standard test-function space, whereas here Φ is characteristic of the system and built from $\mathcal{H}$, which is given *a priori*. However, a possible bridge between the two approaches may be provided by Jaffe's local quantum field theory,[50] where the choice of the test-function space also reflects some properties of the system.

B. System with a Unique, Nonnormalizable Vacuum

If we suppose that all creation and destruction operators are continuous on Φ and leave it invariant, we can transpose them to Φ' by duality (this procedure has been suggested by Kristensen *et al.*[15]). If the vacuum is defined as the "state" annihilated by all destruction operators, it is then possible to include it in Φ'. (Its invariance under the group of relativity can be treated similarly.) In this case the theory can be developed as usual, the canonical commutation relations being understood over Φ or Φ'; but only the *universal* observables, i.e., those continuous from Φ' into Φ, can now have a well-defined vacuum expectation value. This shows that such a vacuum is in fact a *bare* vacuum, a state physically inaccessible to the system. This kind of frame is probably well adapted for a rigorous formulation of "current algebra" theories[51]: since all the relevant operators (currents and current densities) are unbounded on $\mathcal{H}$, they will be most easily treated in Φ and Φ', where they become continuous.

C. System where an Infinite Number of Realizations of the Space of States are Considered Simultaneously

This is typically the situation of a system defined by a representation of a group or an algebra which has a noncountable number of inequivalent representations. Such are, for instance, the BCS model of superconductivity[33] (gauge group), the infinite system of harmonic oscillators,[52] or the boson gas[53] (fundamental commutation relations), and, more generally, all systems with a "spontaneously broken" symmetry. To each representation corresponds a Hilbert space which *completely* describes the system, but, in order to keep explicitly the freedom in the choice of this representation, one considers all these Hilbert spaces simultaneously, with a direct integral for instance, together with some (nonobservable) operators, mapping them onto each other. But it must be emphasized that the larger Hilbert space thus obtained is *not* the space of states; it is a more general—and, in a sense, artificial—space. In such a situation, one way out is to build a triplet $\Phi_\alpha \subset \mathcal{H}_\alpha \subset \Phi'_\alpha$ in each component α and to gather all these spaces in a big triplet $\Phi \subset \mathcal{H} \subset \Phi'$ with help of Foias's natural operators[11] (see the note at the end of Sec. IV).

These indications are rather vague and sketchy, but it is not unreasonable to hope that the present formalism will be useful in such general situations, as it is in simpler cases. This might then provide an answer to Dirac's recent criticism of the adequacy of Hilbert space to describe field theory.[54] But there remains of course an impressive amount of work to be done!

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Killing Horizons and Orthogonally Transitive Groups in Space-Time

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Some concepts which have been proven to be useful in general relativity are characterized, definitions being given of a local isometry horizon, of which a special case is a Killing horizon (a null hypersurface whose null tangent vector can be normalized to coincide with a Killing vector field) and of the related concepts of invertibility and orthogonal transitivity of an isometry group in an n-dimensional pseudo-Riemannian manifold (a group is said to be orthogonally transitive if its surfaces of transitivity, being of dimension p, say, are orthogonal to a family of surfaces of conjugate dimension $n - p$). The relationships between these concepts are described and it is shown (in Theorem 1) that, if an isometry group is orthogonally transitive then a local isometry horizon occurs wherever its surfaces of transitivity are null, and that it is a Killing horizon if the group is Abelian. In the case of $(n - 2)$-parameter Abelian groups it is shown (in Theorem 2) that, under suitable conditions (e.g., when a symmetry axis is present), the invertibility of the Ricci tensor is sufficient to imply orthogonal transitivity; definitions are given of convection and of the flux vector of an isometry group, and it is shown that the group is orthogonally transitive in a neighborhood if and only if the circulation of convective flux about the neighborhood vanishes. The purpose of this work is to obtain results which have physical significance in ordinary space-time ($n = 4$), the main application being to stationary axisymmetric systems; illustrative examples are given at each stage; in particular it is shown that, when the source-free Maxwell–Einstein equations are satisfied, the Ricci tensor must be invertible, so that Theorem 2 always applies (giving a generalization of the theorem of Papapetrou which applies to the pure-vaccuum case).

1. INTRODUCTION

The purpose of this paper is to develop in a coherent way some concepts which are currently being found useful in work on general relativity in connection with isometries, and to point out some of the relationships between them and show how they may be applied. Although the motive for this study is to obtain physical applications to 4-dimensional space–time, the results are all derived in n dimensions, because, on one hand, very little extra work is required, while, on the other hand, considerably greater mathematical insight is obtained.

The main subject of discussion will be certain types of horizons which we shall now define.

A null hypersurface in a pseudo-Riemannian manifold is said to be a local isometry horizon (which we henceforth abbreviate to LIH) with respect to a group of isometries if (I) it is invariant under the group, and (II) each null-geodesic generator is a trajectory of the group.

The special case of a null surface which is an LIH with respect to a one parameter group (or subgroup) is said to be a Killing horizon. In other words, a Killing horizon is a null surface whose generating null vector can be normalized so as to coincide with a Killing vector field.

The purpose of these definitions is to isolate the characteristic features of the class of functions of which the Schwarzschild horizon[1] is the most familiar example in so far as these features can be described in terms of purely local concepts. The physical significance of an LIH is that on it a particle may at once be travelling at the speed of light (along one of the null generators) and standing still (in the sense that no change in its surroundings can be detected as its affine parameter varies because it is moving along a trajectory of a motion which leaves invariant both the intrinsic structure of space–time and the position of the null surface itself). As a general consequence, infinite red or blue shifts will be observable in relation to the frames of reference naturally determined by the isometry group.

LIH's are worth studying because, in addition to their local significance, they may have considerable importance in the global structure of space–time, for example as event horizons[2] or Cauchy horizons,[3] etc. Killing horizons in particular are interesting in four dimensions because any spacelike 2-surface within such a horizon will be marginally locally trapped according to the definition of Penrose.[4] This is because the null vectors generating the Killing horizon must have zero expansion, rotation, and shear (i.e., $\rho = \sigma = 0$ in Newman–Penrose language).[5] The vanishing of the first of these means that one family of null normals to the 2-surface is not expanding in either direction, and so there must be a sense of time

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direction in which both families of null normals are nonexpanding. If the required sense happened to be the same over the whole 2-surface, then it would follow, in the case of a compact 2-surface, that it would be a closed marginally trapped surface. (A marginally trapped surface is one which satisfies the condition that neither family of null normals diverges, but not the strict condition that both converge.) However, although such global properties as these provide much of the motivation for studying LIH's, we restrict attention to purely local concepts in this paper.

It is worth emphasizing that the conditions (I) and (II) in the definition of an LIH are independent of each other, and that they are both essential if the condition is to be sufficiently restrictive to be useful. In physical terms, they are both necessary if a particle moving along a null generator is to be able to be thought of as also standing still, since if (II) were not satisfied it would have motion with respect to the intrinsic structure of space–time, while if (I) were not satisfied the null surface itself would define a structure with respect to which motion could be defined. These points may be made clearer by consideration of a few simple examples.

A trivial example is provided by the null cone of a point in Minkowski space, which is an LIH with respect to the Lorentz group at that point, but not with respect to the full Poincare group [since (I) would not be satisfied] nor with respect to the rotation group at the point [since (I) would not be satisfied]. It is not a Killing horizon.

The classic example is the Schwarzschild horizon,[1] which is an LIH with respect to the one-parameter group of static displacements, and is therefore a Killing horizon. It is also an LIH with respect to larger groups such as the Abelian group (static displacements) $\oplus$ (rotations about an axis). Within the Schwarzschild horizon there are many null hypersurfaces which satisfy (I), but the definition excludes them from being counted as LIH's because they do not satisfy (II).

A slightly more complicated example is provided by the Kerr solution[6] when $a > m$ (in the standard notation as used in Ref. 4), in which there are LIH's with respect to the Abelian group (stationary displacements) $\oplus$ (rotation about the axis), but not with respect to any larger groups. These LIH's also are Killing horizons, but this is less obvious than in the case of the Schwarzschild solution because the Killing fields involved are not the same as the unique Killing field which is timelike at infinity. This will be further discussed in Sec. 4.

It is now natural to wonder under what conditions LIH's and Killing horizons are likely to occur. A casual glance at the Schwarzschild solution might suggest that they occur where a Killing vector field becomes null. However, a little consideration shows that this is neither sufficient nor (except for a Killing horizon) necessary. For example, in Minkowski space one may form a whole class of Killing vector fields by taking different linear combinations of a static displacement and a rotation about an axis, but the hypersurfaces on which these fields become null are not themselves even null, but are timelike.

Further investigation of this question constitutes the principal content of this paper. With this end in view we introduce, in Sec. 2, the idea of an isometry group being orthogonally transitive, meaning that the surfaces of transitivity are orthogonal to a family of surfaces of conjugate dimension. It is a convenient consequence of orthogonal transitivity that it is possible (where the surfaces of transitivity are not null) to choose coordinates in two sets, constant on the surfaces of transitivity and the orthogonal surfaces, respectively, in such a way that the resulting form of the metric tensor makes manifest, as far as possible, the isometries, and at the same time contains no cross terms between the two sets.

One of the main results of this investigation is given in Sec. 3, where it is shown that, wherever the surfaces of transitivity of an orthogonally transitive group do become null, an LIH occurs. In Sec. 4 it is shown in addition that if the group is Abelian, such an LIH is a Killing horizon.

In Secs. 5 and 6 it is shown that orthogonal transitivity is not merely a condition imposed for mathematical convenience (although it has often been assumed in past investigations without any other justification) but that it may be expected to occur naturally under fairly general conditions, provided the group is Abelian and provided also that its surfaces of transitivity have $(n - 2)$ dimensions where n is the dimension of the manifold [orthogonal transitivity being trivial in the $(n - 1)$-dimensional case]. These conditions are given a physical interpretation in general relativity in terms of the vanishing of the convective circulation of matter around a region.

As the paper progresses the class of groups under consideration has to be progressively restricted: from general groups in Sec. 3 to Abelian groups in Sec. 4 to Abelian $(n - 2)$-parameter groups in Secs. 5 and 6. However, all the results apply to 2-parameter (and trivially to 3-parameter) Abelian groups in

[6] R. H. Boyer and T. G. Price, Proc. Cambridge Phil. Soc. **61**, 531 (1965).

four-dimensional space–time, and therefore to stationary axisymmetric systems in particular.

2. INVERTIBILITY AND ORTHOGONAL TRANSITIVITY

We now introduce the related concepts of orthogonal transitivity and invertibility of a group of isometries.

Consider an open region $\mathfrak{U}$ on an n-dimensional manifold such that there is a continuous group of isometries whose surfaces of transitivity have dimensionality p ($1 \leq p \leq n-1$) in $\mathfrak{U}$.

Then the group is said to be orthogonally transitive in $\mathfrak{U}$ if there exists a family of $(n-p)$-dimensional surfaces which are orthogonal to the surfaces of transitivity at each point in $\mathfrak{U}$.

The group is said to be invertible at a point P in $\mathfrak{U}$ if there is an isometry leaving P fixed which simultaneously inverts the sense of the p independent directions in the surface of transitivity at P, but leaves unaltered the sense of the directions orthogonal to the surface of transitivity at P. If such an isometry exists, it is clear that it is an involution and that it is uniquely determined.

It is important to note that a group cannot be invertible at a point P if the surface of transitivity through P is null, since in this case there is a direction in the surface of transitivity which is also orthogonal to it. This situation is not merely due to an inadequacy in the definition of invertibility, but is a result of the fact that, even when the group is invertible on the other surfaces of transitivity in the immediate neighborhood of P, there is generally a real distinction between the two opposed arrangements of the direction senses in the null surface of transitivity. This somewhat paradoxical state of affairs may be made intelligible by means of an illustration. Consider the 1-dimensional group generated by stationary displacements in Kruskal's completed Schwarzschild solution.[1] This group is invertible everywhere except on the horizon, where the Killing vector becomes null. It is immediately clear that there is a distinction between the two senses of direction along a line of transitivity there, since in one sense the line approaches a fixed point of the group, while in the other it continues to infinity without interruption.

It can easily be seen that orthogonal transitivity is a necessary condition for a group to be invertible in a neighborhood. For suppose we have an n-dimensional manifold with a group of isometries whose surfaces of transitivity are p-dimensional, and which is invertible in the neighborhood of a point P. Construct the set of all differentiable paths in the neighborhood which pass through P and which are everywhere orthogonal to the surfaces of transitivity. This set of paths intersects each surface of transitivity in a unique point: for consider a pair of paths PQ and PQ', where Q and Q' lie on the same surface of transitivity; since the directed compound path QPQ' could be defined without reference to any sense of direction in the surfaces of transitivity, it follows that Q and Q' must coincide, because otherwise the ordered pair Q, Q' would give rise to an intrinsically defined sense of direction in the surface of transitivity at Q. It follows that this set of paths generates an $(n-p)$-surface through P which is orthogonal to the surfaces of transitivity. By a similar construction at each point in the neighborhood of P, a complete family of orthogonal $(n-p)$-surfaces can be built up.

Thus, in order that a group should be invertible, it is necessary that it be orthogonally transitive, and also that the surfaces of transitivity be nonnull. These conditions are not in general sufficient. For consider as a counterexample the 4-dimensional space with metric given by

$$ds^2 = a(z,t)e^{-2y}\,dx^2 + 2b(z,t)e^{-y}\,dx\,dy + c(z,t)\,dy^2 + dz^2 - dt^2, \quad (1)$$

with $a(z,t)c(z,t) > b^2(z,t)$. Then the Killing vectors $\partial/\partial x$ and $x(\partial/\partial x) + (\partial/\partial y)$ generate a non-Abelian group which is orthogonally (and simply) transitive over the 2-surfaces, $z = \text{const}$, $t = \text{const}$, these surfaces being orthogonal to the family of 2-surfaces, $x = \text{const}$, $y = \text{const}$. The surfaces of transitivity are nonnull. Nevertheless, it can easily be checked that, except for some specially simple choices of the functions $a(z,t)$, $b(z,t)$, $c(z,t)$, the group is not invertible.

Suppose, however, that we have an Abelian group. In this case the requirement that the group be orthogonally transitive with nonnull surfaces of transitivity is not only necessary but also sufficient for the group to be invertible.

In order to see this, consider an n-dimensional manifold with an orthogonally transitive Abelian isometry group which has nonnull p-dimensional surfaces of transitivity in some neighborhood. We construct a manifestly invertible coordinate patch as follows. Let $y^1, \cdots, y^{n-p}$ be any well-behaved coordinate system on one of the orthogonal $(n-p)$-surfaces. There will be a nondegenerate induced metric $ds^2 = g_{ij}\,dy^i\,dy^j$, $i,j = 1, \cdots, n-p$. By dragging the system along under the operations of the group, we equip all the orthogonal $(n-p)$-surfaces with coordinates in which the induced metric has an identical form, since, being nonnull, the surfaces of

transitivity through the original orthogonal $(n-p)$-surface span the whole neighborhood. It is for the next stage that we need the group to be Abelian. We choose p linearly independent Killing vector fields generating the group, which we shall suggestively label $\partial/\partial\psi^1, \cdots, \partial/\partial\psi^p$. We proceed to attach a set of coordinate values $\psi^1, \cdots, \psi^p$ to each of the orthogonal $(n-p)$-surfaces in the obvious way, i.e., we first choose one of the $(n-p)$-surfaces as the origin, $\psi^1 = \cdots = \psi^p = 0$; we then drag this one along under the Killing vectors $\partial/\partial\psi^2, \cdots, \partial/\partial\psi^p$, thereby generating a hypersurface (since the Killing vectors commute) which we label $\psi^1 = 0$; from here we form the family of hypersurfaces $\psi^1 = \text{const}$ by dragging this one along under $\partial/\partial\psi^1$ by corresponding values of the parameter ψ^1; finally, we repeat the process for $\psi^2, \cdots, \psi^p$. As a result of the commutation, each hypersurface $\psi^k = \text{const}$ is invariant under the Killing vectors other than $\partial/\partial\psi^k$. It follows that in each p-surface of transitivity the induced metric is given by $ds^2 = h_{kl}\, d\psi^k\, d\psi^l$, $(k, l = 1, \cdots, p)$, where the coefficients h_{kl} are independent of $\psi^1, \cdots, \psi^p$. Due to the orthogonality, the metric on the whole space has the form $ds^2 = g_{ij}\, dy^i\, dy^j + h_{kl}\, d\psi^k\, d\psi^l$. Now consider the inversion mapping $(y^1, \cdots, \psi^p) \to (\tilde{y}^1, \cdots, \tilde{\psi}^p)$ where $\tilde{\psi}^i = y^i$ $(i = 1, \cdots, n-p)$ and

$$\tilde{\psi}^k = -\psi^k \quad (k = 1, \cdots, p).$$

Since g_{ij} and h_{kl} are independent of $\psi^1, \cdots, \psi^p$, this is clearly an isometry; thus the group is invertible.

We note in passing that the concept of being static is the special case of orthogonal transitivity which refers to a 1-parameter group (applying in the stricter sense only when the Killing vector is time like). Since a 1-parameter group is automatically Abelian, orthogonal transitivity and invertibility are equivalent here when the Killing vector is nonnull.

By a rough analogy we can transfer these ideas from groups to tensors. Let ${}_{(i)}\zeta^\lambda$ $(i = 1, \cdots, p)$ be a set of independent vectors spanning a p-dimensional surface element at a point P, and let ${}^{(j)}\eta_\mu$ $(j = p+1, \cdots, n)$ be a set of independent vectors spanning the orthogonal $(n-p)$ element at P. Then a tensor T is said to be orthogonal to the p-surface element at P with respect to a particular subset of s of its indices if, when we form the mixed components $T^{\mu_1 \cdots \mu_r}{}_{\lambda_1 \cdots \lambda_s}$, which are covariant in the indices of the subset and contravariant in the others, the contraction

$${}^{(\alpha_1)}\eta_{\mu_1}, \cdots, {}^{(\alpha_r)}\eta_{\mu_r} T^{\mu_1 \cdots \mu_r}{}_{\lambda_1 \cdots \lambda_s}\, {}_{(\beta_1)}\zeta^{\lambda_1}, \cdots, {}_{(\beta_s)}\zeta^{\lambda_s}$$

vanishes for all possible choices of $\alpha_1, \cdots, \alpha_s$ and $\beta_1, \cdots, \beta_s$. The tensor is said to be invertible in the p element at P [or invertible about the orthogonal $(n-p)$ element at P] if each of the scalars obtained by contracting any combinations of its indices with any choice of the ${}_{(i)}\zeta^\lambda$ and the ${}^{(j)}\eta_\mu$ is invariant when ${}_{(i)}\zeta^\lambda \to -{}_{(i)}\zeta^\lambda$ and ${}^{(j)}\eta_\mu \to {}^{(j)}\eta_\mu$ for all i, j. Obviously, these definitions are independent of the choice of basis vectors in the elements. Clearly also, the statement that a tensor is invertible in an element is equivalent to the statement that it is orthogonal to the element with respect to every subset consisting of an odd number of its indices. The definition of invertibility is quite straightforward when the element is nonnull, so that ${}_{(i)}\zeta^\lambda$ and the ${}^{(j)}\eta^\lambda$ are linearly independent. It is slightly more subtle when the element is null, since there then exist directions common to these sets. The definition requires that such a direction be inverted when represented by a contravariant vector and left unaltered when represented by a covariant vector. In this way a tensor can be invertible even in a null element, although a group cannot be invertible on a null surface of transitivity.

A tensor is said to be orthogonal (with respect to a subset of indices) to a group or invertible in a group if it is orthogonal (with respect to the subset of indices) to the surfaces of transitivity or invertible in them respectively. Clearly, if a group is invertible, then any intrinsically defined tensor (such as the Ricci tensor or the Weyl tensor) must be invertible in it.

3. AN EXISTENCE THEOREM FOR LOCAL ISOMETRY HORIZONS WHERE AN ORTHOGONALLY TRANSITIVE GROUP HAS NULL SURFACES OF TRANSITIVITY

We can use the concepts of the previous section to proceed further with the question raised in Sec. 1.

Before doing so we explain our notation and state Frobenius's theorem, which is fundamental to questions of orthogonality. We use square brackets to denote antisymmetrization and round brackets for symmetrization; when two such operations are to be performed in a context where the order is important, we shall indicate the operation to be performed first by using boldface brackets as, e.g., $[\cdots \mathbf{[}\cdots]\cdots]$. We define the p vector generated by a set of vectors ${}_{(1)}\zeta^\mu, \cdots, {}_{(p)}\zeta^\mu$ as

$$w^{\kappa_1 \cdots \kappa_p} = {}_{(1)}\zeta^{[\kappa_1} \cdots {}_{(p)}\zeta^{\kappa_p]} \tag{2}$$

and define the orthogonal conjugate in n dimensions as

$$*w_{\mu_{p+1} \cdots \mu_n} = \frac{1}{p!}\, \epsilon_{\kappa_1 \cdots \kappa_p \mu_{p+1} \cdots \mu_n} w^{\kappa_1 \cdots \kappa_p}, \tag{3}$$

where $\epsilon_{\mu_1 \cdots \mu_n}$ is the alternating tensor. Frobenius's Theorem (see, e.g., Schouten[7]) states that a necessary

[7] J. A. Schouten, *Ricci Calculus* (Springer-Verlag, Berlin, 1954), p. 81.

and sufficient condition for a field of such p vectors to be orthogonal (locally) to a family of $(n-p)$-surfaces in n dimensions is

$$w^{[\kappa_1 \cdots \kappa_p ; \mu} w^{\nu] \lambda_2 \cdots \lambda_p} = 0. \tag{4}$$

It is convenient for future reference to have the expansion

$$w^{[\kappa_1 \cdots \kappa_p ; \mu} w^{\nu] \lambda_2 \cdots \lambda_p} = \frac{1}{p} \sum_{i=1}^{p} (-1)^{i-1} w^{[\kappa_1 \cdots \kappa_p}{}_{(i)} \zeta^{\mu ; \nu]} \times {}_{(1)}\zeta^{[\lambda_1} \cdots {}_{(i-1)}\zeta^{\lambda_i}{}_{(i+1)}\zeta^{\lambda_{i+1}} \cdots {}_{(p)}\zeta^{\lambda_p]}. \tag{5}$$

The following theorem (which covers the cases of the Schwarzschild and Kerr solutions) shows that LIH's may be expected to occur in a fairly wide class of circumstances.

Theorem 1: Let $\mathfrak{U}$ be an open subregion of an n-dimensional C^2 manifold with a C^1 pseudo-Riemannian metric, such that there is a continuous group of isometries whose surfaces of transitivity have constant dimension p $(1 \leq p \leq n-1)$ in $\mathfrak{U}$.

Let $\mathcal{N}$ be the subset (which must obviously be closed in $\mathfrak{U}$) where the surfaces of transitivity become null, and suppose that they are never more than singly null (i.e., the rank of the induced metric on the surfaces of transitivity drops from p to $p-1$ on $\mathcal{N}$, but is never lower).

Then, if the group is orthogonally transitive in $\mathfrak{U}$, it follows that $\mathcal{N}$ is the union of a family of non-intersecting hypersurfaces which are LIH's with respect to the group, and consequently (since $\mathcal{N}$ is closed) that the boundaries of $\mathcal{N}$ are members of the family.

Proof: In the neighborhood of any point in $\mathfrak{U}$ we choose a linearly independent set ${}_{(i)}\zeta^{\mu}$ $(i = 1, \cdots, p)$ of the Killing vectors generating the group, and form the Killing p vector tangent to the surfaces of transitivity

$$w^{\kappa_1 \cdots \kappa_p} = {}_{(1)}\xi^{[\kappa_1} \cdots {}_{(p)}\xi^{\kappa_p]}. \tag{6}$$

We now substitute this in the identity (5), make a further expansion of the right-hand side, and finally antisymmetrize the whole over the indices μ, ν, $\lambda_2, \cdots, \lambda_p$. Most of the terms then drop out, leaving the reduced identity

$$w^{[\kappa_1 \cdots \kappa_p ; [\mu} w^{\nu] \lambda_2 \cdots \lambda_p]} = \frac{2}{p(p+1)(p+2)} \Big\{ 2 w^{\kappa_1 \cdots \kappa_p ; [\mu} w^{\nu \lambda_2 \cdots \lambda_p]} - w^{\kappa_1 \cdots \kappa_p} w^{[\nu \lambda_2 \cdots \lambda_p ; \mu]} - 2 \sum_{i=1}^{p} {}_{(1)}\xi^{[\kappa_1} \cdots {}_{(i-1)}\xi^{\kappa_{i-1}}{}_{(i+1)}\xi^{\kappa_{i+1}} \cdots {}_{(p)}\xi^{\kappa_p} \times {}_{(i)}\xi^{(\kappa_i ; [\mu} w^{\nu \lambda_2 \cdots \lambda_p]} \Big\}. \tag{7}$$

Since the surfaces of transitivity are $(n-p)$-surface orthogonal, Eq. (4) holds, and so the left-hand side of Eq. (7) vanishes. Since the ${}_{(i)}\xi^{\mu}$ satisfy Killing's equation ${}_{(i)}\xi^{(\mu ; \nu)} = 0$, it follows that the last term vanishes also. This leaves the relation

$$2 w^{\kappa_1 \cdots \kappa_p ; [\mu} w^{\lambda_1 \cdots \lambda_p]} = w^{\kappa_1 \cdots \kappa_p} w^{[\lambda_1 \cdots \lambda_p ; \mu]}. \tag{8}$$

Contracting with $w_{\kappa_1 \cdots \kappa_p}$ and setting

$$W = \frac{1}{p!} w^{\kappa_1 \cdots \kappa_p} w_{\kappa_1 \cdots \kappa_p}, \tag{9}$$

we obtain the result

$$W^{;[\mu} w^{\lambda_1 \cdots \lambda_p]} = W w^{[\lambda_1 \cdots \lambda_p ; \mu]}. \tag{10}$$

We shall use the orthogonal conjugate form of this equation, i.e.,

$$W_{,\rho} \, {}^{*}w^{\rho \kappa_{p+2} \cdots \kappa_n} = W \, {}^{*}w^{\rho \kappa_{p+2} \cdots \kappa_n}{}_{;\rho}. \tag{11}$$

Now the vanishing of W at a point is a necessary and sufficient condition for the p surface of transitivity to be null there, or, in other words, $W = 0$ is the equation of the set $\mathcal{N}$.

Hence in the open region $\mathfrak{U} - \mathcal{N}$ we may divide by W to obtain

$$(\ln W)_{,\rho} \, {}^{*}w^{\rho \kappa_{p+2} \cdots \kappa_n} = {}^{*}w^{\rho \kappa_{p+2} \cdots \kappa_n}{}_{;\rho}. \tag{12}$$

Since the right-hand side is continuous in $\mathfrak{U}$, this equation may be interpreted as implying that the left-hand side is locally bounded in $\mathfrak{U} - \mathcal{N}$.

Now let us restrict attention to a particular one of the orthogonal $(n-p)$-surfaces. Suppose that this surface lies partly in $\mathcal{N}$ and partly outside. Then in the neighborhood of any point on the boundary ln W must be unbounded, and consequently the restriction of its gradient to the $(n-p)$-surface must be unbounded. But ${}^{*}w^{\kappa_{p+1} \cdots \kappa_n}$ is the tangent element to the orthogonal $(n-p)$-surface and is locally non-vanishing. Thus (12) implies that the restriction of the gradient of ln W to the $(n-p)$-surface is bounded, contrary to the deduction we have just made. It follows that if any part of one of the orthogonal $(n-p)$-surfaces lies in $\mathcal{N}$, then the whole of it must lie in $\mathcal{N}$.

Consider one such $(n-p)$-surface through a point P in $\mathcal{N}$. At each point on this surface $w^{\kappa_1 \cdots \kappa_p}$ and ${}^{*}w^{\kappa_{p+1} \cdots \kappa_n}$ together generate an $(n-1)$ element, since, being singly null, they have a unique (null) direction in common. Therefore, by dragging along the $(n-p)$-surface under the operations of the group, we obtain a uniquely defined null hypersurface through P which is contained in $\mathcal{N}$. Its null geodesic generators lie everywhere in $w^{\kappa_1 \cdots \kappa_p}$ and consequently are trajectories of the group. They cannot intersect since otherwise the member of the family passing through a point of intersection would not be unique.

We remark on a few points arising from this theorem.

(1) In Lorentz spaces (i.e., those with signature $n-2$), and in general relativity in particular, the restriction that the p-surfaces should be at most singly null is unnecessary, since higher nullity is not possible in these spaces anyway.

(2) When $p = n-1$, the orthogonality condition is automatically satisfied, and the conclusion of the theorem is also a trivial result.

(3) When $p = n-1$, and also when $p = 1$, a converse theorem holds as a trivial result. The converse theorem may be stated as follows: If $\mathcal{K}$ is an LIH with respect to a group which is transitive over p-surfaces in n dimensions, then these p-surfaces are $(n-p)$-surface orthogonal on $\mathcal{K}$. However, this converse does not hold for the intermediate values $p = 2, \cdots, n-2$.

In the case $n = 4$, $p = 2$, a simple counterexample is given by the space (which has Lorentz signature when $x < 1$) with metric

$$ds^2 = dx^2 + dy^2 + dz^2 - 2\,dx\,dt + 2y\,dz\,dt - (x - y^2)\,dt^2. \quad (13)$$

Here $x = 0$ is an LIH with respect to the group generated by $\partial/\partial t$ and $\partial/\partial z$. Nevertheless, the Killing bivector $\partial/\partial t \wedge \partial/\partial z$ is not 2-surface orthogonal at $x = 0$.

(4) Most commonly, $\mathcal{N}$ will consist of discrete hypersurfaces separating regions of positive and negative W, i.e., regions where the Killing p-vector is nonnull and contains, respectively, an even and an odd number of independent orthogonal timelike directions (or more simply, in a Lorentz space, where the Killing p-vector is, respectively, spacelike and timelike).

A special case, which also arises commonly, is the situation where two such hypersurfaces have coalesced to give one, so that W has the same sign on both sides and has vanishing gradient on the hypersurface.

These possibilities are very well displayed in the hybrid Kerr–Reissner–Nordstrom solution.[8] The metric form in which it was discovered is

$$\begin{aligned} ds^2 = {} & \rho^2\,d\theta^2 + 2a\sin^2\theta\,dr\,d\varphi - 2\,dr\,du \\ & + \{r^2 + a^2 + (2mr - e^2)\rho^{-2}a^2\sin^2\theta\}\sin^2\theta\,d\varphi^2 \\ & - 2a(2mr - e^2)\rho^{-2}\sin^2\theta\,d\varphi\,du \\ & - \{1 - (2mr - e^2)\rho^{-2}\}\,du^2, \end{aligned} \quad (14)$$

where $\rho^2 = r^2 + a^2\cos^2\theta$, and the parameters m, e, ma, and ea are to be interpreted as the mass, charge, angular momentum, and magnetic dipole moment, respectively. Here, and in applications to general relativity throughout this paper, the units are understood to be such that the speed of light c and Newton's gravitational constant γ are both unity.

The Killing bivector $\partial/\partial\varphi \wedge \partial/\partial u$ is 2-surface orthogonal. It becomes null on the hypersurface where $\Delta \equiv r^2 - 2mr + e^2 + a^2 = 0$. Consequently, Theorem 1 implies that the hypersurfaces $\Delta = 0$ are LIH's.

The orthogonality is not immediately apparent in the above coordinate system, but, according to the result demonstrated in Sec. 1, a manifestly invertible coordinate system must exist. It may be obtained explicitly by using the generalized Boyer–Lindquist[9] transformation:

$$dt = -du - (r^2 + a^2)\Delta^{-1}\,dr, \quad d\phi = d\varphi + a\Delta^{-1}\,dr,$$

giving the invertible form

$$\begin{aligned} ds^2 = {} & \rho^2\Delta^{-1}\,dr^2 + \rho^2\,d\theta^2 \\ & + \{r^2 + a^2 + (2mr - e^2)\rho^{-2}a^2\sin^2\theta\}\sin^2\theta\,d\phi^2 \\ & + 2a(2mr - e^2)\rho^{-2}\sin^2\theta\,d\phi\,dt \\ & - \{1 - (2mr - e^2)\rho^{-2}\}\,dt^2. \end{aligned} \quad (15)$$

This form necessarily fails when the Killing bivector becomes null, but the orthogonality is patent elsewhere and it can be deduced by continuity that it holds where $\Delta = 0$ also.

The general and special cases mentioned above correspond to distinct and continuous roots of Δ. When there are no real roots, there are no LIH's. These different cases give rise to significant differences in the global topology (see the diagrams in Carter[10]), which can be applied qualitatively to the charged case provided it is noted that the discriminant of Δ is changed from $m^2 - a^2$ to $m^2 - a^2 - e^2$, and provided $a^2 \neq 0$; when $a^2 = 0$, the appropriate topological diagrams are also given by Carter[11]). In this paper we are not concerned with global matters, but it is the intimate connection between large-scale topology and LIH's which provides one of the motives for studying the latter.

4. EXISTENCE OF A KILLING HORIZON WHERE AN ORTHOGONALLY TRANSITIVE ABELIAN GROUP HAS NULL SURFACES OF TRANSITIVITY

If we are dealing with an Abelian group, the conclusion of Theorem 1 may be considerably strengthened.

Corollary to Theorem 1: Let the postulates of Theorem 1 be satisfied. Then if in addition the group

[8] E. Newman, E. Couch, K. Chinnapared, A. Exton, A. Prakash, and R. Torrence, J. Math. Phys. **6**, 918 (1965).

[9] R. H. Boyer and R. W. Lindquist, J. Math. Phys. **8**, 265 (1967).

[10] B. Carter, Phys. Rev. **141**, 1242 (1966).

[11] B. Carter, Phys. Letters **21**, 243 (1966).

is Abelian, it follows that each of the resulting LIH's is a Killing horizon.

Proof: Consider one of the resulting LIH's and let its null generator be l^μ. Since l^μ lies in the surface of transitivity of the group, we have

$$l^\mu = {}^{(i)}\alpha\ {}_{(i)}\xi^\mu, \tag{16}$$

where the set of scalars ${}^{(i)}\alpha$ is determined up to a constant of proportionality. In order to show that this LIH has a Killing vector field coinciding with its null generator, we need to show that the factor of proportionality may be chosen so that the ${}^{(i)}\alpha$ are constant in the LIH.

Since the surface of transitivity is only singly null, the direction of l^μ is fully determined by the condition that it be orthogonal to the surface of transitivity, i.e., $l_\mu w^{\mu\nu_2\cdots\nu_p} = 0$; thus substituting from (14) we find that the ${}^{(i)}\alpha$ are determined by

$$a_{(i)(j)}\,{}^{(j)}\alpha = 0; \quad a_{(i)(j)} = {}_{(i)}\xi^\mu\,{}_{(j)}\xi_\mu. \tag{17}$$

The solution of these equations is given by

$${}^{(i)}\alpha = kA^{(i)(j)}, \quad \text{for fixed } j, \tag{18}$$

where k is an arbitrary constant of proportionality and $A^{(j)(j)}$ is the cofactor of $a_{(i)(j)}$. Since $a_{(i)(j)}$ is singly null, its adjoint has rank 1 (by a well-known theorem of Jacobi) and therefore this set of solutions is nonvanishing for some values of j and is the same for all such values. For convenience we take $j = p$, reordering the labels if necessary in order to obtain a nonvanishing result.

We need to show that each of the ratios ${}^{(i)}\alpha$ to ${}^{(k)}\alpha$ is constant in the LIH. Since the Killing vectors commute, this is true automatically in the surfaces of transitivity and so we need only show that the ratios do not vary in orthogonal directions, i.e., that

$${}^{[(k)}\alpha^{(i)]}\alpha_{,[\rho}w_{\nu_1\cdots\nu_p]} = 0. \tag{19}$$

Hence, by (18), we have established the required result if we can prove

$$A^{[(\kappa)|(p)|}A^{(i)](p)}{}_{,[\rho}w_{\nu_1\cdots\nu_p]} = 0. \tag{20}$$

The cofactors are given explicitly by

$$A^{(i)(p)} = (-1)^{i+p}(p-1)!\ {}_{(1)}\xi_{\kappa_1}\cdots{}_{(i-1)}\xi_{\kappa_{i-1}} \times {}_{(i+1)}\xi_{\kappa_1}\cdots{}_{(p)}\xi_{\kappa_{p-1}}\,{}_{(1)}\xi^{[\kappa_1}\cdots{}_{(p-1)}\xi^{\kappa_{p-1}]}. \tag{21}$$

Therefore, using Killings equations ${}_{(i)}\xi_{(\mu;\nu)} = 0$ and the commutation conditions

$${}_{(i)}\xi_{\mu;\nu}\,{}_{(j)}\xi^\nu = {}_{(j)}\xi_{\mu;\nu}\,{}_{(i)}\xi^\nu,$$

we obtain

$$A^{(i)(p)}{}_{,\rho} = 2(-1)^{i+p}(p-1)! \times {}_{(1)}\xi_{\kappa_1}\cdots{}_{(i-1)}\xi_{\kappa_{i-1}}\,{}_{(i+1)}\xi_{\kappa_i}\cdots{}_{(p)}\xi_{\kappa_{p-1}} \times \sum_{j=1}^{p-1}{}_{(i)}\xi^{[\kappa_1}\cdots{}_{(j)}\xi^{\kappa_j}{}_{;\rho}\cdots{}_{(p-1)}\xi^{\kappa_{p-1}]}. \tag{22}$$

Again substituting (6) into the orthogonality conditions (4) and using the expansion (5), we see that the orthogonality conditions are equivalent to

$${}_{(j)}\xi^{[\sigma;\rho}w^{\nu_1\cdots\nu_p]} = 0 \quad (\text{each } j). \tag{23}$$

On expansion this gives

$$2\,{}_{(j)}\xi^\sigma{}_{;[\rho}w_{\nu_1\cdots\nu_p]} = \sum_{l=1}^{p}(-1)^l\,{}_{(l)}\xi^\sigma \times {}_{(j)}\xi_{[\rho;\nu_1}\,{}_{(i)}\xi_{\nu_2}\cdots{}_{(l-1)}\xi_{\nu_l}\,{}_{(l+1)}\xi_{\nu_{l+1}}\cdots{}_{(p)}\xi_{\nu_p]}. \tag{24}$$

Consequently we deduce that

$$\begin{aligned}
&2\sum_{j=1}^{p}{}_{(1)}\xi^{[\kappa_1}\cdots{}_{(j)}\xi^{\kappa_j}{}_{;[\rho}\cdots{}_{(p-1)}\xi^{\kappa_{p-1}]}w_{\nu_1\cdots\nu_p]} \\
&= {}_{(1)}\xi^{[\kappa_1}\cdots{}_{(p-1)}\xi^{\kappa_{p-1}]} \\
&\quad\times\sum_{j=1}^{p-1}(-1)^j{}_{(j)}\xi_{[\rho;\nu_1}\,{}_{(1)}\xi_{\nu_2}\cdots{}_{(j-1)}\xi_{\nu_j}\,{}_{(j+1)}\xi_{\nu_{j+1}}\cdots{}_{(p)}\xi_{\nu_p]} \\
&\quad-\sum_{j=1}^{p-1}(-1)^j\,{}_{(1)}\xi^{[\kappa_1}\cdots{}_{(j-1)}\xi^{\kappa_{j-1}}\,{}_{(j+1)}\xi^{\kappa_j}\cdots{}_{(p)}\xi^{\kappa_{p-1}]} \\
&\quad\times{}_{(j)}\xi_{[\rho;\nu_1}\,{}_{(1)}\xi_{\nu_2}\cdots{}_{(p-1)}\xi_{\nu_p]}.
\end{aligned} \tag{25}$$

Substituting into (22) and using (21), we obtain

$$\begin{aligned}
&A^{(i)(p)}{}_{,[\rho}w_{\nu_1\cdots\nu_p]} \\
&\quad= A^{(i)(p)}\sum_{j=1}^{p-1}(-1)^j{}_{(j)}\xi_{[\rho;\nu_1} \\
&\qquad\times{}_{(1)}\xi_{\nu_2}\cdots{}_{(j-1)}\xi_{\nu_j}\,{}_{(j+1)}\xi_{\nu_{j+1}}\cdots\xi_{\nu_p]} \\
&\qquad-(-1)^p\sum_{j=1}^{p}A^{(i)(j)}\xi_{[\rho;\nu_1}\xi_{\nu_2}\cdots\xi_{\nu_{p-1}]}.
\end{aligned} \tag{26}$$

When this is substituted into the left-hand side of (20), it can be seen that each of the terms has as a factor a 2×2 minor of the adjoint matrix $A^{(i)(j)}$. The terms must therefore vanish since, as has been already remarked, this matrix has rank 1. Thus (20) is true and the result is established.

We can apply this result to the charged Kerr solution. In terms of the metric form (14) with coordinates numbered from 1 to 4 in the order r, θ, φ, u, we find that the normal to the hypersurface $\Delta = 0$ has covariant components $l_\mu = \delta^1_\mu$. We can use the inverse metric given in Ref. 8 to obtain the contravariant components of the null generator:

$$l^\mu = \rho^{-2}\{\Delta\delta^\mu_1 - a\delta^\mu_3 - (r^2+a^2)\delta^\mu_4\}.$$

On the surface $\Delta = 0$, r takes constant values $r_\pm$.

Therefore we see that the null generator can be normalized so as to coincide with the Killing vector $\alpha(\partial/\partial\varphi) + (r_{\pm}^2 + a^2)\partial/\partial u$.

It should not be concluded from the result of this section that any null hypersurface which is an LIH with respect to an Abelian group is also a Killing horizon. A counterexample is provided by the metric described in note (3) after Theorem 1. It contains an LIH at $r = 0$ with respect to the Abelian group generated by $\partial/\partial z$ and $\partial/\partial t$. However, since the orthogonal transitivity condition does not hold, there is no reason why it should be also a Killing horizon, and indeed it is not. The null generator is $\partial/\partial t - y\partial/\partial z$. Therefore it cannot be normalized so as to coincide with any Killing vector field.

5. ORTHOGONAL TRANSITIVITY AND INVERTIBILITY OF AN $(n-2)$-PARAMETER ABELIAN ISOMETRY GROUP WITH INVERTIBLE RICCI TENSOR

It is worthwhile to enquire when orthogonal transitivity and invertibility are likely to occur, not only because of their connection with LIH's, but also because they give rise to useful simplifications generally. Since in fact a large proportion of the known solutions of the general relativity equations have been obtained with the aid of various preassumed invertibility conditions (usually introduced with no other justification than algebraic convenience), it would probably be helpful in the future to know when such assumptions are reasonable and when they involve undesired restrictions.

One might also ask the specific question whether the orthogonal transitivity of the Kerr–Reissner–Nordstrom solution is merely a convenient algebraic coincidence, or whether there is a deeper reason for it.

Papapetrou has pointed out[12] that in the uncharged case there is a deeper reason, since he has shown that any stationary axisymmetric space–time satisfying the empty-space equations (i.e., vanishing Ricci tensor) in a region including the axis of symmetry must be orthogonally transitive in that region.

The objective of this section is to show that this rather striking result is a special case of a theorem with considerably wider significance. Thus Papapetrou's result can be extended in several directions: to a wider class of groups, to cases where the condition that the Ricci tensor vanishes is replaced by the very much weaker condition that it be invertible with respect to the group (which covers the charged case above), and to cases where the region under consideration does not include a symmetry axis but satisfies certain alternative conditions (an aspect which is further developed in Sec. 6).

When the general question of orthogonal transitivity of a p-transitive group in n dimensions is examined, it turns out that, for $p = n - 1$, the problem is trivial as has already been remarked, while for $p < n - 3$ the problem becomes very complicated, as it does even for $p = n - 2$ in the non-Abelian case. Therefore in the remainder of this paper we only attempt to deal with Abelian groups, and we are soon obliged to make the restriction $p = n - 2$.

Our results depend on the following lemma which gives a connection between the orthogonality condition and the Ricci tensor.

Lemma: Let $w^{\lambda_1 \cdots \lambda_p} = {}_{(1)}\xi^{[\lambda_1} \cdots {}_{(p)}\xi^{\lambda_p]}$, where ${}_{(1)}\xi^{\lambda}, \cdots, {}_{(p)}\xi^{\lambda}$ are a set of generators of a p-parameter Abelian isometry group on an n-dimensional C^3 manifold with C^2 metric. Then

$$\{w^{[\lambda_1 \cdots \lambda_p}\xi^{\mu;\rho]}\}_{;\rho} = \frac{2}{p+2}\, w^{[\lambda_1 \cdots \lambda_p} R^{\mu]}{}_{\rho}\, {}_{(i)}\xi^{\rho}, \qquad i = 1, \cdots, p, \quad (27)$$

where R_{ν}^{μ} is the Ricci tensor.

Proof: For any set of C^2 vector fields,

$$\begin{aligned}
&{}_{(1)}\xi^{\mu}, \cdots, {}_{(p)}\xi^{\mu}\binom{p+2}{3}\,{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\,{}_{(p)}\xi^{\lambda_p}\,{}_{(p)}\xi^{\lambda_{p+1};\rho]} \\
&= \binom{p+1}{2}\,{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\,{}_{(p)}\xi^{[\lambda_p}\,{}_{(p)}\xi^{\lambda_{p+1}];\rho]} \\
&\quad + \frac{1}{(p-1)}\binom{p+1}{3}\sum_{i=1}^{p-1}(-1)^{p-i} \\
&\quad \times {}_{(1)}\xi^{[\lambda_1} \cdots {}_{(i)}\xi^{|\rho|} \cdots {}_{(p-1)}\xi^{\lambda_{p-2}}\,{}_{(p)}\xi^{\lambda_{p-1}}\,{}_{(p)}\xi^{\lambda_p;\lambda_{p+1}]}.
\end{aligned} \quad (28)$$

When we take the contracted derivative and make suitable rearrangements, we obtain the identity

$$\begin{aligned}
&(p+2)\{{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\,{}_{(p)}\xi^{\lambda_p}\,{}_{(p)}\xi^{\lambda_{p+1};\rho]}\}_{;\rho} \\
&= 3\,{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\{{}_{(p)}\xi^{[\lambda_p}\,{}_{(p)}\xi^{\lambda_{p+1}];\rho]}\}_{;\rho} \\
&\quad + 3\sum_{i=1}^{p-1}{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(i)}\xi^{\lambda_i}{}_{;\rho} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\xi^{[\lambda_p}\xi^{\lambda_{p+1}];\rho]} \\
&\quad - \sum_{i=1}^{p-1}{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(i)}\xi^{|\rho|} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\{{}_{(p)}\xi^{\lambda_i}\,{}_{(p)}\xi^{\lambda_p;\lambda_{p+1}]}\}_{;\rho} \\
&\quad - \sum_{i=1}^{p-1}{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(i)}\xi^{|\rho|}{}_{;\rho} \cdots {}_{(p-1)}\xi^{\lambda_{p-1}}\,{}_{(p)}\xi^{\lambda_i}\,{}_{(p)}\xi^{\lambda_p;\lambda_{p+1}]} \\
&\quad + 2\sum_{i=2}^{p-1}\sum_{j=1}^{i-1}(-1)^{i-j-1} \\
&\quad \times {}_{(1)}\xi^{[\lambda_1} \cdots {}_{(j-1)}\xi^{\lambda_{j-1}}\,{}_{(j+1)}\xi^{\lambda_{j+1}} \cdots {}_{(i-1)}\xi^{\lambda_{i-2}} \\
&\quad \times {}_{(i+1)}\xi^{\lambda_{i-1}} \cdots {}_{(p-1)}\xi^{\lambda_{p-3}}\,{}_{[(i)}\xi^{\lambda_{p-2}}{}_{;\rho}\,{}_{(j)]}\xi^{|\rho|} \\
&\quad \times {}_{(p)}\xi^{\lambda_{p-1}}\,{}_{(p)}\xi^{\lambda_p;\lambda_{p+1}]}.
\end{aligned} \quad (29)$$

[12] A. Papapetrou, Ann. Inst. H. Poincaré A-IV, 83 (1966).

We now use the condition that the ${}_{(i)}\xi^{\mu}$ commute with each other,

$$\underset{[(i)\xi^{\rho}]}{\pounds}\,{}_{(i)}\xi^{\mu} \equiv 2\,{}_{[(i)}\xi^{\mu}{}_{;\rho}\,{}_{(j)]}\xi^{\rho} = 0. \tag{30}$$

This implies that the last term in (29) vanishes. Applying Killing's equation ${}_{(i)}\xi^{(\mu;\nu)} = 0$, we deduce that ${}_{(i)}\xi^{\rho};\rho = 0$ and hence that the second last term in (29) vanishes. Combining Killing's equation with (30) we obtain

$$\underset{[(i)\xi^{\rho}]}{\pounds}\left\{{}_{(p)}\xi^{[\lambda}\,{}_{(p)}\xi^{\mu;\nu]}\right\} \equiv \left\{{}_{(p)}\xi^{[\lambda}\,{}_{(p)}\xi^{\mu;\nu]}\right\}_{;\rho}\,{}_{(i)}\xi^{\rho} - 3\,{}_{(i)}\xi^{[\lambda}{}_{;\rho}\,{}_{(p)}\xi^{[\mu}\,{}_{(p)}\xi^{\nu];\rho]} = 0, \tag{31}$$

from which it follows that the third and fourth last terms in (29) cancel each other out.

Since we could have singled out any one of the ${}_{(i)}\xi^{\mu}$ $(i = 1, \cdots, p-1)$ instead of ${}_{(p)}\xi^{\mu}$, it follows that for each i we have

$$\left\{W^{[\lambda_1 \cdots \lambda_p}\,{}_{(i)}\xi^{\mu;\rho]}\right\}_{;\rho} = \frac{3}{p+2}\,{}_{(1)}\xi^{[\lambda_1} \cdots {}_{(i-1)}\xi^{\lambda_{i-1}}\,{}_{(i+1)}\xi^{\lambda_{i+1}} \cdots {}_{(p)}\xi^{\lambda_p} \times \left\{{}_{(i)}\xi^{[\lambda_i}\,{}_{(i)}\xi^{\mu];\rho]}\right\}_{;\rho}. \tag{32}$$

At this stage we introduce the Riemann and Ricci tensors defined by

$$\zeta_{\mu;[\nu\rho]} = \tfrac{1}{2}R^{\sigma}{}_{\mu\nu\rho}\zeta_{\sigma}; \quad R_{\mu\nu} = R_{\mu\rho}{}^{\rho}{}_{\nu}. \tag{33}$$

If we substitute any Killing vector ${}_{(i)}\xi^{\mu}$ in (33) and use the full Riemann-tensor symmetries together with Killing's equation, we obtain

$${}_{(i)}\xi^{\mu;\nu\rho} = R^{\mu\nu\rho}{}_{\sigma}\,{}_{(i)}\xi^{\sigma}. \tag{34}$$

Contracting Eq. (21) gives

$${}_{(i)}\xi^{\mu;\rho}{}_{;\rho} = R^{\mu}{}_{\rho}\,{}_{(i)}\xi^{\rho}. \tag{35}$$

From (22), with further use of Killing's equation, we can deduce

$$\left\{{}_{(i)}\xi^{[\mu}\,{}_{(i)}\xi^{\nu;\rho]}\right\}_{;\rho} = \tfrac{2}{3}\,{}_{(i)}\xi^{[\mu}R^{\nu]}{}_{\rho}\,{}_{(i)}\xi^{\rho}. \tag{36}$$

Finally, insertion of (36) into Eq. (32) gives Eq. (27), which is the desired result.

It is convenient to work with the orthogonal conjugate form of Eq. (27), i.e.,

$$(n-p-1)\,{}_{(i)}\chi_{[\kappa_{p+3}\cdots\kappa_n;\sigma]} = 2\,{}_{(i)}\xi^{\rho}R_{\rho}{}^{\mu}\,{}^{*}W_{\mu\kappa_{p+3}\cdots\kappa_n\sigma}, \tag{37}$$

where we have introduced a set of twist tensors ${}_{(i)}\chi_{\kappa_{p+3}\cdots\kappa_n}$ $(i = 1, \cdots, p)$ by

$${}_{(i)}\chi_{\kappa_{p+3}\cdots\kappa_n} = {}_{(i)}\xi^{\mu;\rho}\,{}^{*}W_{\mu\rho\kappa_{p+3}\cdots\kappa_n}. \tag{38}$$

The significance of the twist tensors can be seen by taking the orthogonal conjugate of Eq. (23). Thus Frobenius's Theorem may be expressed in the following alternative form: The elements spanned by ${}_{(1)}\xi^{\rho}, \cdots, {}_{(p)}\xi^{\mu}$ are orthogonal to a family of $(n-p)$-surfaces if and only if all the corresponding twist tensors vanish.

The utility of Eqs. (37) lies in the fact that the right-hand sides vanish for all i if and only if the Ricci tensor is invertible in the p element. However, as the equations control only the rotation of the twist tensors, this restriction is not very strong except when $p \geq n-2$, so that the twist tensors reduce to scalars or vanish trivially. This is why, in order to make further progress, we consider only $p = n-2$. Thus we now reach the main result of this section.

Theorem 2: Let $\mathfrak{D}$ be a connected open subdomain of an n-dimensional C^3 manifold with a C^2 pseudo-Riemannian metric and an Abelian $(n-2)$-parameter isometry group, whose surfaces of transitivity, which in general are $(n-2)$-dimensional, become degenerate on a subset $\mathfrak{F}$ where the group has fixed points.

Then the group will be orthogonally transitive everywhere in $\mathfrak{D}$, and consequently invertible in $\mathfrak{D}$, except where the surfaces of transitivity are null, provided that:

(I) The Ricci tensor is invertible in the group everywhere in $\mathfrak{D}$; and

(II) one of the following holds:

(a) $\mathfrak{F}$ is nonempty;

(b) there is a discrete isometry in some neighborhood in $\mathfrak{D}$ consisting of an inversion in a direction orthogonal to the surfaces of transitivity (in other words, an inversion about a hypersurface to which the surfaces of transitivity are tangent);

(c) it is known, for any other reason, that the group is orthogonally transitive on at least one point in $\mathfrak{D}$.

Proof: Let ${}_{(i)}\xi^{\mu}$, $i = 1, \cdots, n-2$ be a set of independent generators of the group. Then the corresponding twist tensors ${}_{(i)}\chi$ are scalars and, by the preceding work, they satisfy

$${}_{(i)}\chi_{,\sigma} = 2\,{}_{(i)}\xi^{\rho}R_{\rho}{}^{\mu}\,{}^{*}W_{\mu\sigma}. \tag{39}$$

As has already been remarked, the invertibility of the Ricci tensor implies the vanishing of the right-hand side, and so we see that the ${}_{(i)}\chi$ are constant in $\mathfrak{D}$.

Thus the group will be orthogonally transitive everywhere in $\mathfrak{D}$, provided that these constants are all zero. This establishes the result when (c) holds.

To check condition (b) we observe that if there is an inversion isometry in some direction, then it follows, when the direction is orthogonal to the surfaces of transitivity, that the tensors ${}_{(i)}\xi^{\mu;\nu}$ are also invertible in this direction. In the case under consideration, Eq. (38) reduces to

$$ {}_{(i)}\chi = {}_{(i)}\xi^{\mu;\rho} *w_{\mu\rho}, \tag{40} $$

and invertibility of the ${}_{(i)}\xi^{\mu;\nu}$ in a direction orthogonal to the surfaces of transitivity implies that the right-hand side vanishes, leading to the required result.

To check condition (a) we need only to notice that on $\mathcal{F}$ the Killing p vector vanishes, and consequently the ${}_{(i)}\chi$ vanish there also by (40), giving the required result.

This theorem is useful for general relativity because of the physical significance of the conditions. Since the metric tensor is invertible in all circumstances, we could, if we wished, substitute the Einstein tensor for the Ricci tensor in the statement of Theorem 2 and substitute $-G_\mu{}^\rho$ for $R_\mu{}^\rho$ in Eqs. (37) and (39), where the Einstein tensor is defined by

$$ -G_\mu{}^\rho = R_\mu{}^\rho - \tfrac{1}{2}Rg_\mu{}^\rho \tag{41} $$

so that in general relativity, with units as for Eqs. (14) and (15), the energy–momentum tensor satisfies

$$ T_\mu{}^\rho = \frac{1}{8\pi} G_\mu{}^\rho. \tag{42} $$

Since $n = 4$ in ordinary space–time, the physical applications of the theorem are to 2-parameter groups. Several 2-parameter Abelian isometry groups have been used for idealized problems in general relativity, of which cylindrical symmetry is perhaps the most popular. However, the most important case is that of stationary axial symmetry, since this applies to large classes of finite astrophysical objects as a realistic approximation.

As an example of the application of Theorem 2 to this situation, we shall show that the original result of Papapetrou, which applied to solutions of the vacuum Einstein equations, is in fact equally valid for solutions of the source-free Einstein–Maxwell equations.

Let $F_{\mu\nu}$ be the electromagnetic-field tensor and let ${}_{(i)}\xi^\mu$, $i = 1, 2$, be the two commuting Killing vectors in the space. The Lie derivative of the electromagnetic-field tensor with respect to each of these must vanish, i.e.,

$$ \underset{[{}_{(i)}\xi^\rho]}{\mathcal{L}} F_{\mu\nu} \equiv F_{\mu\nu;\rho}\,{}_{(i)}\xi^\rho + 2F_{[\epsilon]\rho]}\,{}_{(i)}\xi^\rho{}_{\nu]} = 0, \tag{43} $$

from which, using the condition (17) that the Killing vectors commute, we obtain

$$ \{F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu\}_{;\sigma} = 3F_{[\mu\nu;\sigma]}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu. \tag{44} $$

Similarly, we can obtain two equations identical to (30) and (31), except that $F_{\mu\nu}$ is replaced by its orthogonal conjugate $*F_{\mu\nu}$. Maxwell's equations take the form

$$ F_{[\mu\nu;\sigma]} = 0, \tag{45} $$

$$ *F_{[\mu\nu;\sigma]} = (4\pi/3)\, *j_{\mu\nu\sigma}, \tag{46} $$

where j^μ is the current vector, and so we obtain

$$ \{F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu\}_{;\sigma} = 0, \tag{47} $$

$$ \{*F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu\}_{;\sigma} = 4\pi\, *j_{\mu\nu\sigma}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu. \tag{48} $$

Equation (34) implies that $F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu$ is always constant, while (48) implies that $*F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu$ is also constant when the right-hand side vanishes, which occurs if and only if the current vector lies in the 2-surface of transitivity. Therefore, if these two quantities vanish at any point in a connected region satisfying this condition, and in particular if there is a symmetry axis within the region where one of the Killing vectors vanishes, then they vanish everywhere in the region, i.e.,

$$ F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu = *F_{\mu\nu}\,{}_{(1)}\xi^\mu\,{}_{(2)}\xi^\nu = 0. \tag{49} $$

This is the condition that the tensor $F_{\mu\nu}$ be skew invertible, i.e., that it be affected only by an overall change of sign when the senses of the Killing vectors are simultaneously inverted. Since the energy momentum tensor of the electromagnetic field is homogeneous quadratic in the electromagnetic field tensor $F_{\mu\nu}$, it follows that condition (49) implies that the energy–momentum tensor is invertible, and consequently, when no matter other than the electromagnetic field is present, that the Einstein tensor is invertible so that the conditions of Theorem 2 are satisfied.

Thus from Theorem 2 we deduce the following result:

If the vacuum Einstein–Maxwell equations are satisfied in a connected region of a 4-dimensional space–time with a 2-parameter Abelian group, if a symmetry axis is present in the region, and if the source current is parallel to the 2-surfaces of transitivity (and, in particular, if there is no source current, as is usually assumed to be the case when no ponderable matter is present), then the group is orthogonally transitive.

When no electromagnetic field is present, this reduces to Papapetrou's result. The more general result shows that the orthogonal transitivity of the Kerr–Reissner–Nordstrom solution could have been predicted at once, even though it was not immediately apparent in the original form (12) of the solution.

6. CONVECTIVE CIRCULATION

We have not yet fully exploited the information in Eq. (39). In order to do so, we make some further definitions with ultimate astrophysical applications in mind.

A vector is said to be nonconvective with respect to an isometry group if it is invertible in the element orthogonal to the surface of transitivity at a point; otherwise it is said to be convective; i.e., it is nonconvective if and only if it is tangent to the surface of transitivity.

We define the flux vector of a group as the two-index quantity

$$ {}_{(i)}F^{\mu} = \frac{1}{8\pi}\, {}_{(i)}\xi^{\rho} G_{\rho}{}^{\mu}, \tag{50} $$

where the ${}_{(i)}\xi^{\rho}$ are a set of generators of the group. This quantity transforms as an ordinary vector with respect to μ in the manifold, and as a covariant vector with respect to (i) under a change of basis of the Lie algebra of the group. We say that the group is nonconvective if ${}_{(i)}F^{\mu}$ is nonconvective with respect to the group for each (i). We note that the statement that the group is nonconvective is invariant in the Lie algebra, and that it is equivalent to the statement that the Ricci tensor is invertible in the group.

Suppose that in an n-dimensional manifold with an Abelian isometry group transitive over p-surfaces, we have a finite segment $\mathcal{K}$ of an invariant hypersurface generated as follows. We take a finite segment $\mathcal{S}$ of an $(n-p-1)$-surface which cuts across the surfaces of transitivity, and drag it along under a set

$$ {}_{(1)}\xi^{\mu}, \cdots, {}_{(p)}\xi^{\mu} $$

of independent generators of the group by finite values, $\Delta\psi^{(1)}, \cdots, \Delta\psi^{(p)}$ of the group parameters where the group parameters $\psi^{(1)}, \cdots, \psi^{(p)}$ may be taken to be a set of functions defined on the space in such a manner that

$$ {}_{(i)}\xi^{\mu} = \partial x^{\mu}/\partial\psi^{(i)} \tag{51} $$

($x^1, \cdots, x^n$ being the coordinate patch in the manifold to which the tensor indices refer). Then we define the convective circulation through $\mathcal{K}$ as the surface integral of the normal component of the flux vector over $\mathcal{K}$. The circulation transforms as a covariant vector in the Lie algebra.

If $\mathcal{K}$ is generated by unit parameter changes $\Delta\psi^{(1)} = \cdots = \Delta\psi^{(p)} = 1$, we say that it is the unit hypersurface $\mathfrak{I}(\mathcal{S})$ through $\mathcal{S}$ and that the circulation over it is the unit convective circulation over $\mathcal{S}$, which we denote by ${}_{(i)}C(\mathcal{S})$. We see that ${}_{(i)}C(\mathcal{S})$ transforms as the product of a covariant vector and a density in the Lie algebra.

When $p = n - 2$, $\mathcal{S}$ will be a line. We can now state the following result.

Corollary to Theorem 2: Let the postulates of Theorem 2 be satisfied except for the conditions (I) and (II). Then the unit convective circulation between two points in $\mathfrak{D}$ is independent of the path over which it is taken; and if the group is orthogonally transitive at a point P in $\mathfrak{D}$, then it is orthogonally transitive at a point Q in $\mathfrak{D}$ if and only if the unit convective circulation over a path PQ between then vanishes.

Proof: By Eqs. (39) and the definitions (41) and (50) we have

$$ {}_{(i)}\chi_{,\sigma} = 16\pi\, {}_{(i)}F^{\mu}\, {}^{*}w_{\sigma\mu}. \tag{52} $$

Expanding this and expressing it in terms of differential forms, we obtain

$$ d\, {}_{(i)}\chi = \frac{16\pi}{(n-2)!}\, {}_{(i)}F^{\mu}\epsilon_{\kappa_1\cdots\kappa_{n-2}\sigma\mu}\, {}_{(1)}\xi^{[\kappa_1}\cdots{}_{(n-2)}\xi^{\kappa_{n-2}]}\, dx^{\sigma}. \tag{53} $$

Now by (51) we have

$$ dx^{\kappa_1}\wedge\cdots\wedge dx^{\kappa_{n-2}} = (n-2)!\, {}_{(1)}\xi^{[\kappa_1}\cdots{}_{(n-2)}\xi^{\kappa_{n-2}]}\, d\psi^{(1)}\wedge\cdots\wedge d\psi^{(n-2)}. \tag{54} $$

Therefore,

$$ {}_{(i)}F^{\mu}\, d\Sigma_{\mu} = \frac{(n-2)!}{16\pi(n-1)}\, d\psi^{(1)}\wedge\cdots\wedge d\psi^{(n-2)}\wedge d\, {}_{(i)}\chi, \tag{55} $$

where we have defined the $(n-1)$-form

$$ d\Sigma_{\mu} = \frac{1}{(n-1)!}\,\epsilon_{\kappa_1\cdots\kappa_{n-2}\sigma\mu}\, dx^{\kappa_1}\wedge\cdots\wedge dx^{\kappa_{n-2}}\wedge dx^{\sigma}. \tag{56} $$

To obtain the unit convective circulation between P and Q we integrate (35) over the unit hypersurface $\mathfrak{I}(PQ)$ which gives

$$ {}_{(i)}C(PQ) \equiv \int_{\mathfrak{I}(PQ)} {}_{(i)}F^{\mu}\, d\Sigma_{\mu} = \frac{(n-2)!}{16\pi(n-1)}\int_P^Q d\, {}_{(i)}\chi = \frac{(n-2)!}{16\pi(n-1)}\{{}_{(i)}\chi(Q) - {}_{(i)}\chi(P)\}. \tag{57} $$

We can see at once that the result is independent of the path PQ (even if $\mathfrak{D}$ is not simply connected), and that if ${}_{(i)}\chi$ vanishes at P, it will vanish at Q if and only if ${}_{(i)}C(P, Q)$ vanishes. This establishes the required result.

The mathematical significance of Theorem 2 and its corollary seems to be that, in the circumstances to which the results apply, the existence of orthogonal transitivity is controlled almost entirely by the Ricci tensor. One might have expected *a priori* that the Weyl tensor would be able to transmit the effects of noninvertibility of the Ricci tensor in a nearby region and thereby prevent orthogonal transitivity from obtaining in a region where locally the Ricci tensor is invertible. Our results show that this can in fact happen, but only in a very restricted way, governed by the total circulation.

As we have remarked, the most suitable application for these results in general relativity is to stationary axisymmetric rotating bodies. Let us consider, in such a case, a region where the Killing bivector is timelike. (For a simple situation, such a region would have to include the whole space, or else by Theorem 1 there would exist an LIH, with, in general, dramatic consequences.) Then locally it is possible to choose a pair of Killing fields generating the group such that one of them ${}_{(1)}\xi^{\mu}$ is timelike, and the other ${}_{(2)}\xi^{\mu}$ is spacelike. We can define momentum and stress flux vectors P^{μ} and Γ^{μ} by

$$P^{\mu} = {}_{(1)}F^{\mu} = {}_{(1)}\xi^{\rho}T_{\rho}{}^{\mu}; \quad \Gamma^{\mu} = {}_{(2)}F^{\mu} = {}_{(2)}\xi^{\rho}T_{\rho}{}^{\mu}.$$

The convective components of P^{μ} and Γ^{μ} correspond to momentum across the surfaces of transitivity and shearing stress between the surfaces of transitivity, respectively. The corollary to Theorem 2 gives conservation equations for the convective components of P^{μ} and Γ^{μ}. They can be regarded as equations of conservation of momentum and balance of torque forces in the body. (Conservation of nonconvective components is trivial in consequence of the group.) The effects of gravitational potential energy and the adjustment of the correct radial factor in the torque are automatically taken care of by the varying magnitude of the Killing vector with which the energy momentum tensor is contracted.

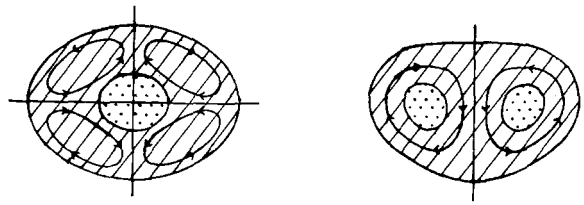

FIG. 1. Cross sections of two examples of stationary axisymmetric bodies are represented. The convective regions are shaded, with convective flow lines marked. The nonconvective regions are dotted, the only flow lines being directly into or out of the paper.

Figure 1 shows two simple examples of rotating bodies to which Theorem 2 and its corollary may be applied. We know at once in such cases that the group is orthogonally transitive in empty space outside the body, since the exterior must always contain part of the symmetry axis. (This is Papapetrou's result.) Now let us consider the interior. The first example is an object which has a nonconvective core, but which has a convective envelope containing two large convection cells, one on each side of a plane of equatorial symmetry. We can deduce that the group will be orthogonally transitive in the core either by applying condition (IIa), since the symmetry axis passes through the core, or by applying condition (IIb), since the equatorial plane also passes through the core. Hence, by the Corollary, the unit convective circulation over any line passing from the core to the outside must be zero. The second example is a smoke-ringlike object containing an annular nonconvective core about which the matter outside circulates; we conclude, by the corollary, that the group is certainly not orthogonally transitive in the annulus.

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High-Frequency Scattering by a Transparent Sphere. I. Direct Reflection and Transmission

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This is Paper I of a series on high-frequency scattering of a scalar plane wave by a transparent sphere (square potential well or barrier). It is assumed that $(ka)^{\frac{1}{3}} \gg 1$, $|N-1|^{\frac{1}{2}}(ka)^{\frac{1}{3}} \gg 1$, where k is the wavenumber, a is the radius of the sphere, and N is the refractive index. By applying the modified Watson transformation, previously employed for an impenetrable sphere, the asymptotic behavior of the exact scattering amplitude in any direction is obtained, including several angular regions not treated before. The distribution of Regge poles is determined and their physical interpretation is given. The results are helpful in explaining the reason for the difference in the analytic properties of scattering amplitudes for cutoff potentials and potentials with tails. Following Debye, the scattering amplitude is expanded in a series, corresponding to a description in terms of multiple internal reflections. In Paper I, the first term of the Debye expansion, associated with direct reflection from the surface, and the second term, associated with direct transmission (without any internal reflection), are treated, both for $N > 1$ and for $N < 1$. The asymptotic expansions are carried out up to (not including) correction terms of order $(ka)^{-2}$. For $N > 1$, the behavior of the first term is similar to that found for an impenetrable sphere, with a forward diffraction peak, a lit (geometrical reflection) region, and a transition region where the amplitude is reduced to generalized Fock functions. For $N < 1$, there is an additional shadow boundary, associated with total reflection, and a new type of surface waves is found. They are related to Schmidt head waves, but their sense of propagation disagrees with the geometrical theory of diffraction. The physical interpretation of this result is given. The second term of the Debye expansion again gives rise to a lit region, a shadow region, and a Fock-type transition region, both for $N > 1$ and for $N < 1$. In the former case, surface waves make shortcuts across the sphere, by critical refraction. In the latter one, they excite new surface waves by internal diffraction.

1. INTRODUCTION

This is the first in a series of papers dealing with the scattering of a plane wave by a transparent sphere at high frequencies. [A preliminary account of this work[1] and a survey of the main results[2] have already been given.] The assumptions are

$$\beta^{\frac{1}{3}} \gg 1, \quad |N-1|^{\frac{1}{2}}\beta^{\frac{1}{3}} \gg 1, \tag{1.1}$$

where

$$\beta = ka \tag{1.2}$$

is the dimensionless parameter associated with the wavenumber k and the radius a of the sphere, and N is the refractive index.

The lower limit on β for which the results are applicable depends on the degree of accuracy desired. It is hoped that they provide useful quantitative information down to $\beta \sim 100$ and at least qualitative information down to $\beta \sim 10$.

The sphere is assumed to be perfectly transparent, so that N is real. Both $N > 1$ and $N < 1$ are considered, but more attention is devoted to the former case. Additional limitations on N will be set in Paper II.[3] Extension of the results to complex values of N, to account for absorption, should not be unduly difficult.

As a rule, we shall also exclude

$$N \gg 1, \quad N \ll 1, \tag{1.3}$$

although the results can be at least partially applied in these cases. The reason for the second limitation in (1.1) will be discussed in Sec. 2. We note here that it implies

$$2\,|N-1|\,\beta \gg \beta^{\frac{1}{3}} \gg 1, \tag{1.4}$$

where the left-hand side is the phase shift of a central ray going through the sphere. This excludes the domain of Rayleigh–Gans scattering (where the Born approximation is applicable) and part of the anomalous diffraction region. The terminology is explained in Van de Hulst's beautiful book (Ref. 4, p. 133). In Van de Hulst's chart of the N–β domain (Ref. 4, Fig. 20), the region we treat corresponds to the right-hand side of the square, excluding the neighborhood of the corners.

For the sake of simplicity, we discuss only the scattering of a scalar field in the first two papers of this series. The whole treatment can be extended to electromagnetic scattering, as will be shown in the third paper.[5]

[1] H. M. Nussenzveig, Bull. Am. Phys. Soc. **11**, 372 (1966).
[2] H. M. Nussenzveig, to appear in *Proceedings of the Theoretical Physics Conference for R. E. Peierls's 60th Birthday.*
[3] H. M. Nussenzveig, J. Math. Phys. **10**, 125 (1969) (following paper), to be referred to hereafter as II.
[4] H. C. Van de Hulst, *Light Scattering by Small Particles* (John Wiley & Sons, New York, 1957).
[5] H. M. Nussenzveig (to be published); hereafter referred to as III.

The scalar wavefunction may be interpreted either as the velocity potential of sound waves or as the Schrödinger wavefunction in quantum mechanics. In the latter case, the problem corresponds to the scattering of nonrelativistic particles of momentum $p = \hbar k$ by a square potential well or barrier of radius a and depth (height) given by V_0,

$$V(r) = -V_0 \quad (0 \leq r < a);$$
$$V(r) = 0 \quad (r > a). \tag{1.5}$$

The refractive index is given by

$$N = [1 + (2mV_0/\hbar^2k^2)]^{\frac{1}{2}}, \tag{1.6}$$

where m is the mass of the particle. Note that $N > 1$ corresponds to a well and $N < 1$ to a barrier. This analogy, of course, is valid only at fixed energy, i.e., fixed k. For a fixed V_0, N is frequency-dependent (dispersion), while fixed N corresponds to an energy-dependent potential (V_0 proportional to the energy).

The extension of the present model to complex N may be of some interest in connection with the optical model in nuclear and high-energy physics. Of course, it would still be unrealistic in several respects: at high energies, inelastic and relativistic effects become important, and the simple potential-well picture no longer applies. Furthermore, some of the effects to be described depend on the existence of a sharp edge in the potential, which again might be unrealistic for nuclear forces. Nevertheless, we shall see that at least some of these effects appear to have analogs in the nuclear case.

We are dealing with a classic problem in scattering theory, the literature on which ranges over several decades.[6] An excellent survey up to 1957 is given by Van de Hulst.[4]

The exact solution of the electromagnetic problem in the form of a partial-wave series is usually associated with Mie.[7] As is well known, this series converges very slowly at high frequencies. One can then associate with the lth partial wave an "impact parameter"

$$p_l = (l + \tfrac{1}{2})/k, \tag{1.7}$$

and partial waves with $p_l \lesssim a$ are appreciably distorted, so that one has to keep at least β terms in the series. Experience with numerical computations has shown that the actual number of terms that must be retained is

$$l_+ \sim \beta + c\beta^{\frac{1}{3}}, \tag{1.8}$$

where c is a constant of order unity (empirically, $c \gtrsim 3$).

[6] N. A. Logan, Proc. I.E.E.E. **53**, 73 (1965).
[7] G. Mie, Ann. Physik **25**, 377 (1908).

This result can be understood in terms of the penetration of the centrifugal barrier up to the surface. The effective potential for radial motion is

$$U(r) = V(r) + \hbar^2 l(l + 1)/2mr^2, \tag{1.9}$$

where $V(r)$ is given by (1.5). [Actually, in order to apply the WKB approximation, $l(l + 1)$ should be replaced by $(l + \frac{1}{2})^2$.[8]] The discontinuity at $r = a$ gives rise to a barrier, and $p_l > a$, according to (1.7), corresponds to an energy below the top of this barrier. The transmissivity of the barrier up to $r = a - 0$ is then given by[8]

$$T_l = \frac{4N}{1 + N^2} \exp(2\psi_l), \tag{1.10}$$

where

$$\psi_l = -\int_\beta^{l+\frac{1}{2}} [(l + \tfrac{1}{2})^2 - x^2]^{\frac{1}{2}} \frac{dx}{x}. \tag{1.11}$$

In particular, near the top of the barrier, we find that

$$\psi_l \approx -\tfrac{1}{3}[2(l + \tfrac{1}{2} - \beta)/\beta^{\frac{1}{3}}]^{\frac{3}{2}}, \tag{1.12}$$

so that the transmissivity for $p_l > a$ is appreciable only within the range $\beta < l < l_+$.

The difficulty in employing the partial-wave expansion at high frequencies is apparent from (1.8). Nevertheless, in view of the practical importance of the problem, numerical computations have been carried out in this way up to values of β of the order of a few hundred. Besides the fact that computer calculations are no substitute for a physical understanding of the behavior of the solution, however, there are also practical difficulties: The results are very rapidly varying functions of β, N, and the scattering angle, so that very closely spaced points would be required for accurate interpolation.

Several approximation methods have been proposed to overcome these difficulties; they are reviewed in Ref. 4. The "localization principle" (1.7) leads to a subdivision of the terms of the partial-wave series into three domains:

(i) $$0 \leq l \lesssim l_- \sim \beta - c\beta^{\frac{1}{3}}; \tag{1.13}$$

(ii) $$l_- \lesssim l \lesssim l_+; \tag{1.14}$$

(iii) $$l_+ \lesssim l. \tag{1.15}$$

Partial waves in the domain (iii) are damped faster than exponentially by the centrifugal barrier and give a negligible contribution. The domain (i) gives rise to the forward diffraction peak, as well as to the contributions of reflected and refracted rays, according to geometrical optics (Ref. 4, Chap. 12).

[8] M. V. Berry, Proc. Phys. Soc. (London) **88**, 285 (1966).

The domain (ii) will be called the *edge domain*, because it corresponds to incident rays passing close to the "edge" of the sphere. We have already seen that the transmissivity of the centrifugal barrier is still appreciable for $\beta < l < l_+$. The domain $l_- < l < \beta$ corresponds to near-grazing incidence, so that strong reflection occurs, as well as strong interference between incident and reflected waves (Ref. 4, Sec. 17.21). We shall see that the edge domain gives rise to some of the most interesting effects.

According to classical mechanics, a particle with $l + \frac{1}{2} \sim \beta$ would have vanishing radial velocity at $r = a$, and it might be expected to circle indefinitely around the scatterer, a phenomenon known as *orbiting*.[9] We shall see that the edge domain indeed gives rise to surface waves, circling around the sphere any number of times. In addition, for $N > 1$, they can also penetrate through the sphere, leading to several striking effects, as will be seen later.

The most far-reaching attempts to derive the high-frequency asymptotic behavior of the exact solution have been based upon Watson's transformation.[10–12] However, the results have never gone much beyond other previously known approximations, and they have been subject to several limitations. Only some disconnected angular regions have been treated, with no discussion of the transition between them. In particular, the neighborhood of the forward and backward directions, where several important diffraction effects take place, has not been treated.

Light scattering by water droplets in the atmosphere gives rise to two of the most beautiful natural phenomena: the rainbow and the glory. The best approximate theory of the rainbow so far available is still Airy's classic theory,[13] despite the fact that it is known to suffer from several shortcomings (Ref. 4, p. 249). No satisfactory quantitative treatment of the glory has ever been given.

A modified form of the Watson transformation has recently been developed and applied by the author to the problem of scattering by an impenetrable sphere (Ref. 14, hereafter referred to as N). This method enables one to derive the asymptotic behavior of the exact solution at any distance from the sphere and in any direction, including near-forward and near-backward directions.

In the present series of papers, the modified Watson transformation is applied to the transparent sphere problem. We shall consider only the scattering amplitude; the behavior of the wavefunction in the near region is not discussed. The main result is that the asymptotic high-frequency behavior of the exact scattering amplitude in any direction can be determined by this method. The different types of transition regions that occur are discussed. In particular, an improved treatment of the rainbow and a quantitative theory of the glory will be given.

In Sec. 2, the distribution of poles of the S function in the complex angular-momentum plane is determined. Their physical interpretation is discussed and their relation to the usual Regge poles that appear in potential scattering is examined. This helps to clarify a long-standing puzzle in scattering theory, namely, the question of why cutoff potentials and potentials with exponential tails give rise to scattering amplitudes having widely different analytic properties. However, it is found that the Watson transformation, applied directly to the partial-wave expansion, is not at all helpful, because the residue series associated with the poles of the S function, in contrast with the case of an impenetrable sphere, are not rapidly convergent.

This difficulty is circumvented in Sec. 3, by means of a procedure first applied by Debye[15] in the case of a circular cylinder. The interaction of the incident wave with the sphere is decomposed into an infinite series of interactions with the surface, analogous to the multiple internal reflection treatment of the Fabry–Perot interferometer. The terms of this Debye expansion are also closely related with the rays appearing in the geometrical-optics (ray-tracing) method that undergo multiple internal reflections. The poles in the complex-angular-momentum plane associated with the terms of the Debye expansion are determined. It is found that, in contrast with the poles of the S function, they give rise to rapidly convergent residue series. The relation with previous treatments of the problem is also discussed.

The modified Watson transformation can be applied to each term of the Debye expansion. The asymptotic behavior of each term, as in the impenetrable sphere problem, is usually dominated by contributions of two types: (a) *saddle-point contributions:* these are associated with geometrical-optic rays and the WKB expansion, and they are related with partial waves in the domain (i); (b) *residue-series contributions:* these correspond to surface waves, and they are related with partial waves in the edge domain (ii).

Each class of rays gives rise to "shadow" and "lit" regions for the corresponding term of the Debye

[9] K. W. Ford and J. A. Wheeler, Ann. Phys. (N.Y.) **7**, 259 (1959).
[10] B. Van der Pol and H. Bremmer, Phil. Mag. **24**, 141, 825 (1937).
[11] P. Beckmann, Z. Naturforsch. **12a**, 960 (1957).
[12] S. I. Rubinow, Ann. Phys. (N.Y.) **14**, 305 (1961).
[13] G. B. Airy, Trans. Cambridge Phil. Soc. **6**, 379 (1838).
[14] H. M. Nussenzveig, Ann. Phys. (N.Y.) **34**, 23 (1965).
[15] P. J. Debye, Physik. Z. **9**, 775 (1908).

expansion. In lit regions, the amplitude is usually (though not always) dominated by the geometrical-optic contributions, whereas the surface-wave contributions are usually dominant in shadow regions. For $N > 1$, each term gives rise to different shadow boundaries, but for $N < 1$ there exists a shadow boundary common to all terms of the Debye expansion.

For each term, we also find transition regions between light and shadow, and the most interesting diffraction phenomena occur in these regions. In addition to "Fock-type" transition regions, such as were found for an impenetrable sphere (N, Fig. 14), we shall find new types of transition regions, such as those associated with the rainbow and the glory. In terms of the particle picture, shadow regions are classically forbidden, and transition effects may be interpreted as a sort of "inertial barrier" penetration.

As to the convergence of the Debye expansion, the geometrical-optic contributions usually converge quite rapidly, because of the attenuation due to successive internal reflections, provided that we exclude the cases (1.3). The surface-wave contributions do not converge so rapidly, because of their high internal reflection coefficient. Nevertheless, we shall be able to estimate their combined effect, and we shall see that, for $N > 1$, they give rise to rapid intensity fluctuations, which become quite large in the case of the glory.

The present paper is concerned with the evaluation of the first two terms in the Debye expansion. The behavior of these terms is discussed both for $N > 1$ and for $N < 1$. In Sec. 4, we consider the first term, which corresponds to rays reflected directly from the surface. For $N > 1$, the results are quite similar to those found for an impenetrable sphere. For $N < 1$, however, we find a new type of diffracted rays, that cannot be interpreted according to the usual formulation of Keller's geometrical theory of diffraction.[16] The physical interpretation of these terms is given. In Sec. 5, the second term of the Debye expansion, corresponding to rays directly transmitted through the sphere, without any internal reflection, is treated in a similar manner.

Paper II is concerned mainly with the third term, and it contains the theory of the rainbow and the glory (for the scalar problem). The effect of higher-order terms will also be discussed. The conclusions for both papers will be given at the end of Paper II.

[16] J. B. Keller, in "Calculus of Variations and its Applications," *Proceedings of Symposia in Applied Mathematics*, L. M. Graves, Ed. (McGraw-Hill, New York, 1958), Vol. 8, p. 27.

2. THE POLES OF THE S FUNCTION

The total scattering amplitude $F(k, \theta)$ is given by the partial-wave expansion

$$F(k, \theta) = \frac{1}{ik} \sum_{l=0}^{\infty} (l + \tfrac{1}{2})[S_l(k) - 1]P_l(\cos\theta), \quad (2.1)$$

where S_l is the S function and P_l is the lth Legendre polynomial. We shall find it convenient to work with a dimensionless scattering amplitude $f(\beta, \theta)$, defined by

$$f(\beta, \theta) = F(k, \theta)/a. \quad (2.2)$$

The continuity conditions for the wavefunction and its normal derivative at the boundary lead to the well-known expression (cf. e.g., Ref. 17):

$$S_l = -\frac{h_l^{(2)}(\beta)}{h_l^{(1)}(\beta)}\left[\frac{\ln' h_l^{(2)}(\beta) - N \ln' j_l(\alpha)}{\ln' h_l^{(1)}(\beta) - N \ln' j_l(\alpha)}\right], \quad (2.3)$$

where ln′ denotes the logarithmic derivative, j_l and h_l are spherical Bessel and Hankel functions, and we have introduced, in addition to (1.2), the dimensionless parameter α associated with the internal wave number:

$$\alpha = Nka = N\beta. \quad (2.4)$$

Applying Poisson's sum formula [N, Eq. (9.57)] to Eq. (2.1), we find

$$f(\beta, \theta) = \frac{i}{\beta} \sum_{m=-\infty}^{\infty} (-1)^m \times \int_0^{\infty} [1 - S(\lambda, \beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)e^{2im\pi\lambda}\lambda\, d\lambda, \quad (2.5)$$

where

$$S(\lambda, \beta) = -\frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)}\left(\frac{[2\,\beta] - N[\alpha]}{[1\,\beta] - N[\alpha]}\right), \quad (2.6)$$

and we have introduced the following notations:

$$[x] = \ln' J_\lambda(x), \quad (2.7)$$

$$[1\,x] = \ln' H_\lambda^{(1)}(x), \quad (2.8)$$

$$[2\,x] = \ln' H_\lambda^{(2)}(x). \quad (2.9)$$

We have also gone over from spherical to cylindrical Bessel and Hankel functions. The physical values of λ are $\lambda = l + \frac{1}{2}$, $l = 0, 1, 2, \cdots$.

The ordinary Watson transformation [N, Eqs. (2.7) and (2.11)] yields

$$f(\beta, \theta) = \frac{i}{2\beta}\int_C [1 - S(\lambda, \beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)e^{-i\pi\lambda}\frac{\lambda\, d\lambda}{\cos(\pi\lambda)} \quad (2.10)$$

[17] H. M. Nussenzveig, Nucl. Phys. **11**, 499 (1959).

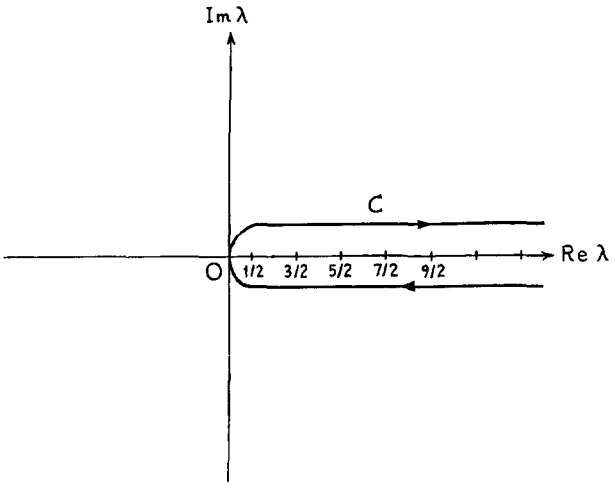

FIG. 1. The contour C.

or, equivalently,

$$f(\beta, \theta) = \frac{1}{2\beta} \int_C [1 - S(\lambda, \beta)] P_{\lambda-\frac{1}{2}}(-\cos\theta) \frac{\lambda \, d\lambda}{\cos(\pi\lambda)}, \tag{2.11}$$

where C is the contour shown in Fig. 1.

The representation (2.10) is equivalent to (2.5), as we see by employing, along the upper half of C, the expansion

$$\frac{1}{\cos(\pi\lambda)} = 2 \sum_{m=0}^{\infty} (-1)^m \exp[i(2m+1)\pi\lambda] \tag{2.12}$$

and, along the lower half,

$$\frac{1}{\cos(\pi\lambda)} = -2 \sum_{m=-\infty}^{-1} (-1)^m \exp[i(2m+1)\pi\lambda]. \tag{2.13}$$

By substituting the same expansions in (2.11), we find that (2.5) is also equivalent to

$$f(\beta, \theta) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} [1 - S(\lambda, \beta)] P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[i(2m+1)\pi\lambda] \lambda \, d\lambda. \tag{2.14}$$

In order to apply the modified Watson transformation (N, Sec. IX.D) directly to (2.5), we have to locate the poles of the meromorphic function $S(\lambda, \beta)$ in the complex λ plane. According to (2.6), they are the roots of

$$[1\ \beta] = N[\alpha]. \tag{2.15}$$

By interpreting N in accordance with (1.6), they may also be identified with the Regge poles for a square potential well ($N > 1$) or barrier ($N < 1$).

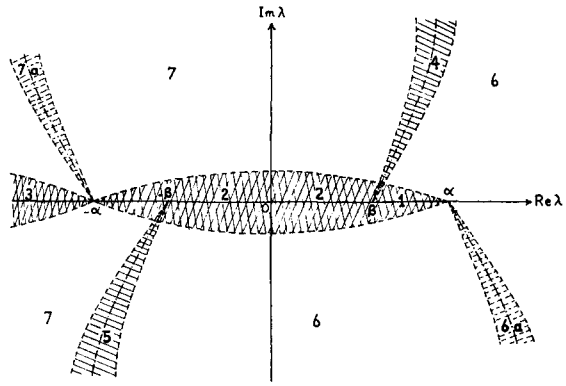

FIG. 2. Subdivision of the λ plane into regions (regions 6a and 7a refer only to Sec. 3B).

The Regge poles associated with the square-well potential have been investigated by many authors.[18–21] For $N < 1$, they have also been investigated in connection with the scattering by a dielectric cylinder.[22]

A detailed discussion of the pole distribution turns out not to be very relevant for the present problem, although some features of it will be required later on. On the other hand, such a discussion is very instructive in connection with the analytic properties of scattering amplitudes in potential scattering. The reader who is not interested in this connection may proceed directly to Sec. 3.

Instead of solving (2.15) to determine the poles $\lambda_n(\beta)$ of $S(\lambda, \beta)$ for fixed (physical) β, one can also fix λ at a physical value, $\lambda = l + \frac{1}{2}$, and solve with respect to β, to find the poles $\beta_n(l)$ in the complex β plane. This has been done explicitly for the lowest values of l.[17] The two sets of poles are related to each other (Ref. 21, Chap. 14), and we shall make use of the known results on the poles β_n to help in the physical interpretation of the poles λ_n.

We are interested mainly in the Regge-pole distribution for $\beta \gg 1$. The case $N > 1$ will be considered first. The physical interpretation of the results becomes simpler for $N \gg 1$, corresponding to an optically very dense material or to a very deep potential well. Accordingly, we shall assume that

$$\alpha \gg \beta \gg 1. \tag{2.16}$$

To solve (2.15), we replace the cylindrical functions by their asymptotic expansions, given in N (Appendix A). Corresponding to N, Fig. 15, the λ plane is subdivided into seven regions, as shown in Fig. 2.

[18] C. J. Bollini and J. J. Giambiagi, Nuovo Cimento **26**, 619 (1962); **28**, 341 (1963).
[19] A. O. Barut and F. Calogero, Phys. Rev. **128**, 1383 (1962).
[20] A. Z. Patashinskii, V. L. Pokrovskii, and I. M. Khalatnikov, Sov. Phys.—JETP **17**, 1387 (1963).
[21] R. G. Newton, *The Complex j-Plane* (W. A. Benjamin, New York, 1964), Chap. 12.
[22] W. Streifer and R. D. Kodis, Quart. Appl. Math. **23**, 27 (1965).

(In the present section, regions 6a and 7a are not to be distinguished from 6 and 7, respectively; this distinction will arise only in Sec. 3B.)

Outside of the shaded regions, we find:

$$[\alpha] \approx (\lambda^2 - \alpha^2)^{\frac{1}{2}}/\alpha, \tag{2.17}$$

$$[1\ \beta] \approx -(\lambda^2 - \beta^2)^{\frac{1}{2}}/\beta, \quad \text{in region 6,} \tag{2.18}$$

$$[1\ \beta] \approx (\lambda^2 - \beta^2)^{\frac{1}{2}}/\beta, \quad \text{in region 7,} \tag{2.19}$$

so that (2.15) becomes $(\lambda^2 - \alpha^2)^{\frac{1}{2}} = \pm(\lambda^2 - \beta^2)^{\frac{1}{2}}$, and therefore has no solutions.

The solutions must be located in the shaded regions, where either the left- or the right-hand side of (2.15) is rapidly varying, because they contain the zeros of $H_\lambda^{(1)}(\beta)$ or $J_\lambda(\alpha)$.

Let us begin with regions 1, 2, and 3, where the zeros of $J_\lambda(\alpha)$ are located. In 1 and 2, for

$$\alpha - |\lambda| \gg \alpha^{\frac{1}{3}}, \tag{2.20}$$

we have, according to N, Eq. (A16):

$$[\alpha] \approx -\frac{(\alpha^2 - \lambda^2)^{\frac{1}{2}}}{\alpha} \tan\left[\varphi(\lambda, \alpha) - \frac{\pi}{4}\right], \tag{2.21}$$

where

$$\varphi(\lambda, x) = (x^2 - \lambda^2)^{\frac{1}{2}} - \lambda \cos^{-1}(\lambda/x), \tag{2.22}$$

with

$$(x^2 - \lambda^2)^{\frac{1}{2}} > 0, \quad 0 < \cos^{-1}(\lambda/x) < \pi/2, \quad \text{for} \quad -x < \lambda < x. \tag{2.23}$$

In region 1, for

$$|\lambda| - \beta \gg \beta^{\frac{1}{3}}, \tag{2.24}$$

Eq. (2.18) is valid as a first approximation; however, in this approximation, we would find poles located on the real axis. To get the imaginary part of the poles, which is a small correction, we need an improved approximation for $[1\ \beta]$ in region 1. Under the condition (2.24), we have[23]

$$H_\lambda^{(1)}(\beta) \approx (2/\pi)^{\frac{1}{2}}(\lambda^2 - \beta^2)^{-\frac{1}{4}} \times \{\exp[\psi(\lambda, \beta)] - i \exp[-\psi(\lambda, \beta)]\}, \tag{2.25}$$

where [cf. N, Eq. (A2)]:

$$\psi(\lambda, x) = (\lambda^2 - x^2)^{\frac{1}{2}} - \lambda \ln\left[\frac{\lambda}{x} + \frac{(\lambda^2 - x^2)^{\frac{1}{2}}}{x}\right]. \tag{2.26}$$

The branches of the many-valued functions that have to be taken are specified in N (Appendix A). In region 1, with (2.24), we have

$$\operatorname{Re} \psi(\lambda, \beta) < 0, \quad |\psi(\lambda, \beta)| \gg 1, \tag{2.27}$$

so that

$$[1\ \beta] \approx -\frac{(\lambda^2 - \beta^2)^{\frac{1}{2}}}{\beta}\{1 - 2i \exp[2\psi(\lambda, \beta)]\}, \tag{2.28}$$

where the exponential term is the small correction to (2.18) that is required to determine the imaginary part of the poles.

Substituting (2.21) and (2.28) in (2.15), we find

$$\tan\left[\varphi(\lambda, \alpha) - \frac{\pi}{4}\right] = \left(\frac{\lambda^2 - \beta^2}{\alpha^2 - \lambda^2}\right)^{\frac{1}{2}}\{1 - 2i \exp[2\psi(\lambda, \beta)]\}. \tag{2.29}$$

Let

$$\lambda_n = \xi_n + i\eta_n \tag{2.30}$$

be the roots of (2.29), where $|\eta_n/\xi_n| \ll 1$. Then, to a very good approximation,

$$\varphi(\xi_n, \alpha) \approx n\pi + \frac{\pi}{4} + \tan^{-1}\left[\left(\frac{\xi_n^2 - \beta^2}{\alpha^2 - \xi_n^2}\right)^{\frac{1}{2}}\right], \tag{2.31}$$

$$\eta_n \approx \frac{2[(\alpha^2 - \xi_n^2)(\xi_n^2 - \beta^2)]^{\frac{1}{2}}}{(\alpha^2 - \beta^2)\cos^{-1}(\xi_n/\alpha)} \exp[2\psi(\xi_n, \beta)], \tag{2.32}$$

where n takes on integer values. To determine the real part of the poles, the real transcendental equation (2.31) must be solved. The corresponding imaginary part is then given by (2.32). In particular, for

$$\beta \ll \xi_n \ll \alpha, \tag{2.33}$$

these equations simplify to

$$\alpha - (\xi_n + \tfrac{1}{2})(\pi/2) \approx n\pi, \tag{2.34}$$

$$\eta_n \approx \frac{4\xi_n}{\pi\alpha}\left(\frac{e\beta}{2\xi_n}\right)^{2\xi_n}. \tag{2.35}$$

Thus, we find in region 1 a series of poles located very close to the real axis. The spacing between two consecutive poles, according to (2.31), is given by

$$\Delta\xi_n \approx \pi/\cos^{-1}(\xi_n/\alpha) \quad (\approx 2 \quad \text{for} \quad \xi_n \ll \alpha). \tag{2.36}$$

According to (2.35), the poles get closer to the real axis as ξ_n increases.

These poles have a simple physical interpretation in terms of resonances. Optically, they correspond to the "free modes of vibration of a dielectric sphere" [see Refs. 24 (p. 73) and 25]. Their long lifetime is made possible by the high internal reflectivity, due to the large refractive index, and by the high centrifugal barrier, due to the large angular momentum. The resonance appears when the corresponding pole lies close to a physical value of λ.

In the quantum-mechanical interpretation, (2.16) corresponds to a very deep potential well, and the poles (2.30) correspond to resonances lying below the top of the centrifugal barrier. Under these conditions,

[23] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1962), 2nd ed., p. 267.

[24] P. J. Debye, Ann. Physik Ser. 4, **30**, 57 (1909).

[25] G. Beck and P. Wenzel, Z. Physik **84**, 335 (1933).

the effective potential (1.9) represents a deep well surrounded by a high barrier, thus giving rise to sharp resonances.

The corresponding poles in the β plane are obtained by setting $\lambda = l + \frac{1}{2}$ in (2.29) and solving for β. We find that $\operatorname{Re}\beta_n$ is determined by the well-known resonance condition (Ref. 26, p. 382):

$$N \operatorname{Re}\beta_n - (l + \tfrac{1}{2})\frac{\pi}{2} \approx n\pi, \tag{2.37}$$

which is equivalent to (2.34). We also find a result analogous to (2.32) for $\operatorname{Im}\beta_n$:

$$\operatorname{Im}\beta_n \propto \exp[2\psi(l + \tfrac{1}{2}, \operatorname{Re}\beta_n)] = \exp(2\psi_l) = v_l, \tag{2.38}$$

where ψ_l is given by (1.11) and v_l represents the penetration factor of the centrifugal barrier in the WKB approximation [cf. Eq. (1.10) and Ref. 26, p. 361]. This leads to the usual expression for the width Γ_n of the resonance (Ref. 26, p. 389).

In region 2, also assuming (2.24), we have, by N, Eq. (A16),

$$[1\ \beta] \approx i(\beta^2 - \lambda^2)^{\frac{1}{2}}/\beta, \tag{2.39}$$

so that (2.15) becomes

$$\tan[\varphi(\lambda, \alpha) - \pi/4] \approx -i\left(\frac{\beta^2 - \lambda^2}{\alpha^2 - \lambda^2}\right)^{\frac{1}{2}}, \tag{2.40}$$

or, since $\beta \ll \alpha$,

$$\varphi(\lambda_n, \alpha) \approx n\pi + \frac{\pi}{4} - i\left(\frac{\beta^2 - \lambda_n^2}{\alpha^2 - \lambda_n^2}\right)^{\frac{1}{2}}. \tag{2.41}$$

In particular, for $|\lambda_n| \ll \beta$, this gives

$$\lambda_n \approx \frac{2\alpha}{\pi} - \left(2n + \frac{1}{2}\right) + \frac{2i}{\pi N}, \quad |\lambda_n| \ll \beta. \tag{2.42}$$

This corresponds to another series of poles with spacing $|\Delta\lambda_n| \approx 2$, not so close to the real axis and with almost constant imaginary part. Their real part is again determined by the resonance condition (2.34).

These poles are associated with broad resonances above the top of the centrifugal barrier. For the corresponding poles in the β plane, we find

$$\operatorname{Im}\beta_n \approx -1. \tag{2.43}$$

This again agrees with the usual expression (Ref. 26, p. 389) for the resonance width, with the barrier penetration factor v_l set equal to unity, so that the width is determined only by the refractive index. For $l = 0$, these poles have been discussed in Ref. 17.

In region 3, setting

$$\lambda = -\mu, \tag{2.44}$$

we find, by N, Eq. (A15),

$$[\alpha] \approx -\frac{(\mu^2 - \alpha^2)^{\frac{1}{2}}}{\alpha} \times \left\{\frac{2\sin(\pi\mu) - \cos(\pi\mu)\exp[2\psi(\mu, \alpha)]}{2\sin(\pi\mu) + \cos(\pi\mu)\exp[2\psi(\mu, \alpha)]}\right\}, \tag{2.45}$$

and, since $H^{(1)}_{-\mu}(x) = e^{i\pi\mu}H^{(1)}_{\mu}(x)$, Eq. (2.28) gives

$$[1\ \beta] \approx -\frac{(\mu^2 - \beta^2)^{\frac{1}{2}}}{\beta}\{1 - 2i\exp[2\psi(\mu, \beta)]\}. \tag{2.46}$$

Substituting into (2.15), we find, for $\mu \gg \alpha$,

$$\left[\frac{\alpha^2 - \beta^2}{2\mu^2} - 2i\left(\frac{e\beta}{2\mu}\right)^{2\mu}\right]\sin(\pi\mu) \approx -\left[\left(\frac{e\alpha}{2\mu}\right)^{2\mu} - i\left(\frac{e^2\alpha\beta}{4\mu^2}\right)^{2\mu}\right]\cos(\pi\mu),$$

so that the roots are located very close to the integers, $\mu_n = n - \epsilon_n$, $|\epsilon_n| \ll 1$, and we finally get

$$\lambda_n = -\mu_n \approx -n + \frac{2n^2}{\pi(\alpha^2 - \beta^2)}\left(\frac{e\alpha}{2n}\right)^{2n} \times \left[1 + \frac{4in^2}{(\alpha^2 - \beta^2)}\left(\frac{e\beta}{2n}\right)^{2n}\right]. \tag{2.47}$$

Thus, in region 3, there is an infinite number of poles, which approach the negative integers faster than exponentially as $|\lambda_n| \to \infty$.

In region 4, let us consider first the neighborhood of $\lambda = \beta$. Let

$$\lambda = \beta + e^{i\pi/3}\xi/\gamma, \tag{2.48}$$

where we have introduced the parameter

$$\gamma = (2/\beta)^{\frac{1}{3}} \ll 1, \tag{2.49}$$

which is very small according to (1.1), and we assume that $|\xi| = \mathcal{O}(1)$. The asymptotic behavior of the cylindrical functions under these conditions is given in Appendix A. It follows from (A1) and (A2) that

$$[1\ \beta] \approx e^{-i\pi/3}\gamma\ \mathrm{Ai}'(-\xi)/\mathrm{Ai}(-\xi), \tag{2.50}$$

where $\mathrm{Ai}(z)$ is the Airy function.

On the other hand, for $\operatorname{Im}\lambda \gg 1$, Eq. (2.21) gives

$$[\alpha] \approx i(\alpha^2 - \lambda^2)^{\frac{1}{2}}/\alpha, \tag{2.51}$$

so that (2.15) becomes

$$\mathrm{Ai}(-\xi)/\mathrm{Ai}'(-\xi) \approx -e^{i\pi/6}\gamma/M, \tag{2.52}$$

where we have introduced the abbreviation

$$M = (N^2 - 1)^{\frac{1}{2}}, \quad N > 1. \tag{2.53}$$

According to (2.52), the roots lie close to the zeros x_n of $\mathrm{Ai}(-x)$. Let

$$\xi_n = x_n - \epsilon_n, \quad \mathrm{Ai}(-x_n) = 0. \tag{2.54}$$

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

Then, (2.52) yields

$$\epsilon_n \approx -e^{i\pi/6}\gamma/M, \tag{2.55}$$

so that (2.48) becomes

$$\lambda_n \approx \beta + e^{i\pi/3}(x_n/\gamma) + i/M. \tag{2.56}$$

The first two terms of the (2.56) coincide with those found for the Regge poles for an impenetrable sphere [N, Eq. (3.5)]. Thus, as in that case, the poles (2.56) must be associated with surface waves, with an angular damping factor given by Im λ_n (N, Sec. V). The second term of (2.56) contains the radiation damping due to propagation along a curved surface. Since this effect depends only on the geometry (radius of curvature), it is not surprising that it coincides with that found for an impenetrable sphere. The third term in (2.56) is the only one that depends on the refractive index. It represents the additional damping due to refraction of the surface waves into the sphere. This is a small correction, provided that the refractive index is not too close to unity, as expressed in the second condition (1.1). We now see the physical meaning of that condition: it implies that *the damping of the surface waves is determined mainly by the geometry, and is not greatly perturbed by penetration into the sphere.*

Finally, let us consider the asymptotic behavior of the poles for large $|\lambda|$ in region 4. According to N, Eq. (3.7), we then have

$$[1\ \beta] \approx \frac{(\lambda^2-\beta^2)^{\frac{1}{2}}}{\beta}\coth\left[\psi(\lambda,\beta) - i\frac{\pi}{4}\right], \tag{2.57}$$

while $[\alpha]$ is still given by (2.17). Thus, for $|\lambda| \gg \alpha^2$, Eq. (2.15) becomes

$$\coth\left[\lambda\ln\left(\frac{2\lambda}{e\beta}\right) + i\frac{\pi}{4}\right] \approx -1 + (N^2-1)\frac{\beta^2}{2\lambda^2}. \tag{2.58}$$

Let

$$\lambda_n = \rho_n \exp\,[i(\pi/2 - \epsilon_n)], \quad \rho_n \gg \alpha^2. \tag{2.59}$$

Then, equating real and imaginary parts of (2.58), we get

$$\rho_n \ln\,(2\rho_n/e\beta) \approx n\pi, \tag{2.60}$$

$$\epsilon_n \approx \frac{\pi}{2\ln\,(2\rho_n/e\beta)} - \frac{1}{n\pi}\ln\left(\frac{2\rho_n}{M\beta}\right). \tag{2.61}$$

The solution of (2.60) has already been given in N, Eq. (3.12):

$$\rho_n \approx \frac{n\pi}{\ln\,(2n\pi/e\beta)} + \cdots. \tag{2.62}$$

Substituting these results in (2.59), we see that the asymptotic behavior of these poles is again very similar to that found for an impenetrable sphere [N, Eq. (3.13)]. Both Re λ_n and Im λ_n approach infinity with n, but

$$\text{Re}\,\lambda_n/\text{Im}\,\lambda_n = \mathcal{O}[(\ln n)^{-1}]. \tag{2.63}$$

The results for the poles in region 5 are very similar to those found for region 4.

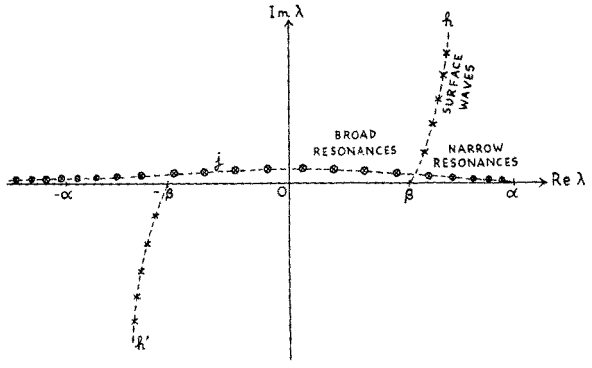

FIG. 3. The Regge poles of $S(\lambda,\beta)$ for $\alpha \gg \beta \gg 1$. The physical interpretation of the poles in the first quadrant is also indicated. ⊗—Class I poles; ×—Class II poles.

The complete pole distribution for $\alpha \gg \beta \gg 1$ is schematically shown in Fig. 3. We see that the poles fall into two sharply differentiated classes: those located near the real axis, along the curve j, will be called *Class I poles*, whereas those located along the curves h and h' will be called *Class II poles.*

The Regge trajectories for these two classes of poles also show quite different behavior.[20] For Class I poles (called "physical" in Ref. 20), they behave similarly to the well-known pattern of Regge trajectories for Yukawa-type potentials.[21] For a sufficiently deep well, the "right-most" poles in the right half-plane move along the real axis at negative energies, giving rise to bound states, and they leave the real axis, going into the first quadrant, at positive energies, giving rise to resonances. At finite energy, there is only a finite number of Class I poles in the right half-plane. However, in contrast with Yukawa-type potentials, the trajectories do not turn back as $\beta \to \infty$, but proceed to infinity in the right half-plane.

The trajectories of Class II poles (called "unphysical" in Ref. 20) behave quite differently. At finite energy, there is an infinite number of these poles, with unbounded real parts, in the first quadrant. As $\beta \to 0$, they all move towards the origin, so that they have "0-type" trajectories, in contrast with Class-I poles, which have "C-type" trajectories (cf. Ref. 21, pp. 66, 99, 100).

The physical origin of the different behavior of the two classes of poles is now clear. Class I poles are associated with the "interior" of the potential, i.e.,

with its behavior for $r < a$. This is why they resemble the usual Regge poles for Yukawa-type potentials. Class II poles, on the other hand, are by no means unphysical. They are associated with surface waves, as has been discussed in detail in N. They are insensitive to the behavior of the potential in the internal region, and are almost entirely determined by the geometrical shape of the surface.

These results help us to understand the origin of a very puzzling feature in dispersion theory, namely, the radically different analytic behavior of scattering amplitudes for cutoff potentials and for potentials with tails extending to infinity (e.g., Yukawa type). One can argue that cutting off an exponentially decreasing potential at sufficiently large distances should produce negligibly small physical effects, and yet it drastically alters the analytic behavior. This has always been regarded as an unphysical aspect of dispersion theory, reflecting the instability of analytic continuation.

It is now seen that the effect is at least partially due to the appearance of surface waves as soon as a cutoff is made. For Yukawa-type potentials, it is the finiteness of the number of Regge poles in the right half-plane that leads to polynomial boundedness of the scattering amplitude in momentum transfer and therefore to the Mandelstam representation. For cutoff potentials, the existence of an infinite number of Class II poles in the right half-plane at any finite energy gives rise to an essential singularity at infinity in the momentum transfer plane, so that the Mandelstam representation is no longer valid.[27]

It can still be argued that a sufficiently rapid exponential decrease is physically indistinguishable from a sharp cutoff, and should therefore give rise to effects resembling those of surface waves. However, this can only be true over a bounded energy range. In fact, "sufficiently rapid" means that the range of the exponential is much shorter than the wavelength, which ceases to be true at sufficiently high energy. On the other hand, cutoff potentials can support surface waves at arbitrarily high energy. This is related with the existence of an infinite number of Class II poles.

Finally, let us briefly consider the pole distribution for $N < 1$. We restrict ourselves to the case $N \ll 1$ (corresponding to a very high potential barrier), so that

$$\beta \gg \alpha \gg 1. \tag{2.64}$$

A detailed investigation of the pole distribution for $N < 1$ has been made by Streifer and Kodis.[22] Figure 4, based on their results, gives a schematic representation of the pole distribution when (2.64) is valid.

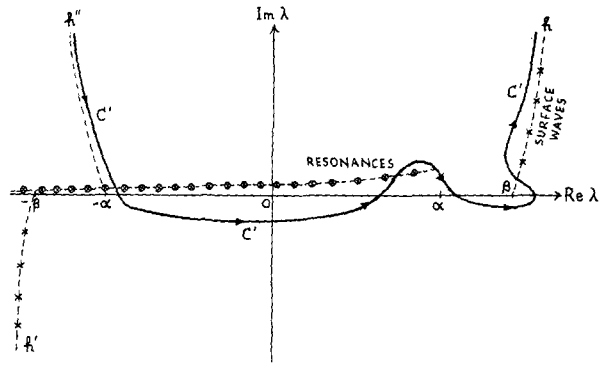

FIG. 4. The Regge poles of $S(\lambda, \beta)$ for $\beta \gg \alpha \gg 1$. The physical interpretation of the poles in the first quadrant is also indicated. ⊗—Class I poles; ×—Class II poles. C' is the path used by Chen (cf. Sec. 3D).

The main difference with respect to Fig. 3 is that narrow resonances now occur also at low values, rather than only at high values of the angular momentum. In fact, for $|\lambda| \ll \alpha$, the poles are approximately given by [cf. Eq. (2.42)]:

$$\lambda_n \approx (2\alpha/\pi) - (2n + \tfrac{1}{2}) + (2i/\pi)N, \tag{2.65}$$

which is close to the real axis for $N \ll 1$.

These poles correspond to Fabry–Perot type resonances immediately above the top of the barrier. The corresponding poles in the β plane, for $l = 0$, are given by Ref. 17 [Eq. (18)].

In the second quadrant, the poles again tend to approach the negative integers; (2.47) remains valid for $N < 1$.

3. THE DEBYE EXPANSION

A. Derivation

If we try to apply the modified Watson transformation, as developed in N (Sec. IX.D), directly to (2.5), we are immediately confronted with the following difficulty: in contrast with the case of an impenetrable sphere, a large number of Regge poles lie close to the real axis (cf. Figs. 3 and 4). Therefore, if we succeeded in reducing (2.5) to rapidly convergent contour integrals plus series of residues at the Regge poles, as in N, the residue series would still be slowly convergent. According to (2.36), the number of poles located very close to the real axis in the first quadrant is of the order of $(N - 1)\beta$. Thus, the minimum number of terms to be retained in the residue series (even without considering the infinite number of poles in the second quadrant) would be of the same order as in the original partial-wave series. Physically, this corresponds to the fact that a large number of partial waves can be near resonance at high frequency.

[27] H. M. Nussenzveig, Ann. Phys. (N.Y.) **21**, 344 (1963).

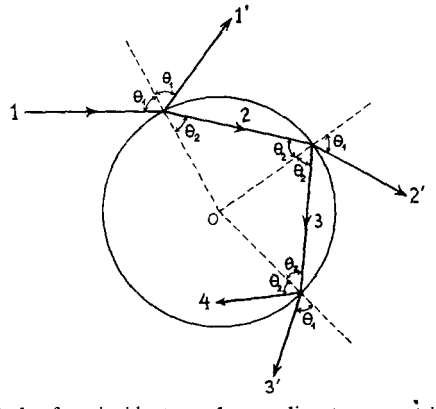

FIG. 5. Path of an incident ray 1 according to geometrical optics ($N > 1$).

Another way to see the origin of this difficulty, which also provides a clue to its solution, is to consider the contour integrals resulting from the transformation. In N, these contour integrals were evaluated by the saddle-point method, and the saddle-point contributions were found to correspond, in first approximation, to the results given by geometrical optics.

In order to apply geometrical optics to the present problem, we have to consider the path followed by a ray incident upon the sphere. This path is indicated in Fig. 5. An incident ray 1 is partially reflected (ray 1') and partially transmitted into the sphere (ray 2). Ray 2 in its turn undergoes partial internal reflection (ray 3) and partial transmission to the external region (ray 2'), and so on. This gives rise to an infinite series of multiple internal reflections, analogous to multiple-beam formation in a plane-parallel plate. The geometrical-optic solution outside of the sphere is constructed by superposing the contribution from the incident ray 1 with that from the directly reflected ray 1' and those from all transmitted rays 2', 3', $\cdots$.

Thus, in contrast with the impenetrable-sphere case, where only direct reflection takes place, each incident ray generates an infinite series of geometrical-optic rays, which should correspond to an infinite number of saddle points. In the geometrical-optic description, the total interaction of a ray with the sphere is broken up into an infinite number of interactions with the surface.

This is the clue to the resolution of the difficulty: in order to have a parallel with geometrical optics, we must look for *a description in terms of surface interactions*. This was first done by Debye[15] for a circular cylinder; his procedure was applied to the sphere by Van der Pol and Bremmer.[10]

For each multipole order l, we consider an incoming spherical wave of this order that strikes the surface of the sphere at $r = a$ and is partially reflected and partially transmitted. In order to evaluate the reflection and transmission coefficients of the interface purely in terms of a surface interaction, we must regard it as an interface between two unbounded media, by solving the radial equation in a fictitious one-dimensional space, in which r ranges from $-\infty$ to ∞. If 1 and 2 denote the interior and exterior of the sphere, respectively, there will then be only a transmitted wave in medium 1, so that we have

$$\psi_{2,l} = A\left[\frac{h_l^{(2)}(kr)}{h_l^{(2)}(\beta)} + R_{22}(l,\beta)\frac{h_l^{(1)}(kr)}{h_l^{(1)}(\beta)}\right], \tag{3.1}$$

$$\psi_{1,l} = AT_{21}(l,\beta)\frac{h_l^{(2)}(Nkr)}{h_l^{(2)}(\alpha)}, \tag{3.2}$$

where $\psi_{i,l}$ denotes the radial wavefunction in medium i for multipole order l, $R_{22}(l,\beta)$ is the external spherical reflection coefficient, and $T_{21}(l,\beta)$ is the spherical transmission coefficient from 2 to 1. The wavefunction and its radial derivative must be continuous at the interface; the coefficients are determined by this condition. Letting

$$l + \tfrac{1}{2} = \lambda, \tag{3.3}$$

we find

$$R_{22}(\lambda,\beta) = -\frac{[2\,\beta] - N[2\,\alpha]}{[1\,\beta] - N[2\,\alpha]}, \tag{3.4}$$

$$\begin{aligned} T_{21}(\lambda,\beta) &= 1 + R_{22}(\lambda,\beta) \\ &= \frac{[1\,\beta] - [2\,\beta]}{[1\,\beta] - N[2\,\alpha]} \\ &= \frac{4i}{\pi\beta H_\lambda^{(1)}(\beta)H_\lambda^{(2)}(\beta)([1\,\beta] - N[2\,\alpha])}, \end{aligned} \tag{3.5}$$

where we have employed the notations (2.8), (2.9), as well as the Wronskian relation

$$\begin{aligned} &W[H_\lambda^{(1)}(z), H_\lambda^{(2)}(z)] \\ &\quad = H_\lambda^{(1)}(z)H_\lambda^{(2)}(z)([2\,z] - [1\,z]) = -4i/\pi z. \end{aligned} \tag{3.6}$$

Similarly, by considering an outgoing spherical multipole wave of order l in medium 1, we can determine the internal spherical reflection coefficient R_{11} and the spherical transmission coefficient T_{12} from 1 to 2:

$$R_{11}(\lambda,\beta) = -\frac{[1\,\beta] - N[1\,\alpha]}{[1\,\beta] - N[2\,\alpha]}, \tag{3.7}$$

$$\begin{aligned} T_{12}(\lambda,\beta) &= 1 + R_{11}(\lambda,\beta) \\ &= \frac{N([1\,\alpha] - [2\,\alpha])}{[1\,\beta] - N[2\,\alpha]} \\ &= \frac{4i}{\pi\beta H_\lambda^{(1)}(\alpha)H_\lambda^{(2)}(\alpha)([1\,\beta] - N[2\,\alpha])}. \end{aligned} \tag{3.8}$$

For real λ, we have (reciprocity):

$$|R_{11}(\lambda, \beta)| = |R_{22}(\lambda, \beta)|, \quad \lambda \text{ real.} \tag{3.9}$$

On the other hand, for any λ, real or complex, it follows from the reflection properties of the cylindrical functions with respect to the index [cf. N, Eq. (2.15)] that all the coefficients are even functions of λ:

$$R_{ii}(-\lambda, \beta) = R_{ii}(\lambda, \beta); \quad T_{ij}(-\lambda, \beta) = T_{ij}(\lambda, \beta); \quad i, j = 1, 2. \tag{3.10}$$

The conservation of energy (or probability, in the quantum-mechanical interpretation) yields

$$|R_{22}(\lambda, \beta)|^2 + \left| \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(2)}(\alpha)} T_{21}(\lambda, \beta) \right|^2 = |R_{11}(\lambda, \beta)|^2 + \left| \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(1)}(\beta)} T_{12}(\lambda, \beta) \right|^2 = 1. \tag{3.11}$$

These relations are valid for any real λ, as may also be verified directly from the definitions of the spherical reflection and transmission coefficients, with the help of (3.6). Actually, the first equality in (3.11) already follows from (3.5) and (3.8).

In the limit as the radius of the sphere goes to infinity, the above coefficients approach the well-known Fresnel reflection and transmission coefficients for a plane interface at perpendicular incidence, as they should:

$$R_{22} \to -\frac{N-1}{N+1}, \quad T_{21} \to \frac{2}{N+1}, \quad R_{11} \to \frac{N-1}{N+1}, \quad T_{12} \to \frac{2N}{N+1}, \quad a \to \infty. \tag{3.12}$$

In order to expand the S function in terms of surface interactions, we first subtract from (2.6) the external reflection coefficient (3.4), rewriting the result as follows:

$$\frac{H_\lambda^{(1)}(\beta)}{H_\lambda^{(2)}(\beta)} S(\lambda, \beta) - R_{22}(\lambda, \beta) = N T_{21}(\lambda\ \beta) \frac{([\alpha] - [2\,\alpha])}{([1\ \beta] - N[\alpha])} = \frac{N T_{21}(\lambda, \beta) H_\lambda^{(1)}(\alpha)([1\ \alpha] - [2\,\alpha])}{H_\lambda^{(1)}(\alpha)([1\ \beta] - N[1\ \alpha]) + H_\lambda^{(2)}(\alpha)([1\ \beta] - N[2\ \alpha])}. \tag{3.13}$$

With the help of (3.8), this becomes

$$\frac{H_\lambda^{(1)}(\beta)}{H_\lambda^{(2)}(\beta)} S(\lambda, \beta) = R_{22}(\lambda, \beta) + \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(2)}(\alpha)} \frac{T_{21}(\lambda, \beta) T_{12}(\lambda, \beta)}{[1 - \rho(\lambda, \beta)]}, \tag{3.14}$$

where

$$\rho(\lambda, \beta) = \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(2)}(\alpha)} R_{11}(\lambda, \beta). \tag{3.15}$$

The Debye expansion is now obtained by expanding the inverse of the denominator in (3.14) into a geometric series:

$$S(\lambda, \beta) = \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} \left\{ R_{22}(\lambda, \beta) + T_{21}(\lambda, \beta) T_{12}(\lambda, \beta) \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(2)}(\alpha)} \sum_{p=1}^{\infty} [\rho(\lambda, \beta)]^{p-1} \right\}. \tag{3.16}$$

This expansion has a very simple physical interpretation. The over-all phase factor $H_\lambda^{(2)}(\beta)/H_\lambda^{(1)}(\beta)$ expresses the fact that the interaction takes place at $r = a$ (rather than at $r = 0$). The first term R_{22} represents direct reflection from the surface. The pth term corresponds to transmission into the sphere (factor T_{21}), followed by going back and forth between $r = a$ and $r = 0$ p times [factors $H_\lambda^{(1)}(\alpha)/H_\lambda^{(2)}(\alpha)$ in ρ], with $p - 1$ internal reflections at the surface (factors R_{11} in ρ) and a final transmission to the outside (factor T_{12}). The origin acts as a perfect reflector (due to the regularity of the wavefunction at $r = 0$). *The pth term of the Debye expansion represents the effect of $p + 1$ surface interactions.*

Before applying the Debye expansion, we must first make sure that it converges. For any finite real λ, this follows immediately from (3.15) and (3.11):

$$|\rho(\lambda, \beta)| = |R_{11}(\lambda, \beta)| < 1, \quad \lambda \text{ real.} \tag{3.17}$$

In fact, the denominator of (3.8) has no poles for real λ, so that $|T_{12}|$ is strictly positive.

On the other hand, as $\lambda \to \infty$, it follows from the asymptotic behavior of T_{12}, given in Appendix B, and from N (Appendix A), that

$$\frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(1)}(\beta)} T_{12}(\lambda, \beta) \approx -4i \frac{\lambda^2}{\alpha^2 - \beta^2} \left(\frac{e\beta}{2\lambda}\right)^{2\lambda} \left(\frac{e\alpha}{2\lambda}\right)^{2\lambda} \to 0, \quad \lambda \to \infty, \tag{3.18}$$

so that

$$\lim_{\lambda \to \pm\infty} |\rho(\lambda, \beta)| = 1. \tag{3.19}$$

Thus, in order to substitute the Debye expansion in (3.5), where the integrals range from 0 to ∞, we must interpret the integrals in (2.5) as limits of finite integrals:

$$\int_0^\infty d\lambda = \lim_{\Lambda \to \infty} \int_0^\Lambda d\lambda. \tag{3.20}$$

For any finite Λ, according to (3.17), the expansion

is justified, so that we get

$$f(\beta, \theta) = f_0(\beta, \theta) + \sum_{p=1}^{\infty} f_p(\beta, \theta), \tag{3.21}$$

where

$$f_0(\beta, \theta) = \frac{i}{\beta} \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} \left[1 - \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} R_{22}\right] \times P_{\lambda-\frac{1}{2}}(\cos\theta) \exp(2im\pi\lambda)\lambda \, d\lambda, \tag{3.22}$$

$$f_p(\beta, \theta) = -\frac{i}{\beta} \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} U(\lambda, \beta)[\rho(\lambda, \beta)]^{p-1} \times P_{\lambda-\frac{1}{2}}(\cos\theta) \exp(2im\pi\lambda)\lambda \, d\lambda, \quad p \geq 1, \tag{3.23}$$

where we have introduced

$$U(\lambda, \beta) = T_{21}(\lambda, \beta) \frac{H_\lambda^{(1)}(\alpha) H_\lambda^{(2)}(\beta)}{H_\lambda^{(2)}(\alpha) H_\lambda^{(1)}(\beta)} T_{12}(\lambda, \beta) = U(-\lambda, \beta), \tag{3.24}$$

and all integrals in (3.23) are to be interpreted in accordance with (3.20). Actually, when we discuss the asymptotic behavior of the integrand of (3.23) (cf. Sec. 5A and Appendix B), we shall see that it tends to zero faster than exponentially for $\lambda - \beta \gg \beta^{\frac{1}{3}}$, just like the integrand of (2.5), so that contributions to (3.20) are very rapidly damped beyond this point and we do not have to worry about the effect of (3.19). This corresponds to the negligible contribution from the partial waves in the domain (1.15).

Alternatively, one can also substitute (3.16) in (2.14) [or apply to each term of (3.21) the same transformation that led from (2.5) to (2.14)], with the result:

$$f_0(\beta, \theta) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} \left[1 - \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} R_{22}\right] \times P_{\lambda-\frac{1}{2}}(-\cos\theta) \exp[i(2m+1)\pi\lambda]\lambda \, d\lambda, \tag{3.25}$$

$$f_p(\beta, \theta) = -\frac{1}{\beta} \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} U(\lambda, \beta)[\rho(\lambda, \beta)]^{p-1} \times P_{\lambda-\frac{1}{2}}(-\cos\theta) \exp[i(2m+1)\pi\lambda]\lambda \, d\lambda, \quad p \geq 1. \tag{3.26}$$

Although the Debye expansion is convergent with the interpretation (3.20), what matters in practice is whether or not it is rapidly convergent. There are two questions involved: first, whether the application of the modified Watson transformation leads to rapidly convergent results in the evaluation of *each term* in the expansion [in contrast with its direct application to (2.5)]; secondly, how rapidly the Debye expansion itself converges.

We shall defer till later a discussion of the second point. As for the first one, the trouble with (2.5) was the slow convergence of residue series due to the existence of many Regge poles close to the real axis. In order to find out what happens for (3.21), our first task is to determine the distribution of poles in the λ plane associated with each term.

B. The Poles for the Debye Expansion

According to (3.22)–(3.26) and (3.4)–(3.8), the same set of poles is associated with each term in the Debye expansion. The poles are the roots of

$$[1\ \beta] = N[2\ \alpha], \tag{3.27}$$

which differs from (2.15) by the replacement $[\alpha] \to [2\ \alpha]$, corresponding to the transition from standing waves to travelling waves within the sphere, in accordance with the physical interpretation of the Debye expansion. Although the poles are the same for all terms, their order varies from term to term: they are of order $p + 1$ for the pth term ($p = 0, 1, 2, \cdots$).

As we have seen in connection with (2.15), the roots of (3.27) are located in those regions of the λ plane where either the left or the right-hand side is rapidly varying, i.e., close to the zeros of $H_\lambda^{(1)}(\beta)$ (regions 4 and 5, Fig. 2) or to those of $H_\lambda^{(2)}(\alpha)$ (regions 6a and 7a, Fig. 2). We shall denote by λ_n the poles in region 4 and by λ_n' those in region 6a. (As the Regge poles λ_n discussed in Sec. 2 will no longer be considered from now on, no confusion should arise.) These considerations already suggest that there will not be many poles close to the real axis.

Since $[1\ \beta]$ and $[2\ \alpha]$ are even functions of λ [cf. N, Eq. (2.15)], the pole distribution is symmetric with respect to the origin, so that it suffices to determine the poles located in the right half-plane.

In region 4, Eq. (2.50) is valid, whereas we have

$$[2\ \alpha] \approx -i(\alpha^2 - \lambda^2)^{\frac{1}{2}}/\alpha, \quad \text{if} \quad N > 1, \qquad \approx -(\lambda^2 - \alpha^2)^{\frac{1}{2}}/\alpha, \quad \text{if} \quad N < 1, \tag{3.28}$$

assuming that $|\alpha - \beta| \gg \beta^{\frac{1}{3}}$ [cf. (1.4)]. We then find

$$\lambda_n \approx \beta + e^{i\pi/3}(x_n/\gamma) - i/M, \quad N > 1, \tag{3.29}$$

where M has been defined by (2.53). The corresponding result for $N < 1$ is obtained by the substitution

$$M \to -iM', \quad N < 1, \tag{3.30}$$

where we define

$$M' = (1 - N^2)^{\frac{1}{2}} \quad (N < 1). \tag{3.31}$$

As we found in connection with (2.56), the dependence on the refractive index is a small correction when (1.1)

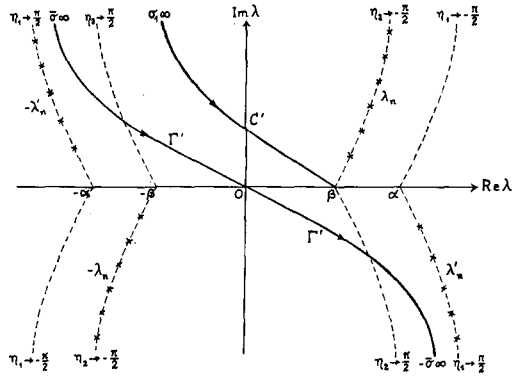

FIG. 6. The poles associated with the Debye expansion for $N > 1$. The path C' refers to (4.10) and the path Γ' to (4.18).

is valid, so that the poles λ_n are still very close to those found for an impenetrable sphere.

Similarly, in region 6a, with

$$\lambda = \alpha + e^{-i\pi/3}(\alpha/2)^{\frac{1}{3}}\xi, \tag{3.32}$$

we find [cf. Eqs. (A1) and (A2)]

$$[2\,\alpha] \approx e^{i\pi/3}(2/\alpha)^{\frac{1}{3}}\mathrm{Ai}'(-\xi)/\mathrm{Ai}(-\xi), \tag{3.33}$$

and

$$\begin{aligned}[1\,\beta] &\approx -(\lambda^2 - \beta^2)^{\frac{1}{2}}/\beta, \quad \text{if} \quad N > 1, \\ &\approx i(\beta^2 - \lambda^2)^{\frac{1}{2}}/\beta, \quad \text{if} \quad N < 1,\end{aligned} \tag{3.34}$$

so that the same procedure yields

$$\lambda'_n \approx \alpha + e^{-i\pi/3}N^{\frac{1}{3}}(x_n/\gamma) + N/M, \quad N > 1, \tag{3.35}$$

to which the substitution (3.30) is to be applied for $N < 1$.

The pole distribution for $N > 1$ is illustrated in Fig. 6. The asymptotic behavior of the poles λ_n as $n \to \infty$ is given by expressions very similar to (2.59)–(2.62), and analogous results (with obvious modifications) hold for the poles λ'_n.

Although the above approximations turn out to be adequate for most purposes in the present paper, we shall later require a better approximation to the poles λ_n. Complete asymptotic expansions for both λ_n and λ'_n have been derived by Streifer and Kodis.[28] Their results for λ_n are reproduced in Appendix A, together with the Schöbe asymptotic expansions for the cylindrical functions, on which their work is based. The case excluded by (1.1), in which $|N - 1| \sim \beta^{-\frac{2}{3}}$, has also been discussed in Ref. 28.

C. Discussion

The poles λ_n shown in Fig. 6 do not differ very much from those found for an impenetrable sphere, so that we expect them to be also associated with surface waves.

The poles λ'_n are located in the fourth quadrant, where ordinary Regge poles cannot appear at positive energy (Ref. 21, p. 51); their appearance is due entirely to the Debye expansion. However, except for their location in different quadrants, the pole distributions for λ_n and λ'_n have several features in common. This suggests that the poles λ'_n may be also associated with surface waves. It will be seen in Sec. 4E that this interpretation is indeed correct.

The next step will be to apply the modified Watson transformation to each term in the Debye expansion. As has already been mentioned in Sec. 1, the dominant contributions to the asymptotic behavior of each term are usually of the same type as for an impenetrable sphere, i.e., saddle-point contributions and residue-series contributions. The former correspond to the geometrical-optic rays in Fig. 5, so that for each term there is a finite (and, at least for the first few terms, small) number of saddle points. The latter, according to Fig. 6, are rapidly convergent, since the imaginary parts of λ_n and λ'_n increase rapidly with n. Thus, the modified Watson transformation leads to rapidly convergent asymptotic expansions for each term of the Debye series, in contrast with (2.5).

There remains to discuss the second problem referred to above, namely, the rapidity of convergence of the Debye series itself. Insofar as saddle-point contributions are concerned, they converge as rapidly as the corresponding geometrical-optic contributions, shown in Fig. 5. Their rate of convergence is determined by the damping produced at each internal reflection, i.e., by the Fresnel reflection coefficient at the interface. (If the sphere is not perfectly transparent, there is an additional damping of successive terms due to absorption, which increases the rapidity of convergence.) This in turn depends on the refractive index and on the angle θ_2 in Fig. 5, i.e., on the impact parameter of the incident ray. If we exclude the cases $N \gg 1$, $N \ll 1$, as in (1.3), the reflection coefficient is small for most directions, leading to fairly rapid convergence.

In the case of water, for instance, which will be of particular interest later on, we have $N \approx 1.33$, and it has been estimated by Van de Hulst (Ref. 4, p. 231) that more than 98.5% of the total intensity goes into the rays 1′, 2′, and 3′ of Fig. 5, corresponding to the first three terms of the Debye expansion. The remaining 1.5% must be distributed among higher-order terms and residue-series contributions.

Thus, in this case, residue-series contributions account only for a small fraction of the total intensity.

[28] W. Streifer and R. D. Kodis, Quart. Appl. Math. **21**, 285 (1964).

This does not preclude them from being large within narrow angular domains, concentrated about special directions. As will be seen in Paper II, this indeed happens in the glory region, where residue-series contributions become dominant over those associated with geometrical-optic rays.

We shall postpone the discussion of the rapidity of convergence of the Debye expansion for the residue-series contributions until we have found out more about their physical interpretation. It can already be expected, however, that they will converge much more slowly than the saddle-point contributions. In fact, as one increases the impact parameter of the incident ray, the reflection coefficient tends to increase, approaching unity in the limiting case of total reflection. This happens at glancing incidence for $N > 1$ and at critical incidence for $N < 1$. While the corresponding incident rays are totally reflected in the geometrical-optics approximation, it will be seen later that they are precisely the limiting rays responsible for the excitation of surface waves. According to the above discussion, high reflectivity implies slow convergence of the surface-wave contributions.

We can also note that $|\rho(\lambda, \beta)|$ in (3.17) is very close to unity within the edge domain (1.14), from which the residue-series contributions originate. Different damping mechanisms also arise in this case. In spite of the relatively slow convergence, however, it is possible to estimate the total residue-series contribution and to find out its physical effects. We shall return to the discussion of this point in Paper II (Sec. 6D).

D. Relation to Previous Treatments

Van de Hulst (Ref. 4, Chap. 12) applies the Debye expansion directly to the partial-wave series. He shows that the geometrical-optic contributions may be obtained by applying the principle of stationary phase to the domain (1.13); the forward diffraction peak also arises from this domain. He also gives a heuristic discussion of the contributions from the edge domain (1.14) (Ref. 4, Chap. 17).

The Debye expansion combined with the Watson transformation has been employed by several authors. The results agree insofar as geometrical-optic contributions are concerned, but they differ considerably in dealing with the remaining contributions.

For $N > 1$, the treatments most closely related to the present one are those given by Van der Pol and Bremmer,[10] Rubinow,[12] and Chen.[29] However, although the method is potentially more powerful, the results do not go beyond the derivation of the geometrical-optics approximation and the evaluation of some residue-series contributions within limited angular domains. No discussion of the domain of validity of the results is given, and the transition regions between different angular domains are not considered. In particular, the neighborhood of the forward and backward directions is not treated. Rubinow and Chen relate their results with Keller's geometrical theory of diffraction. However, the contribution from the poles λ'_n is omitted in their work.

Several investigations of the transparent cylinder or sphere problem have been made by Franz and Beckmann,[11,30–32] who propose somewhat different methods in each of them. They criticize Van der Pol and Bremmer for substituting the Debye expansion directly in the partial-wave series, claiming that $|\rho|$ is necessarily greater than unity for some partial wave near $\lambda = \alpha$, so that the expansion diverges. However, in view of (3.17), this criticism is unjustified: $|\rho| < 1$ for any real λ, and in particular at the physical points $\lambda = l + \frac{1}{2}$. It is true that $|\rho| \to 1$ as $\lambda \to \pm\infty$ [cf. Eq. (3.19)], but this also happens for Franz and Beckmann's contours, as will be seen below, so that an interpretation similar to (3.20) is required, although they are apparently unaware of this.

The starting point of their method is the representation (2.11); actually, they treat Green's function rather than the scattering amplitude. They then deform the lower half of the contour C (Fig. 1) into the lower half-plane, bringing it down to the negative imaginary axis[11] or to the negative real axis.[31,32] The Debye expansion is carried out along the modified contour.

This modification has a twofold purpose: (i) to find a contour along which $|\rho| < 1$. As shown in Appendix B (Fig. 21) one then has

$$\lim_{|\lambda| \to \infty} \rho = 0$$

along the lower part of the modified contour, and it can be shown that $|\rho| < 1$ along the negative imaginary axis. (ii) To avoid the appearance of contributions from the poles λ'_n. In fact, $S(\lambda, \beta)$ has no poles in the fourth quadrant, so that no poles are captured when the lower part of C sweeps across this quadrant, and the Debye expansion is only made afterwards. Franz and Beckmann claim that the residue series at the poles λ'_n have no physical interpretation, so that the poles are unphysical and should not contribute to the solution.

[29] Y. M. Chen, J. Math. Phys. **5**, 820 (1964).

[30] W. Franz and P. Beckmann, Trans. IRE, **AP-4**, 203 (1956).

[31] P. Beckmann and W. Franz, Z. Naturforsch. **12a**, 257 (1957).

[32] W. Franz, "Theorie der Beugung elektromagnetischer Wellen," Erg., Angew. Math., Band 4, §§16 and 19 (Springer-Verlag, Berlin, 1957).

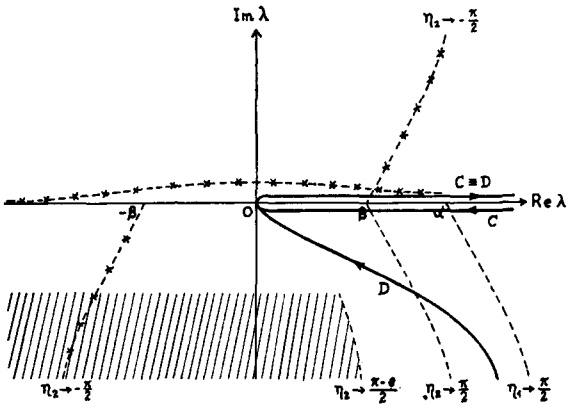

FIG. 7. Modification of the contour C in (2.11) according to Franz and Beckmann. The integrand tends to infinity in the shaded regions, to zero elsewhere, apart from the poles ×. The parameters η_1 and η_2 are defined by (B2).

To find out whether the modification proposed by Franz and Beckman is allowed, we must consider the asymptotic behavior of the integrand of (2.11) as $|\lambda| \to \infty$, which follows from Appendix B (Fig. 18) and from N [Eq. (C8)]. The behavior differs from that shown in Fig. 18 essentially by a factor $\lambda^{\frac{1}{2}}e^{i\lambda\theta}$ for $\operatorname{Im}\lambda > 0$ and $\lambda^{\frac{1}{2}}e^{-i\lambda\theta}$ for $\operatorname{Im}\lambda < 0$. It follows that the integrand tends to zero everywhere, except in the shaded region of Fig. 7.

Thus, while it is not possible to deform the lower half of C onto the negative imaginary axis, as proposed by Beckmann,[11] it is possible to move it across the line of poles λ'_n (curve $\eta_1 \to \pi/2$) and into the region where $\rho \to 0$ as $|\lambda| \to \infty$ (cf. Fig. 21, Appendix B). This leads to the contour D shown in Fig. 7.

Furthermore, after making the Debye expansion on D, it is possible, for the first term of the expansion, to deform the part of D located in the upper half-plane in order to obtain a path symmetric about the origin, which is another requirement in Franz and Beckmann's method. [If we had started from (2.10) instead of (2.11), it would have been possible to deform the lower part of C onto the negative imaginary axis. However, the last requirement could not then be satisfied, because the integrand of (2.10) (as well as the corresponding first term in the Debye expansion) diverges as $|\lambda| \to \infty$ over a portion of the upper half-plane, in such a way that no equivalent contour symmetric about the origin can be found.]

However, a modified contour, such as they propose, is not only unnecessary, but also inappropriate. In fact, as was shown above, the condition $|\rho| < 1$ is already satisfied along any bounded portion of C; it is unnecessary to get away from C in order to make use of the Debye expansion. It is true that $\rho \to 0$ along the part of D located in the lower half-plane, but we still have $|\rho| \to 1$ as $|\lambda| \to \infty$ along the upper portion of D. This is unavoidable, as shown in Appendix B (Fig. 21).

Furthermore, it is neither possible nor desirable to get rid of the contributions from the poles λ'_n. This can be seen already for the first term of the Debye expansion. As will be shown in Sec. 4, different representations are required for $\theta \gg \gamma$ and for $\theta \ll \gamma$. Franz and Beckmann's representation, avoiding the poles λ'_n, might be employed for $\theta \gg \gamma$. However, it cannot be continued to the domain $\theta \ll \gamma$ without including contributions from these poles.

For $N > 1$, we shall see that the contributions from the poles λ'_n are negligibly small (and consequently harmless). However, this is by no means so for $N < 1$. In this case, as will be seen in Sec. 4, the residue series at the poles λ'_n play an important role, and they have a clearcut physical interpretation. It will also be shown (cf. Sec. 4E) that there is no possible way to avoid them, since the contour that gives rise to the saddle-point contributions necessarily sweeps across the poles λ'_n as the scattering angle varies from 0 to π. We conclude that Franz and Beckmann's method is not suitable for the present problem.

For $N < 1$, there appears to be no treatment related to the present one. Chen's procedure for a cylinder, in this case,[33] is to deform the path of integration, before making the Debye expansion, into the path C' shown in Fig. 4, thereby capturing the residues at Regge poles located to the left and to the right of C', as well as at the poles located close to $\lambda = \alpha$ (exactly how many such poles are to be enclosed is not specified). He then applies the Debye expansion on C' and claims that all the integrals over C' can be evaluated by the saddle-point method (without further residue-series contributions, because C' is kept within the lines on which λ_n and λ'_n are located), yielding the geometrical-optic contributions. However, apart from the fact that C' is not suitable for saddle-point evaluation, it is contained within the region where $|\rho| \to \infty$ (cf. Fig. 21, Appendix B), so that the Debye expansion diverges. Thus, Chen's method cannot be applied.

Christiansen[34] starts with a contour similar to that employed by Beckmann[11]; after subtracting out the direct-reflection term, he deforms the path of integration for the remaining term [second term on the right in Eq. (3.14)] into the first quadrant, capturing the residues at the corresponding Regge poles.

[33] Y. M. Chen, J. Math. Phys. **6**, 1332 (1965).

[34] P. L. Christiansen, Report No. 1, Laboratory of Applied Mathematical Physics, Technical University of Denmark, Lingby, 1965.

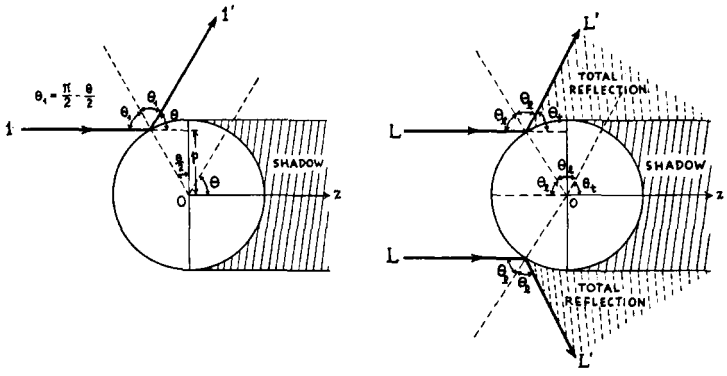

FIG. 8. Structure of the lit and shadow regions in the geometrical-optics approximation, for the first term of the Debye expansion. (a) $N > 1$; p is the impact parameter of the incident ray that is geometrically reflected in the direction θ. (b) $N < 1$; in this case, there is an additional shadow, bounded by the critically reflected rays L' (θ_l = critical angle for total reflection).

He then makes the Debye expansion over the resulting path of integration and applies the saddle-point method. Here again the Debye expansion is divergent on the resulting path. Furthermore, all Regge poles in the first quadrant (Fig. 4) contribute (not only those near $\lambda = \alpha$), and we have seen that the corresponding residue series, for $\alpha \gg 1$, converge no better than the partial-wave expansion.

4. THE FIRST TERM OF THE DEBYE EXPANSION

A. Preliminary Considerations

The first term of the Debye expansion is given by either one of the equivalent representations (3.22) or (3.25). In the geometrical-optics approximation, it is associated with rays directly reflected from the surface, without penetrating into the sphere, like the ray 1′ in Fig. 5.

To each term of the Debye expansion, associated with a certain class of rays, there correspond, in the geometrical-optics approximation, one or more "lit regions" and one or more "shadow regions," the latter being inaccessible to rays of this class (though not necessarily to rays of other classes!). The structure of these regions for the first term of the Debye expansion is shown in Fig. 8.

For $N > 1$, at finite distance, we have the geometrical shadow of the sphere, just as for an impenetrable sphere. For the scattering amplitude, which represents the field at infinity, this corresponds to the single direction $\theta = 0$ [Fig. 8(a)].

For $N < 1$, there is an additional shadow, bounded by the reflected rays L' corresponding to the critically incident rays L, that fall upon the surface at the critical angle,

$$\theta_l = \sin^{-1} N, \quad N < 1. \tag{4.1}$$

Beyond this region [Fig. 8(b)], total reflection occurs. It will be seen in Sec. 5 that the complementary region, $\theta > \pi - 2\theta_l$, is a shadow region for transmitted rays, and this remains true for all terms of the Debye expansion.

We shall see that around each shadow boundary there is a domain of angular width $\Delta\theta$, where the transition from the lit region to the shadow takes place. For an impenetrable sphere (N), such transitions were found to be described by "Fock-type" functions, and the corresponding angular width was given by (N, Fig. 14):

$$\Delta\theta \sim \gamma, \tag{4.2}$$

where γ is defined by (2.49). Transitions of this type will be called "normal." The scattering amplitude is given by different approximations within a transition region and on either side of it.

We shall consider first the case $N > 1$. The structure of the first term should then be very similar to that found for an impenetrable sphere, since the corresponding class of rays does not penetrate within the sphere. According to Fig. 8(a), different approximations should hold for $0 \leq \theta \leqslant \Delta\theta$ and for $\Delta\theta \ll \theta \leq \pi$; for an impenetrable sphere, $\Delta\theta$ was given by (4.2) (N, Sec. IX.D), and the same is true here.

The corresponding representations for $f_0(\beta, \theta)$ can be derived from (3.22) and (3.25) by the same procedure applied in N (Sec. IX.D). Let us define

$$S_0(\lambda, \beta) = \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} R_{22}(\lambda, \beta) = e^{2i\pi\lambda} S_0(-\lambda, \beta). \tag{4.3}$$

Then, as in N [Eq. (9.59)], it follows from (3.22) that

$$f_0(\beta,\theta)=\frac{i}{\beta}\sum_{m=0}^{\infty}(-1)^m \times\left\{\int_{-\infty}^{0}[e^{2i\pi\lambda}-S_0(\lambda,\beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)e^{2im\pi\lambda}\lambda\,d\lambda +\int_0^{\infty}[1-S_0(\lambda,\beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)e^{2im\pi\lambda}\lambda\,d\lambda\right\}. \quad (4.4)$$

The asymptotic behavior of $R_{22}(\lambda,\beta)$ as $|\lambda|\to\infty$ follows from Appendix B (Fig. 19). We find that $R_{22}\to -1$ in all regions, except for $-\pi/2<\eta_2<\pi/2$, where $R_{22}\to 0$ like λ^{-2}. Thus, except in this region, we have

$$S_0(\lambda,\beta)\approx S_{\text{imp}}(\lambda,\beta)=-H_\lambda^{(2)}(\beta)/H_\lambda^{(1)}(\beta), \quad \text{as } |\lambda|\to\infty, \quad (4.5)$$

where $S_{\text{imp}}(\lambda,\beta)$ is the S function for an impenetrable sphere [N, Eq. (3.1)].

Combining the above results with those given in N for the asymptotic behavior of $S_{\text{imp}}(\lambda,\beta)$, we find that $e^{2i\pi\lambda}-S_0(\lambda,\beta)$ tends to zero at least as fast as $e^{i\pi\lambda}$ in the second quadrant, so that the path of integration in the first integral of (4.4) may be shifted to the positive imaginary axis. To do this, we have to sweep across the poles $-\lambda_n'$ (Fig. 6), so that we get a corresponding residue-series contribution. Let

$$r_{0n}'=\text{residue } S_0(\lambda,\beta)\big|_{\lambda=\lambda_n'}.$$

Then, according to (4.3), we have

$$\text{residue } S_0(\lambda,\beta)\big|_{\lambda=-\lambda_n'}=-e^{-2i\pi\lambda_n'}r_{0n}', \quad (4.6)$$

so that we find

$$f_0(\beta,\theta)=\frac{i}{\beta}\sum_{m=0}^{\infty}(-1)^m \times\left\{\int_{i\infty}^{0}[e^{2i\pi\lambda}-S_0(\lambda,\beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)e^{2im\pi\lambda}\lambda\,d\lambda +\int_0^{\infty}[1-S_0(\lambda,\beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)e^{2im\pi\lambda}\lambda\,d\lambda\right\} +\frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n\lambda_n'r_{0n}' \times\exp[-2i(m+1)\pi\lambda_n']P_{\lambda_n'-\frac{1}{2}}(\cos\theta). \quad (4.7)$$

Writing

$$e^{2i\pi\lambda}-S_0(\lambda,\beta)=e^{2i\pi\lambda}-1+1-S_0(\lambda,\beta)$$

in the sum from $m=1$ to ∞, and employing N [Eq. (9.61)], we get, just as in N [Eqs. (9.62)–(9.65)],

$$\begin{aligned}f_0(\beta,\theta)=&-\frac{i}{\beta}\int_{i\infty}^{0}S_0(\lambda,\beta)P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda\\&+\frac{i}{\beta}\int_0^{\infty}[1-S_0(\lambda,\beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda\\&+\frac{2i}{\beta}\int_{i\infty}^{0}\frac{e^{2i\pi\lambda}}{1+e^{2i\pi\lambda}}P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda\\&+\frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n\lambda_n'r_{0n}'\\&\times\exp[-2i(m+1)\pi\lambda_n']P_{\lambda_n'-\frac{1}{2}}(\cos\theta)\\&+\frac{i}{\beta}\sum_{m=1}^{\infty}(-1)^m\left(\int_{i\infty}^{0}+\int_0^{\infty}\right)[1-S_0(\lambda,\beta)]\\&\times e^{2im\pi\lambda}P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda. \quad (4.8)\end{aligned}$$

It follows from (4.3)–(4.5) that the asymptotic behavior of $1-S_0(\lambda,\beta)$ in the first quadrant is the same as that for an impenetrable sphere, so that, as in N [Eq. (9.65)], the path of integration in the last term of (4.8) can be closed at infinity, reducing it to a residue series at the poles λ_n in the first quadrant (Fig. 6). Similarly, we can split the path of integration in the second term of (4.8) at $\lambda=\beta$ and combine it with the first term, as in N [Eqs. (9.67)–(9.69)], so that we finally get

$$f_0(\beta,\theta)=f_{01}+f_{02}+f_{03}+\tilde{f}_{0,\text{res}}+\tilde{f}_{0,\text{res}}', \quad (4.9)$$

where

$$\begin{aligned}f_{01}(\beta,\theta)+f_{02}(\beta,\theta)=&-\frac{i}{\beta}\int_{\sigma_1\infty}^{\beta}S_0(\lambda,\beta)P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda\\&+\frac{i}{\beta}\int_\beta^{\infty}[1-S_0(\lambda,\beta)]P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda, \quad (4.10)\end{aligned}$$

$$f_{03}(\beta,\theta)=\frac{i}{\beta}\int_0^{\beta}P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda+\Delta_1, \quad (4.11)$$

$$\Delta_1(\beta,\theta)=\frac{2i}{\beta}\int_{i\infty}^{0}\frac{e^{2i\pi\lambda}}{1+e^{2i\pi\lambda}}P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda, \quad (4.12)$$

$$\begin{aligned}\tilde{f}_{0,\text{res}}(\beta,\theta)=&\frac{2\pi}{\beta}\sum_{m=1}^{\infty}(-1)^m\sum_n\lambda_nr_{0n}\\&\times\exp(2im\pi\lambda_n)P_{\lambda_n-\frac{1}{2}}(\cos\theta), \quad (4.13)\end{aligned}$$

$$\begin{aligned}\tilde{f}_{0,\text{res}}'(\beta,\theta)=&\frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n\lambda_n'r_{0n}'\\&\times\exp[-2i(m+1)\pi\lambda_n']P_{\lambda_n'-\frac{1}{2}}(\cos\theta), \quad (4.14)\end{aligned}$$

and

$$r_{0n}=\text{residue } S_0(\lambda,\beta)\big|_{\lambda=\lambda_n}. \quad (4.15)$$

The path C' from $\sigma_1\infty$ to β is shown in Fig. 6. According to the above discussion on the behavior of $S_0(\lambda, \beta)$, the path must begin at infinity to the left of $\eta_2 \to -(\pi - \theta)/2$ (cf. also Fig. 10); in particular, any direction $\sigma_1\infty$ in the second quadrant may be chosen.

The representation (4.9)–(4.14) is exact and, just like its counterpart N, Eq. (9.78), it will be employed for

$$0 \leq \theta \ll \gamma. \tag{4.16}$$

To obtain the counterpart of N, Eq. (9.79), we might proceed just as in N, by transforming (4.7), but it is simpler to start from (3.25). By the same procedure that led from (2.11) to (2.14), we find that (3.25) is equivalent to

$$f_0(\beta, \theta) = \frac{1}{2\beta}\int_C [1 - S_0(\lambda, \beta)]P_{\lambda-\frac{1}{2}}(-\cos\theta)\frac{\lambda\, d\lambda}{\cos(\pi\lambda)}, \tag{4.17}$$

where C is the contour shown in Fig. 1.

The asymptotic behavior of the integrand as $|\lambda| \to \infty$ is essentially the same as that of (2.11), illustrated in Fig. 7. Thus, we can deform the lower half of C into the lower half of the contour Γ' shown in Fig. 6, going from $-\bar{\sigma}\infty$ to 0 (Γ' is symmetric about the origin). This gives rise to a residue-series contribution from the poles λ'_n. Similarly, the upper half of C can be deformed into the upper half of Γ', from 0 to $\bar{\sigma}\infty$, giving rise to a residue-series contribution from the poles λ_n. The result is

$$\begin{aligned} f_0(\beta, \theta) = &-\frac{1}{2\beta}\int_{\Gamma'}[1 - S_0(\lambda, \beta)]P_{\lambda-\frac{1}{2}}(-\cos\theta) \\ &\times \frac{\lambda\, d\lambda}{\cos(\pi\lambda)} - \frac{i\pi}{\beta}\sum_n \lambda_n r_{0n}\frac{P_{\lambda_n-\frac{1}{2}}(-\cos\theta)}{\cos(\pi\lambda_n)} \\ &- \frac{i\pi}{\beta}\sum_n \lambda'_n r'_{0n}\frac{P_{\lambda_n'-\frac{1}{2}}(-\cos\theta)}{\cos(\pi\lambda'_n)}. \end{aligned} \tag{4.18}$$

The integral can be split into two, corresponding to the two terms within square brackets (both are convergent for $\theta > 0$). The first of the resulting integrals identically vanishes, because its integrand is odd. The second integral can again be split into two according to the identity [N, Eq. (C5)]:

$$\begin{aligned} P_{\lambda-\frac{1}{2}}(-\cos\theta) = &\, ie^{-i\pi\lambda}P_{\lambda-\frac{1}{2}}(\cos\theta) \\ &- 2i\cos(\pi\lambda)Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta). \end{aligned} \tag{4.19}$$

Again, both integrals are separately convergent for $\theta > 0$, and the first one identically vanishes due to the antisymmetry of the integrand [cf. Eq. (4.3)]. Finally, substituting (2.12) in the first residue series of (4.18) and (2.13) in the second one, we get

$$f_0(\beta, \theta) = f_{0,g} + f_{0,\mathrm{res}} + f'_{0,\mathrm{res}}, \tag{4.20}$$

where

$$f_{0,g}(\beta, \theta) = -\frac{i}{\beta}\int_{\Gamma'} S_0(\lambda, \beta)Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda, \tag{4.21}$$

$$\begin{aligned} f_{0,\mathrm{res}}(\beta, \theta) = &-\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n \lambda_n r_{0n} \\ &\times \exp[i(2m+1)\pi\lambda_n]P_{\lambda_n-\frac{1}{2}}(-\cos\theta), \end{aligned} \tag{4.22}$$

and

$$\begin{aligned} f'_{0,\mathrm{res}}(\beta, \theta) = &-\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n \lambda'_n r'_{0n} \\ &\times \exp[-i(2m+1)\pi\lambda'_n]P_{\lambda_n'-\frac{1}{2}}(-\cos\theta). \end{aligned} \tag{4.23}$$

In view of the symmetry property (4.3), we may rewrite (4.21) as (cf. N, Eqs. (9.75)–(9.76)]:

$$\begin{aligned} f_{0,g}(\beta, \theta) = &\frac{i}{\beta}\int_{\bar{\sigma}\infty}^{0} S_0(\lambda, \beta)P_{\lambda-\frac{1}{2}}(-\cos\theta) \\ &\times e^{-i\pi\lambda}\tan(\pi\lambda)\lambda\, d\lambda, \end{aligned} \tag{4.24}$$

thus rendering manifest the regularity of all the above expressions at $\theta = \pi$.

The exact representation (4.20)–(4.24) is the counterpart of N, Eq. (9.79), and it will be employed for

$$\gamma \ll \theta \leq \pi. \tag{4.25}$$

Together with (4.9)–(4.14), it allows us to determine the asymptotic behavior of $f_0(\beta, \theta)$ for $0 \leq \theta \leq \pi$ and $N > 1$. The case $N < 1$ will be discussed in Sec. 4E.

B. Behavior for $N > 1$, $\theta \gg \gamma$, $\pi - \theta \gg \beta^{-\frac{1}{2}}$

Let us consider first the behavior of $f_0(\beta, \theta)$ for $N > 1$ and θ not too close to 0 or π. As in N [Eq. (9.9)], we shall see that the approximations below are valid for

$$\theta \gg \gamma, \quad \pi - \theta \gg \beta^{-\frac{1}{2}}. \tag{4.26}$$

In this domain, we employ (4.20)–(4.24).

Let us discuss first the behavior of (4.21), which is quite similar to that of N, Eq. (9.8), representing the directly reflected wave in the geometrical-optics approximation. As in N, Eq. (9.8), the main contribution to (4.21) arises from the neighborhood of a saddle point, located at [cf. N, Eq. (9.2)]

$$\bar{\lambda} = kp = \beta\cos(\theta/2). \tag{4.27}$$

The physical interpretation is the same as in N (Fig. 11): p is the impact parameter of the incident ray that is geometrically reflected from the surface in the direction θ; this is also shown in Fig. 8(a). We may again employ the approximation N, Eq. (6.14) for

$H_\lambda^{(2)}(\beta)/H_\lambda^{(1)}(\beta)$ and N, Eq. (C7) for $Q_{\lambda-\frac{1}{2}}^{(1)}(\cos\theta)$. There remains only to approximate R_{22} in (4.3).

In the neighborhood of $\lambda = \bar{\lambda}$, we can employ the Debye asymptotic expansion N, Eq. (A16), to evaluate $[1\,\beta]$, $[2\,\beta]$, and $[2\,\alpha]$ in (3.4), with the following result:

$$\beta[1\,\beta] = i(\beta^2 - \lambda^2)^{\frac{1}{2}} - \frac{\beta^2}{2(\beta^2 - \lambda^2)} + \mathcal{O}\left[\frac{\beta^2}{(\beta^2 - \lambda^2)^{\frac{3}{2}}}\right]. \tag{4.28}$$

To obtain $[2\,\beta]$, it suffices to replace i by $-i$, and $[2\,\alpha]$ is obtained by replacing β by α. Substituting these approximations in (3.4), we find

$$R_{22}(\lambda, \beta) \approx -\left(\frac{(\alpha^2 - \lambda^2)^{\frac{1}{2}} - (\beta^2 - \lambda^2)^{\frac{1}{2}}}{(\alpha^2 - \lambda^2)^{\frac{1}{2}} + (\beta^2 - \lambda^2)^{\frac{1}{2}}}\right) \times \left[1 + \frac{i\lambda^2}{(\beta^2 - \lambda^2)^{\frac{1}{2}}(\alpha^2 - \lambda^2)} + \cdots\right]. \tag{4.29}$$

Finally, substituting all the above approximations in (4.21) and making the change of variable

$$\lambda = \beta \cos w, \tag{4.30}$$

we get

$$f_{0,g}(\beta, \theta) = -e^{i\pi/4}\left(\frac{\beta}{2\pi \sin\theta}\right)^{\frac{1}{2}} \times \int B(w, \beta, \theta) \exp\left[i\beta\delta(w, \theta)\right] dw, \tag{4.31}$$

where

$$\delta(w, \theta) = 2\left[\left(w - \frac{\theta}{2}\right)\cos w - \sin w\right], \tag{4.32}$$

$$B(w, \beta, \theta) = \sin w(\cos w)^{\frac{1}{2}}\left(\frac{\sqrt{N^2 - \cos^2 w} - \sin w}{\sqrt{N^2 - \cos^2 w} + \sin w}\right) \times \left\{1 + \frac{i}{4\beta}\left[\frac{1}{\sin w} + \frac{\cot\theta}{2\cos w} + \frac{5}{3}\frac{\cos^2 w}{\sin^3 w} + \frac{4\cos^2 w}{\sin w(N^2 - \cos^2 w)}\right] + \mathcal{O}(\beta^{-2})\right\}, \tag{4.33}$$

and the path of integration is the image of Γ' (Fig. 6) in the w plane. For the application of the saddle-point method, the path is shifted so as to cross the real axis at the saddle point (4.27), i.e., at $\bar{w} = \theta/2$, $0 < \bar{w} < \pi/2$, at an angle of $-\pi/4$ with the real axis.

The formula for the saddle-point evaluation of (4.31), including the first correction term, has already been given in N [Eq. (6.21)]:

$$f_{0,g}(\beta, \theta) = -\frac{Be^{i\delta\beta}}{(|\delta''|\sin\theta)^{\frac{1}{2}}}\left\{1 - \frac{i}{2\beta\,|\delta''|}\left[\frac{B''}{B} + \frac{B'}{B}\frac{\delta'''}{|\delta''|} + \frac{5}{12}\left(\frac{\delta'''}{\delta''}\right)^2 + \frac{1}{4}\frac{\delta''''}{|\delta''|}\right] + \mathcal{O}(\beta^{-2})\right\}, \tag{4.34}$$

where B, δ, and their derivatives are to be evaluated at the saddle point $\bar{w} = \theta/2$. Substituting (4.32) and (4.33) in (4.34), we finally get

$$f_{0,g}(\beta, \theta) = -\frac{1}{2}\left(\frac{\sqrt{N^2 - \cos^2(\theta/2)} - \sin(\theta/2)}{\sqrt{N^2 - \cos^2(\theta/2)} + \sin(\theta/2)}\right) \times \exp\left(-2i\beta\sin(\theta/2)\right)\left\{1 + \frac{i}{2\beta}\left[\frac{1}{\sin^3(\theta/2)} - \frac{2N^2 - \cos^2(\theta/2)}{(N^2 - \cos^2(\theta/2))^{\frac{3}{2}}}\right] + \mathcal{O}(\beta^{-2})\right\}. \tag{4.35}$$

The main term of (4.35) is well known [cf. Ref. 12, Eq. (39)]. In the limit $N \to i\infty$, which would formally correspond to an impenetrable sphere, both the main term and the first correction term agree with the result found in N [Eq. (9.4)]. The main term differs from that result only by the replacement of the reflection coefficient $R = -1$ for an impenetrable sphere by the Fresnel reflection coefficient corresponding to the angle of incidence $\theta_1 = (\pi - \theta)/2$ [Fig. 8(a)]:

$$R = -\frac{\sin(\theta_1 - \theta_2)}{\sin(\theta_1 + \theta_2)} = -\frac{\sqrt{N^2 - \cos^2(\theta/2)} - \sin(\theta/2)}{\sqrt{N^2 - \cos^2(\theta/2)} + \sin(\theta/2)}. \tag{4.36}$$

Let us consider next the residue-series contribution from the poles λ_n, given by (4.22). The poles λ_n are given by (3.29), with sufficiently good approximation for our present purpose (a more accurate expansion is given in Appendix A). The residues r_{0n} follow from (4.15), (4.3), and (3.4):

$$r_{0n} = 4i/\{\pi\beta[H_{\lambda_n}^{(1)}(\beta)]^2\,\dot{d}(\lambda_n, \beta)\} \tag{4.37}$$

where

$$d(\lambda, \beta) = [1\,\beta] - N[2\,\alpha], \tag{4.38}$$

and the dot denotes a derivative with respect to λ; we have also made use of (3.6).

The asymptotic expansion of all functions required for the evaluation of (4.37) is given in Appendix A. If we keep only the dominant term in each expansion, we find

$$r_{0n} \approx e^{-i\pi/6}/2\pi\gamma a_n'^2, \tag{4.39}$$

where we have introduced the abbreviation

$$a_n' = \mathrm{Ai}'(-x_n), \tag{4.40}$$

and x_n is defined by (2.54). If necessary, higher-order

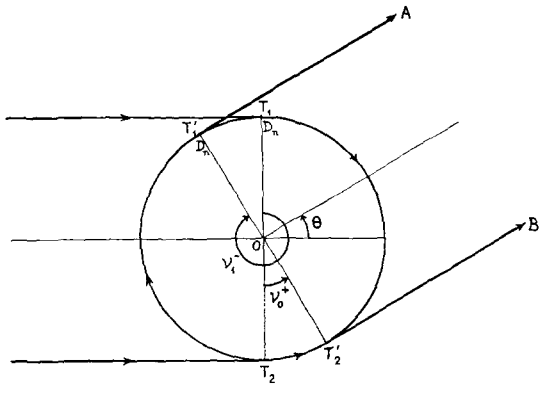

FIG. 9. Diffracted rays $T_1T_1'A$ and $T_2T_2'B$ in the direction θ.

corrections to (4.39) can easily be computed, with the help of Appendix A.

Substituting $P_{\lambda_n-\frac{1}{2}}(-\cos\theta)$ in (4.22) by its asymptotic expansion N, Eq. (C8), we finally get

$$f_{0,\mathrm{res}}(\beta,\theta) = \frac{1}{\beta}\left(\frac{2\pi}{\sin\theta}\right)^{\frac{1}{2}}\left\{e^{-i\pi/4}\sum_n \sqrt{\lambda_n}\, r_{0n}\exp(i\lambda_n\nu_0^+) + \sum_{m=1}^{\infty}(-1)^m\sum_n\sqrt{\lambda_n}\, r_{0n} \times\left[\exp\left(i\lambda_n\nu_m^- + i\frac{\pi}{4}\right) + \exp\left(i\lambda_n\nu_m^+ - i\frac{\pi}{4}\right)\right]\right\}, \quad (4.41)$$

where

$$\nu_m^{\pm} = 2m\pi \pm \theta, \quad m = 0, 1, 2, \cdots. \quad (4.42)$$

In particular, in the lowest-order approximation, in which r_{0n} is given by (4.39), the above result becomes formally identical to N, Eq. (9.5), the only difference (apart from notation) being in the expression for the poles λ_n.

The physical interpretation of this result is again the same as in N: the incident rays tangential to the sphere at T_1 and T_2 (Fig. 9) excite surface waves that travel around the sphere any number of times, giving rise to diffracted rays in the direction θ. The angles $\nu_m^{\pm}$ correspond to the total arc described along the surface (Fig. 9).

In the language of the geometrical theory of diffraction,[35] we can rewrite (4.41) as follows:

$$f_{0,\mathrm{res}}(\beta,\theta) = \frac{1}{(\sin\theta)^{\frac{1}{2}}}\left\{-i\sum_n D_n^2\exp(i\lambda_n\nu_0^+) + \sum_{m=1}^{\infty}(-1)^m\sum_n D_n^2 \times[\exp(i\lambda_n\nu_m^-) - i\exp(i\lambda_n\nu_m^+)]\right\}, \quad (4.43)$$

where

$$D_n^2 = e^{i\pi/4}(2\pi\lambda_n)^{\frac{1}{2}}r_{0n}/\beta \quad (4.44)$$

is the square of the *diffraction coefficient*. (Our diffraction coefficient differs from that of Levy and Keller[35] by an extra factor $a^{-\frac{1}{2}}$, to render it dimensionless.) One factor D_n corresponds to the excitation of a diffracted ray (e.g., at T_1, Fig. 9), and the other one to its reconversion into a tangentially emerging ray (e.g., at T_1', Fig. 9).

In the first-order approximation (4.39), Eq. (4.44) becomes

$$D_n^2 \approx \frac{e^{i\pi/12}}{(2\pi\beta)^{\frac{1}{2}}\gamma a_n'^2} = \frac{e^{i\pi/12}}{2\sqrt{\pi}\, a_n'^2}\left(\frac{2}{\beta}\right)^{\frac{1}{6}}. \quad (4.45)$$

This is identical to the result for an impenetrable sphere [cf. N, Eq. (9.5), and Ref. 35, p. 170]. [Chen's result for a cylinder [Ref. 29, Eq. (1.42)], although apparently different, can be shown to be equivalent to (4.45), by employing Ref. 29, Eq. (1.44).] Thus, to first order, not only the decay exponents, but also the diffraction coefficients associated with this class of rays are the same as those for an impenetrable sphere.

Finally, let us consider $f_{0,\mathrm{res}}'(\beta,\theta)$, which is given by (4.23). The expression for r_{0n}' differs from (4.37) only by the replacement of λ_n by λ_n'. Taking into account (3.33)–(3.35), we find

$$r_{0n}' \approx 2i(N/M)\exp(2M\beta - 2\lambda_n'\cosh^{-1}N) \quad (4.46)$$

and, similarly to (4.41),

$$f_{0,\mathrm{res}}'(\beta,\theta) \approx \frac{1}{\beta}\left(\frac{2\pi}{\sin\theta}\right)^{\frac{1}{2}} \times\sum_{m=0}^{\infty}(-1)^m\sum_n\sqrt{\lambda_n'}\, r_{0n}'\exp(-2im\pi\lambda_n') \times\{\exp[-i\lambda_n'(2\pi-\theta) - i(\pi/4)] - \exp[-i\lambda_n'\theta + i(\pi/4)]\}. \quad (4.47)$$

Since $\mathrm{Im}\,\lambda_n' < 0$, this is again a superposition of rapidly damped surface waves; however, as $\mathrm{Re}\,\lambda_n' > 0$, they travel around the sphere in the opposite sense to those in (4.41).

In order to estimate the order of magnitude of this contribution, we may substitute λ_n' by (3.35), taking into account only the contributions from the first few poles. We then find

$$f_{0,\mathrm{res}}'(\beta,\theta) \approx 2\frac{N^{\frac{3}{2}}}{M}\left(\frac{2\pi}{\beta\sin\theta}\right)^{\frac{1}{2}}\exp[-2\beta(N\cosh^{-1}N - M)] \times\sum_{m=0}^{\infty}(-1)^m\sum_n\exp[-2e^{-i\pi/3}x_n\cosh^{-1}N(\alpha/2)^{\frac{1}{3}}] \times\exp(-2im\pi\lambda_n')\{\exp[-i\lambda_n'\theta - i(\pi/4)] + \exp[-i\lambda_n'(2\pi-\theta) + i(\pi/4)]\}. \quad (4.48)$$

[35] B. R. Levy and J. B. Keller, Commun. Pure Appl. Math. **12**, 159 (1959).

Due to the presence of the over-all exponential factor outside of the sum, as well as the rapidly damped exponentials within the sum, $f'_{0,\mathrm{res}}(\beta, \theta)$ is exponentially small in comparison with $f_{0,\mathrm{res}}(\beta, \theta)$ [cf. Eq. (4.41)], and may therefore be neglected. This is true even for N close to unity, provided that condition (1.1) is verified.

Although $f'_{0,\mathrm{res}}(\beta, \theta)$ is completely negligible for $N > 1$, it will be seen in Sec. 4E that this is no longer true for $N < 1$. The result found in that case has a well-defined physical interpretation. It will then become clear that (4.48) represents the analytic continuation of that result to $N > 1$, in which process real rays are replaced by imaginary rays, giving rise to the real exponentials in (4.48). Thus, there is no reason either for calling this contribution unphysical or for trying to avoid it, as was done by Franz and Beckmann (cf. Sec. 3D).

Finally, let us show that the domain of validity of the above approximations is indeed given by (4.26). This follows from the following facts: (i) The Debye asymptotic expansion (4.28) employed in the neighborhood of $\bar{\lambda}$ is no longer valid when $\beta - \bar{\lambda} = \mathcal{O}(\gamma)$, i.e., by (4.27), when $\theta \leqslant \gamma$. Correspondingly, the WKB expansion (4.35) is rapidly convergent only for $\theta \gg \gamma$. (ii) The asymptotic expansions of the Legendre functions employed above are valid only for $\pi - \theta \gg \beta^{-\frac{1}{2}}$.

C. Behavior for $N > 1$, $\pi - \theta \leqslant \beta^{-\frac{1}{2}}$

The procedure to be employed near the backward direction is exactly the same as in N (Sec. IX.C). We start from (4.24) to compute $f_{0,g}(\beta, \theta)$. The only difference with respect to N [Eq. (9.45)] is an additional factor $-R_{22}(\lambda, \beta)$ in the integrand. Since the main contribution to the integral arises from $|\lambda| \leqslant \beta^{\frac{1}{2}}$ [N, Eq. (9.48); there was a misprint in this equation: the exponent should read $\frac{1}{2}$ instead of $-\frac{1}{2}$], we expand $-R_{22}$ in powers of λ, keeping only terms that yield corrections up to $\mathcal{O}(\beta^{-1})$. The result [cf. Eq. (4.29)] is

$$-R_{22}(\lambda, \beta) = \left(\frac{N-1}{N+1}\right)\left(1 + \frac{\lambda^2}{N\beta^2} + \cdots\right). \quad (4.49)$$

Let

$$\theta = \pi - \epsilon, \quad \epsilon \leqslant \beta^{-\frac{1}{2}}. \quad (4.50)$$

Then, proceeding exactly as in N (Sec. IX.C), and employing precisely the same notation, we find that $f_{0,g}(\beta, \pi - \epsilon)$ is given by N [Eq. (9.51)], multiplied by the over-all correction factor $(N-1)/(N+1)$, and with the following additional term within the square brackets:

$$-\frac{i}{N\beta}\int_0^\infty \exp(-x^2) J_0(\omega x) \tan(\pi\alpha x) x^3\, dx = \frac{1}{2N\beta}\left(1 + i\beta\frac{\epsilon^2}{4}\right)\exp\left(i\beta\frac{\epsilon^2}{4}\right) + \mathcal{O}(\beta^{-2}), \quad (4.51)$$

which arises from the term $\lambda^2/(N\beta^2)$ in (4.49). The integral has been evaluated by the procedure given in N, Appendix F.

Thus, we finally obtain, in the place of N [Eq. (9.53)],

$$f_{0,g}(\beta, \pi - \epsilon) = -\frac{1}{2}\left(\frac{N-1}{N+1}\right)\exp\left[-2i\beta\left(1 - \frac{\epsilon^2}{8}\right)\right] \times \left[1 + \frac{i}{2\beta} - \frac{i\beta\epsilon^4}{192} - \frac{i}{N\beta}\left(1 + i\beta\frac{\epsilon^2}{4}\right) + \mathcal{O}(\beta^{-2})\right], \quad 0 \leq \epsilon \leqslant \beta^{-\frac{1}{2}}. \quad (4.52)$$

This coincides with the expansion of (4.35) in powers of ϵ^2, within the domain $\epsilon \leqslant \beta^{-\frac{1}{2}}$. Thus, precisely as in N, we see that (4.35) is uniformly valid up to $\theta = \pi$. In the backward direction, we get the reflection coefficient (3.12).

The only modification that is necessary in $f_{0,\mathrm{res}}$ and $f'_{0,\mathrm{res}}$ is the substitution of the asymptotic expansion [N, Eq. (C8)] of the Legendre functions by the uniform asymptotic expansion [N, Eq. (C11)]. Finally, putting together all these results in (4.20), we obtain

$$\begin{aligned} f_0(\beta, \theta) \approx & -\frac{1}{2}\left(\frac{[N^2 - \cos^2(\theta/2)]^{\frac{1}{2}} - \sin(\theta/2)}{[N^2 - \cos^2(\theta/2)]^{\frac{1}{2}} + \sin(\theta/2)}\right)\exp(-2i\beta\sin(\theta/2)) \\ & \times \left\{1 + \frac{i}{2\beta}\left[\frac{1}{\sin^3(\theta/2)} - \frac{2N^2 - \cos^2(\theta/2)}{[N^2 - \cos^2(\theta/2)]^{\frac{3}{2}}}\right] + \mathcal{O}(\beta^{-2})\right\} \\ & - \frac{e^{i\pi/3}}{\gamma}\left(\frac{\pi - \theta}{\sin\theta}\right)^{\frac{1}{2}}\sum_{m=0}^{\infty}(-1)^m \sum_n (a'_n)^{-2}\exp[i(2m+1)\pi\lambda_n] J_0[\lambda_n(\pi - \theta)] \\ & + 4\pi\frac{N^2}{M}\left(\frac{\pi - \theta}{\sin\theta}\right)^{\frac{1}{2}}\exp[-2\beta(N\cosh^{-1}N - M)] \\ & \times \sum_{m=0}^{\infty}(-1)^m \sum_n \exp[-2e^{-i\pi/3}\cosh^{-1}N(\alpha/2)^{\frac{1}{3}}x_n]\exp[-i(2m+1)\pi\lambda'_n] J_0[\lambda'_n(\pi - \theta)], \\ & N > 1, \quad \gamma \ll \theta \leq \pi, \quad (4.53) \end{aligned}$$

which is uniformly valid throughout the whole domain (4.25). We have employed the approximation (4.39) for r_{0n}; a better approximation may be obtained, if necessary, from (4.37) and Appendix A.

The contribution from the residue series $f_{0,\mathrm{res}}$ is very small, except perhaps at the lower end of the range $\gamma \ll \theta$; that from the residue series $f'_{0,\mathrm{res}}$ is always negligible when (1.1) is satisfied.

D. Behavior for $N > 1$, $0 \leq \theta \leqslant \gamma$

In the domain $0 \leq \theta \leqslant \gamma$, we employ the representation (4.9)–(4.14). Let us evaluate first the contribution from (4.10). As we have seen in connection with the analogous terms in N, the main contribution to the integrals in (4.10) arises from the neighborhood of $\lambda = \beta$, so that we may employ the asymptotic expansions given in Appendix A.

In particular, it follows from (A11) and from the corresponding expansion for $H_\lambda^{(2)}(x)$ (obtained by changing $i \to -i$ everywhere) that

$$\frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} = e^{2i\pi/3}\frac{\bar{A}(\zeta)}{A(\zeta)} + \frac{e^{i\pi/6}\zeta^2}{120\pi A^2(\zeta)}\gamma^2 + \mathcal{O}(\gamma^4), \quad (4.54)$$

where

$$\zeta = \gamma(\lambda - \beta), \quad (4.55)$$

and we have introduced the abbreviations

$$A(\zeta) = \mathrm{Ai}\,(e^{2i\pi/3}\zeta), \quad \bar{A}(\zeta) = \mathrm{Ai}\,(e^{-2i\pi/3}\zeta). \quad (4.56)$$

We have also made use of the Wronskian relation (Ref. 36, p. 446):

$$W[A(\zeta), \bar{A}(\zeta)] = i/2\pi. \quad (4.57)$$

Similarly, employing (3.4), (A11), (A12), and the analogue of (4.28) for [2 α], we find

$$-R_{22}(\lambda, \beta) = 1 - \frac{\gamma}{2\pi M\bar{A}A} - \frac{e^{i\pi/6}A'}{2\pi M^2\bar{A}A^2}\gamma^2 - \frac{1}{2\pi M\bar{A}A}\left[\left(\frac{2}{15} + \frac{1}{2M^2}\right)\zeta + \frac{e^{i\pi/3}}{M^2}\frac{A'^2}{A^2} - \frac{\zeta^2}{60}\left(2e^{-i\pi/3}\frac{A'}{A} - \frac{i}{2\pi\bar{A}A}\right)\right]\gamma^3 + \mathcal{O}(\gamma^4), \quad (4.58)$$

where

$$A' = \mathrm{Ai}'\,(e^{2i\pi/3}\zeta). \quad (4.59)$$

Finally, combining (4.3) with (4.54) and (4.58), we find

$$-S_0(\lambda, \beta) = e^{2i\pi/3}\frac{\bar{A}}{A} + \frac{e^{-i\pi/3}}{2\pi MA^2}\gamma + \frac{1}{2\pi}\left(\frac{e^{i\pi/6}}{60}\frac{\zeta^2}{A^2} + \frac{e^{-i\pi/6}}{M^2}\frac{A'}{A^3}\right)\gamma^2 + \frac{e^{-i\pi/3}}{2\pi M}\left[\left(\frac{2}{15} + \frac{1}{2M^2}\right)\frac{\zeta}{A^2} + \frac{e^{i\pi/3}}{M^2}\frac{A'^2}{A^4} - \frac{e^{-i\pi/3}}{30}\frac{A'}{A^3}\zeta^2\right]\gamma^3 + \mathcal{O}(\gamma^4). \quad (4.60)$$

The corresponding expansion for $1 - S_0(\lambda, \beta)$ can be obtained by noting that [cf. N, Eq. (D3)]:

$$1 - e^{2i\pi/3}\frac{\bar{A}}{A} = e^{i\pi/3}\frac{\mathrm{Ai}\,(\zeta)}{A}. \quad (4.61)$$

In the angular domain under consideration, the uniform asymptotic expansion [N, Eq. (C11)] of the Legendre function becomes

$$P_{\lambda-\frac{1}{2}}(\cos\theta) = (\theta/\sin\theta)^{\frac{1}{2}}J_0 + \mathcal{O}(\gamma^4), \quad (4.62)$$

where we have employed the abbreviation

$$J_0 = J_0(\beta\theta + (\theta/\gamma)\zeta) = J_0[\beta\theta(1 + \tfrac{1}{2}\zeta\gamma^2)]. \quad (4.63)$$

Substituting the above results in(4.10), we obtain

$$f_{01}(\beta, \theta) + f_{02}(\beta, \theta) = \frac{i}{\gamma}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\left\{e^{2i\pi/3}\int_{\sigma_1\infty}^{0}(1 + \tfrac{1}{2}\zeta\gamma^2)\frac{\bar{A}}{A}J_0\,d\zeta + e^{i\pi/3}\int_0^\infty(1 + \tfrac{1}{2}\zeta\gamma^2)\frac{\mathrm{Ai}\,(\zeta)}{A}J_0\,d\zeta + \frac{e^{-i\pi/3}}{2\pi M}\gamma\int_\Gamma\frac{J_0}{A^2}d\zeta + \frac{\gamma^2}{2\pi}\left(\frac{e^{i\pi/6}}{60}\int_\Gamma\frac{\zeta^2}{A^2}J_0\,d\zeta + \frac{e^{-i\pi/6}}{M^2}\int_\Gamma\frac{A'}{A^3}J_0\,d\zeta\right) + \frac{e^{-i\pi/3}\gamma^3}{2\pi M}\left[\left(\frac{2}{15} + \frac{N^2}{2M^2}\right)\int_\Gamma\frac{\zeta}{A^2}J_0\,d\zeta + \frac{e^{i\pi/3}}{M^2}\int_\Gamma\frac{A'^2}{A^4}J_0\,d\zeta - \frac{e^{-i\pi/3}}{30}\int_\Gamma\zeta^2\frac{A'}{A^3}J_0\,d\zeta\right] + \mathcal{O}(\gamma^4)\right\}, \quad (4.64)$$

where

$$\int_\Gamma = \int_{\sigma_1\infty}^0 + \int_0^\infty. \quad (4.65)$$

As we have seen in connection with (4.10), $\sigma_1\infty$ may be any direction in the second quadrant. It is convenient to choose it in such a way that the integrands in (4.64) decrease as rapidly as possible away from $\zeta = 0$. It follows from the asymptotic behavior of the Airy function [N, Eq. (D4)] that the best choice is

$$\sigma_1 = e^{2i\pi/3}, \quad (4.66)$$

[36] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (National Bureau of Standards, Washington, 1964).

so that the path Γ is composed of a straight line from $e^{2i\pi/3}\infty$ to 0 and the positive real axis from 0 to ∞, as in N (Fig. 10). All the integrands in (4.64) then behave like

$$\exp\left(-\tfrac{4}{3}|\zeta|^{\frac{3}{2}}\right)$$

for large $|\zeta|$, so that only the domain $|\zeta| \leqslant 1$ gives an appreciable contribution.

The first two integrals in (4.64) correspond to the Fock-type functions that appeared in N [Eq. (9.13)]. Both these and the remaining integrals can be reduced, by partial integration, to *generalized Fock functions*, defined by

$$F_{m,n}(\beta, \theta) = \frac{e^{i\pi/6}}{2\pi}\int_\Gamma \frac{\zeta^m}{\mathrm{Ai}^2(e^{2i\pi/3}\zeta)} J_n(\beta\theta + (\theta/\gamma)\zeta)\, d\zeta, \tag{4.67}$$

where m and n are integers. The reduction is performed in Appendix C. Taking into account (C3)–(C7), Eq. (4.64) becomes

$$\begin{aligned} f_{01}(\beta, \theta) + f_{02}(\beta, \theta) &= i\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\left[-\frac{J_1(\beta\theta)}{\theta} + \frac{1}{\theta}\left(1 + \frac{\theta^2}{2M^2}\right)F_{0,1}\right. \\ &\quad + \frac{\gamma^2}{2\theta}F_{1,1} - \frac{i}{M}\left(1 + \frac{e^{-i\pi/3}\theta^2}{12M^2}\right)F_{0,0} \\ &\quad + \frac{\gamma}{60}F_{2,0} - \frac{i(4N^2-3)\gamma^2}{6M^3}F_{1,0} \\ &\quad \left. - \frac{e^{i\pi/6}\theta^2}{12M^3}F_{0,2} + \frac{i\theta\gamma}{60M}F_{2,1} + \mathcal{O}(\gamma^3)\right]. \end{aligned} \tag{4.68}$$

On the other hand, $f_{03}(\beta, \theta)$, as defined in (4.11)–(4.12), has already been evaluated in N [Eqs. (9.21) and (9.70)]:

$$f_{03}(\beta, \theta) = i\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\frac{J_1(\beta\theta)}{\theta} + \mathcal{O}(\gamma^3), \tag{4.69}$$

which corresponds to the well-known forward diffraction peak.

The residue-series contributions are given by (4.13) and (4.14), where the Legendre function may be replaced by N, Eq. (C11). Taking into account (4.39) and (4.46), and adding the results to (4.68) and (4.69), we finally get from (4.9)

$$\begin{aligned} f_0(\beta, \theta) &= i\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\left\{\frac{1}{\theta}\left(1 + \frac{\theta^2}{2M^2}\right)F_{0,1} + \frac{\gamma^2}{2\theta}F_{1,1} - \frac{i}{M}\left(1 + \frac{e^{-i\pi/3}\theta^2}{12M^2}\right)F_{0,0} + \frac{\gamma}{60}F_{2,0}\right. \\ &\quad - \frac{i(4N^2-3)\gamma^2}{6M^3}F_{1,0} - \frac{e^{i\pi/6}\theta^2}{12M^3}F_{0,2} + \frac{i\theta\gamma}{60M}F_{2,1} + \mathcal{O}(\gamma^3) - \frac{e^{i\pi/3}}{\gamma} \\ &\quad \times \sum_{m=1}^{\infty}(-1)^m \sum_n (a_n')^{-2}\exp(2im\pi\lambda_n)J_0(\lambda_n\theta) + \frac{4\pi N^2}{M}\exp\left[-2\beta(N\cosh^{-1}N - M)\right] \\ &\quad \left. \times \sum_{m=0}^{\infty}(-1)^m \sum_n \exp\left[-2i(m+1)\pi\lambda_n'\right]\exp\left[-2e^{-i\pi/3}\cosh^{-1}N(\alpha/2)^{\frac{1}{3}}x_n\right]J_0(\lambda_n'\theta)\right\}, \quad N > 1, \quad 0 \leq \theta \leqslant \gamma. \end{aligned} \tag{4.70}$$

For $N \to i\infty$, this reduces to the result found for an impenetrable sphere in N [Eq. (9.42)], where only the first two terms of (4.64) were taken into account.

In particular, within the diffraction peak region $0 \leq \theta \ll \gamma$, we can expand the generalized Fock functions in power series in the small parameter θ/γ, by substituting in (4.67) the Taylor expansion

$$J_n(\beta\theta + (\theta/\gamma)\zeta) = \sum_{p=0}^{\infty} J_n^{(p)}(\beta\theta)(\theta\zeta/\gamma)^p/p!. \tag{4.71}$$

Since the main contribution to the integrals arises from $|\zeta| \leqslant 1$, the resulting series is rapidly convergent for $\theta/\gamma \ll 1$.

It follows from N [Eqs. (8.23) and (8.26)] that

$$\frac{e^{i\pi/6}}{2\pi}\int_\Gamma \frac{\zeta^p}{\mathrm{Ai}^2(e^{2i\pi/3}\zeta)}\, d\zeta = pM_{p-1}, \tag{4.72}$$

where

$$pM_{p-1} = 1 \quad \text{for} \quad p = 0, \quad M_0 = 1.2551e^{i\pi/3},$$
$$M_1 = 0.5323e^{2i\pi/3}, \quad M_2 = 0.09352. \tag{4.73}$$

The values of the coefficients M_p are taken from Wu,[37] who also computed them for higher values of p.

Substituting (4.71) and (4.72) in (4.67), we find

$$F_{m,n}(\beta, \theta) = \sum_{p=0}^{\infty}\frac{(m+p)}{p!}M_{m+p-1}J_n^{(p)}(\beta\theta)\left(\frac{\theta}{\gamma}\right)^p. \tag{4.74}$$

Replacing the generalized Fock functions in (4.70)

[37] T. T. Wu, Phys. Rev. **104**, 1201 (1956).

by their expansions (4.74), we find

$$f_0(\beta,\theta) = i\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\left\{\frac{J_1(\beta\theta)}{\theta} + \left[\frac{M_0}{\gamma} - \frac{i}{M} + \tfrac{8}{15}M_1\gamma - \frac{iM_0(4N^2-3)}{6M^3}\gamma^2 + \mathcal{O}(\gamma^3)\right.\right.$$
$$\left. - \frac{e^{i\pi/3}}{\gamma}\sum_{m=1}^{\infty}(-1)^m\sum_n (a_n')^{-2}\exp(2im\pi\lambda_n)\right]J_0(\beta\theta)$$
$$\left. - \left[\frac{M_1}{\gamma} - \frac{iM_0}{M} + \frac{1}{2}\left(\tfrac{8}{5}M_2 - \frac{1}{M^2}\right)\gamma + \mathcal{O}(\gamma^2)\right]\frac{\theta}{\gamma}J_1(\beta\theta) + \mathcal{O}\left(\frac{\theta^2}{\gamma^2}\right)\right\}, \quad N > 1, \quad 0 \leq \theta \ll \gamma. \quad (4.75)$$

Here, we have approximated $J_0(\lambda_n\theta) \approx J_0(\beta\theta)$ in the first residue series of (4.70), and we have entirely neglected the contribution from the second residue series, which is indeed negligible under the present conditions.

For $N \to i\infty$, (4.75) agrees with N [Eq. (9.33)], to the order of accuracy computed there. The first term of (4.75), which corresponds to the forward diffraction peak, again dominates the amplitude for $\theta \ll \gamma$.

Finally, for $\theta \gg \gamma$, (4.70) goes over smoothly into (4.53). This has already been proved in N [Eq. (9.41)], for the dominant term in the amplitude, which is the same as here, so that the proof need not be repeated.

The results (4.53) and (4.70) give the value of $f_0(\beta, \theta)$ for all directions, $0 \leq \theta \leq \pi$. We see that the domain $\theta \sim \gamma$ is a normal (Fock-type) transition region. In this region, tables of generalized Fock functions would be required for a numerical evaluation.

E. Behavior for $N < 1$

Let us now take $N < 1$. In this case, as shown in Fig. 8(b), all rays incident at an angle $\theta_1 > \theta_t$ are totally reflected, where θ_t is the critical angle, given by (4.1). There is a corresponding shadow boundary at $\theta = \theta_t$, where

$$\theta_t = \pi - 2\theta_t = 2\cos^{-1}N. \quad (4.76)$$

The same shadow boundary, as will be seen later, appears in all the terms of the Debye expansion.

The existence of this shadow boundary leads to a subdivision into three different angular regions:

$$\begin{aligned} &\text{(i)} && \theta - \theta_t \gg \Delta\theta; \\ &\text{(ii)} && |\theta - \theta_t| \lesssim \Delta\theta; \\ &\text{(iii)} && \theta_t - \theta \gg \Delta\theta. \end{aligned} \quad (4.77)$$

We shall see that the width $\Delta\theta$ of the transition region is again given by (4.2), although it is not a normal transition. From the point of view of geometrical optics, region (iii) is where total reflection occurs, whereas only partial reflection takes place in (i). Furthermore, there is still a forward diffraction peak in region (iii), so that we still have to distinguish $\theta \gg \gamma$ and $\theta \lesssim \gamma$ within it.

As shown in Fig. 10, the distinction between regions (i) and (iii) is reflected in the position of the saddle point associated with (4.21). The saddle point $\bar{\lambda}$ is still given by (4.27), so that $\bar{\lambda} < \alpha$ in region (i) (point $\bar{\lambda}_1$ in Fig. 10) and $\bar{\lambda} > \alpha$ in region (iii) (point $\bar{\lambda}_2$ in Fig. 10). The path of integration Γ' crosses the real axis at the saddle point, at an angle of $-\pi/4$, and it must begin and end at infinity outside of the shaded regions in Fig. 10. [The asymptotic behavior of the integrand of (4.21) follows from Appendix B and from N (Appendices A and C). The shaded regions are those where the integrand diverges at infinity, where η_1 and η_2 are defined by (B2).] Thus, as we go through the transition region (ii), the path Γ' sweeps across the poles λ_n'; consequently, as had already been mentioned in Sec. 3D, there is no way to avoid the contributions from these poles.

Let us consider first the behavior of $f_0(\beta, \theta)$ in region (i), still using the representation (4.20)–(4.23). The corresponding path of integration Γ_1' in (4.21) (Fig. 10) does not differ in any way from the path for $N > 1$, so that we obtain precisely the same result (4.35) as before. The only question to be considered is that of the domain of validity of this result.

The expression (4.29) for R_{22} depends upon the validity of the Debye asymptotic expansion for

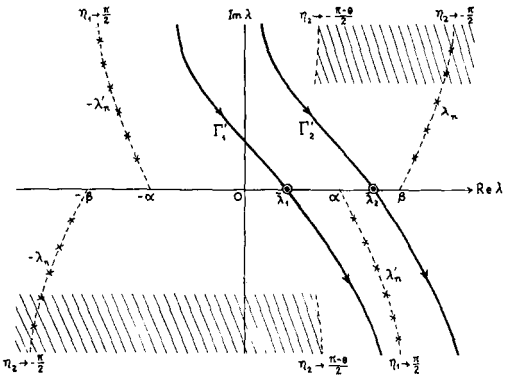

FIG. 10. For $N < 1$, the path of integration in (4.21) must begin in the upper half-plane, to the left of the shaded region, and end in the lower half-plane, to the right of the shaded region, going over a saddle point ○ that, for $\theta > \theta_t$, is to the left of $\lambda = \alpha$ (e.g., at $\bar{\lambda}_1$) and, for $\theta < \theta_t$, is to the right of $\lambda = \alpha$ (e.g., at $\bar{\lambda}_2$). ×—poles.

[2 α]. Thus,

$$|\alpha - \lambda| \gg \alpha^{\frac{1}{3}} \tag{4.78}$$

must be satisfied within the relevant portion of the domain of integration. The distance of closest approach from $\lambda = \alpha$ to the path of integration is of the order of $\alpha - \bar{\lambda}$, so that (4.78) must be valid for $\lambda = \bar{\lambda}$. Taking into account (4.27) and (4.76), this leads to

$$\theta - \theta_t \gg N^{\frac{1}{3}}\gamma^2/M' \tag{4.79}$$

where M' is defined by (3.31). Exactly the same condition is found from the requirement that the first correction term in the WKB expansion (4.35), involving the denominator

$$\beta(N^2 - \cos^2\theta/2)^{\frac{3}{2}} = \beta(\cos^2(\theta_t/2) - \cos^2(\theta/2))^{\frac{3}{2}}, \tag{4.80}$$

must be small.

According to (1.1), the domain (4.79) falls within region (i). [It may overlap with (ii), depending on the value of N.] On the other hand, as we have seen in (4.52), the approximation (4.35) remains valid up to $\theta = \pi$.

The contribution $f_{0,\text{res}}$ from the poles λ_n is still given by (4.41), the only difference being that the substitution (3.30) must be made in the expression (3.29) for the poles. The physical interpretation remains unchanged: these terms correspond to the surface waves excited by the tangentially incident rays, and, as before, their damping is determined almost completely by the geometry.

In contrast with the case $N > 1$, however, the poles λ'_n now give a significant contribution, corresponding to an entirely new type of surface waves. The result for $f'_{0,\text{res}}$ is given by (4.23), where (4.46) is now to be replaced by

$$r'_{0n} \approx -(2N/M')\exp(-2iM'\beta + 2i\lambda'_n\cos^{-1}N), \tag{4.81}$$

so that (4.48) becomes

$$f'_{0\text{res}}(\beta,\theta) \approx \frac{2e^{i\pi/4}N^{\frac{3}{2}}}{M'}\left(\frac{2\pi}{\beta\sin\theta}\right)^{\frac{1}{2}}\exp(-2iM'\beta) \times\left\{\sum_n \exp(-i\lambda'_n\zeta^+_{1,0}) + \sum_{m=1}^{\infty}(-1)^m \times\sum_n[\exp(-i\lambda'_n\zeta^+_{1,m}) - i\exp(-i\lambda'_n\zeta^-_{1,m})]\right\}, \quad \pi - \theta \gg \beta^{-\frac{1}{2}}, \tag{4.82}$$

where

$$\zeta^{\pm}_{1,m} = 2m\pi - \theta_t \pm \theta, \quad m = 0, 1, 2, \cdots, \tag{4.83}$$

and θ_t is given by (4.76).

The geometrical interpretation of the angles $\zeta^+_{1,0}$ and $\zeta^-_{1,1}$ is shown in Fig. 11(a). The surface waves in

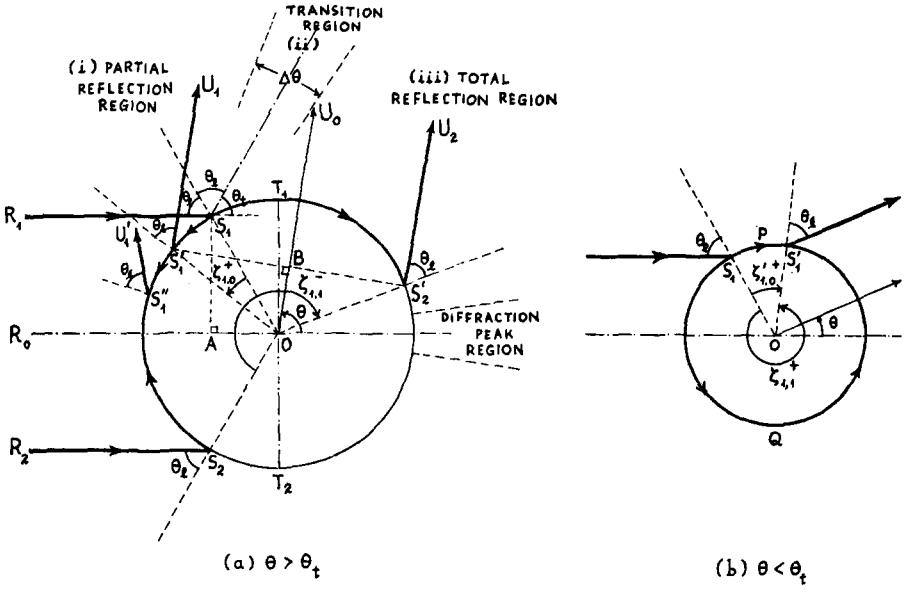

FIG. 11. Geometrical interpretation of (4.82) and (4.83). (a) The angles $\zeta^+_{1,0}$ and $\zeta^-_{1,1}$ correspond to the rays $R_1S_1S'_1U_1$ and $R_2S_2S'_2U_2$, respectively ($\theta > \theta_t$). The path difference with respect to the central path R_0OU_0 is $\overline{OA} + \overline{OB}$. The subdivision into regions is also indicated. The diffracted ray $R_1S_1S'_1S''_1U'_1$ appears in the second term in the Debye expansion [cf. Eq. (5.66)]. (b) For $\theta < \theta_t$, $\zeta^+_{1,0}$ is to be replaced by $\zeta^+_{1,1} = 2\pi + \zeta^+_{1,0}$. According to the geometrical theory of diffraction, the diffracted ray would propagate clockwise, as $S_1PS'_1$, corresponding $\zeta^+_{1,0} = 2\pi - \zeta^+_{1,1} = -\zeta^+_{1,0}$.

(4.82) are excited by the critically incident rays R_1S_1, R_2S_2. Their complex propagation constant λ'_n is given by (3.35), so that they travel along the surface on the inner side, with phase velocity slightly smaller than c/N and angular damping constant

$$\approx (\sqrt{3}/2)(\alpha/2)^{\frac{1}{3}}x_n.$$

In terms of diffracted rays, the surface ray excited by the critically incident ray R_1S_1 gives rise to the diffracted ray S'_1U_1 in the direction θ, leaving the surface at the critical angle θ_i, so that the arc $S_1S'_1$ travelled along the surface corresponds to the angle $\zeta^+_{1,0}$; similarly $\zeta^+_{1,m}$ includes m additional turns around the sphere. The path difference with respect to the central ray R_0OU_0 [Fig. 11(a)] is $\overline{OA} + \overline{OB} = 2a\cos\theta_i = 2M'a$, which accounts for the phase factor $\exp(-2iM'\beta)$ in (4.82). Similar considerations apply to the ray $R_2S_2S'_2U_2$.

These diffracted rays obey a peculiar "law of refraction": although the *magnitudes* of the angles of incidence and refraction are given by Snell's law, they have opposite signs: both upon entering and upon leaving the surface, *the incident and "refracted" rays lie on the same side of the normal!*

This result is in disagreement with the geometrical theory of diffraction.[16,33] According to this theory, the diffracted rays associated with the critically incident rays R_1S_1 and R_2S_2 would obey the ordinary law of refraction both at the point of excitation and at the point where they leave the surface. This is illustrated in Fig. 11(b), which refers to the case $\theta < \theta_i$: according to the geometrical theory of diffraction, the diffracted ray would travel *clockwise*, along the path $S_1PS'_1$, corresponding to the angle $\zeta'^+_{1,0} = -\zeta^+_{1,0}$; according to the present results, it follows the *anticlockwise* path $S_1QS'_1$, corresponding to the angle $\zeta^+_{1,1}$. Thus, although the entry and exit points are the same, the results are quite different.

In the case of a plane interface (Fig. 12), a critically incident ray RS gives rise, as is well known, to a surface wave SV travelling along the interface in the optically rare medium, so that the corresponding ray obeys Snell's law. At each point along its path (such as S', S'' in Fig. 12), the surface wave sheds rays back into the dense medium at the critical angle, again obeying Snell's law. This gives rise to a conical wave in the dense medium, the Schmidt head wave, which has been investigated theoretically and experimentally (Ref. 4, pp. 366 and 380).

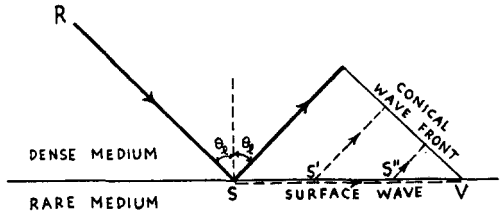

FIG. 12. The Schmidt head wave.

Thus, if we approximate the sphere surface locally by its tangent plane at the entry and exit points (as is done in geometrical optics), we are led to the prediction of the geometrical theory of diffraction. It seems at first sight very surprising that the surface waves actually found in (4.82) travel in the opposite sense around the sphere.

It was precisely to avoid the seemingly "unphysical" contributions from the poles λ'_n that Franz and Beckmann proposed their modified contours. However, as has already been seen in Sec. 3D, their proposal does not achieve its purpose, nor does it lead to the diffracted rays predicted by the geometrical theory of diffraction. Such rays would correspond to poles in the *first* quadrant, near $\lambda = \alpha$.

Chen[33] has tried to identify such poles with the Regge poles closest to $\lambda = \alpha$ in Fig. 4, by enclosing them with the contour C' *before* making the Debye expansion. However, as was mentioned in Sec. 3D, this is not allowed, because the Debye expansion diverges on C' (also, C' is not suitable for applying the saddle-point method). Furthermore, according to the discussion in Secs. 2 and 3, the Regge poles associated with the original partial-wave series have a very different physical interpretation as compared with those associated with the Debye expansion.

Streifer and Kodis[38] found surface waves similar to those of Fig. 11(a) in the case of a dielectric cylinder, but considered their physical interpretation unsatisfactory.

Since the path of integration in the saddle-point method must sweep across the poles λ'_n (Fig. 10), it is clear that one cannot obtain the geometrical-optics contribution without including also the contributions from these poles, so that any attempt to get rid of them is of no avail.

The interpretation of the surface waves found in (4.82) in terms of diffracted rays disagrees with the geometrical theory of diffraction only with respect to the sense of propagation around the sphere. There is, however, a very good physical reason why this should indeed be so.

Physically, the role played by the surface waves is to describe *the field penetration into shadow regions:* their exponential damping is characteristic of the shadow produced by a curved surface (cf. N, p. 83).

[38] W. Streifer and R. D. Kodis, Quart. Appl. Math. **22**, 193 (1964).

They are always excited at the border between lit and shadow regions on the surface. Therefore, one must expect that *surface waves always travel away from the shadow boundary into the shadow* (rather than into the lit region). Otherwise, a smooth transition between lit and shadow regions, with the exponential damping starting at the boundary and proportional to the angle of penetration into the shadow, would not be possible.

For an impenetrable sphere (N, p. 39), as well as for a transparent sphere with $N > 1$, the requirement of propagation into the shadow always leads to agreement with the geometrical theory of diffraction. For $N < 1$, however, the domain $\theta > \theta_t$ is a shadow region for transmitted rays [cf. Fig. 13(b)], and the requirement that the surface waves excited at S_1 and S_2 (Fig. 11) must propagate into the shadow leads precisely to the sense of propagation that we have found. The geometrical theory of diffraction would lead to surface waves propagating into the lit region, which is physically unacceptable.

Since the geometrical theory has met with considerable success in the treatment of a large class of problems, it would be interesting to modify its formulation, taking into account the physical requirements about the sense of propagation of surface waves. The local behavior of a ray is determined not only by the tangential plane, but also by the distinction between shadow and lit sides.

We also see now that, although $f'_{0,\mathrm{res}}(\beta, \theta)$ is negligible for $N > 1$, the expression (4.48) is simply the analytic continuation of the result (4.82) found for $N < 1$ [cf. Eq. (3.30)].

The domain where the residue series (4.82) is rapidly convergent is determined by the condition

$$|\mathrm{Im}\ \lambda'_1|\ \zeta^+_{1,0} \gg 1,$$

i.e., according to (3.35) and (4.83),

$$\theta - \theta_t \gg (N\beta)^{-\frac{1}{3}} \sim \gamma. \tag{4.84}$$

Finally, in order to obtain expressions that remain valid up to $\theta = \pi$, it is necessary to employ the uniform asymptotic expansion [N, Eq. (C11)] of the Legendre functions. Putting together all of the above results, we finally obtain

$$\begin{aligned} f_0(\beta, \theta) \approx & -\frac{1}{2}\left(\frac{[N^2 - \cos^2(\theta/2)]^{\frac{1}{2}} - \sin(\theta/2)}{[N^2 - \cos^2(\theta/2)]^{\frac{1}{2}} + \sin(\theta/2)}\right) \exp(-2i\beta \sin(\theta/2)) \\ & \times \left\{1 + \frac{i}{2\beta}\left[\frac{1}{\sin^3(\theta/2)} - \frac{2N^2 - \cos^2(\theta/2)}{(N^2 - \cos^2(\theta/2))^{\frac{3}{2}}}\right] + \mathcal{O}(\beta^{-2})\right\} - \frac{e^{i\pi/3}}{\gamma}\left(\frac{\pi - \theta}{\sin\theta}\right)^{\frac{1}{2}} \\ & \times \sum_{m=0}^{\infty}(-1)^m \sum_n (a'_n)^{-2} \exp[i(2m+1)\pi\lambda_n] J_0[\lambda_n(\pi - \theta)] + 4\pi i \frac{N^2}{M'}\left(\frac{\pi - \theta}{\sin\theta}\right)^{\frac{1}{2}} \exp(-2iM'\beta) \\ & \times \sum_{m=0}^{\infty}(-1)^m \sum_n \exp[i\lambda'_n\theta_t - i(2m+1)\pi\lambda'_n] J_0[\lambda'_n(\pi - \theta)], \quad N < 1, \quad \theta - \theta_t \gg \gamma. \end{aligned} \tag{4.85}$$

Let us now go over to region (iii) [cf. Eq. (4.77)], where, according to geometrical optics, total reflection takes place. We again have to treat separately the diffraction peak region $0 \leq \theta \lesssim \gamma$. For $\theta \gg \gamma$, we can still employ the representation (4.20)–(4.23), but the saddle-point path Γ'_2 for the evaluation of (4.21) is now on the other side of the line (Fig. 10) where the poles λ'_n are located. Thus, we have to take into account their additional residue-series contribution, and (4.21) becomes

$$\text{where} \qquad f_{0,g}(\beta, \theta) = \tilde{f}_{0,g}(\beta, \theta) - f'_{0,0}(\beta, \theta), \tag{4.86}$$

$$\tilde{f}_{0,g}(\beta, \theta) = -\frac{i}{\beta}\int_{\Gamma_2'} S_0(\lambda, \beta) Q^{(1)}_{\lambda - \frac{1}{2}}(\cos\theta)\lambda\, d\lambda, \tag{4.87}$$

$$\begin{aligned} f'_{0,0}(\beta, \theta) = & -\frac{2\pi}{\beta}\sum_n \lambda'_n r'_{0n} Q^{(1)}_{\lambda'_n - \frac{1}{2}}(\cos\theta) \\ & \approx 2e^{i\pi/4}\frac{N^{\frac{3}{2}}}{M'}\left(\frac{2\pi}{\beta\sin\theta}\right)^{\frac{1}{2}} \exp(-2iM'\beta) \\ & \times \sum_n \exp(-i\lambda'_n\zeta^+_{1,0}), \end{aligned} \tag{4.88}$$

and we have made use of (4.81) and N [Eq. (C7)]. The last term should be grouped together with $f'_{0,\mathrm{res}}(\beta, \theta)$, so that we have to make the following replacements in (4.20):

$$f_{0,g} \to \tilde{f}_{0,g}; \quad f'_{0,\mathrm{res}} \to \tilde{f}'_{0,\mathrm{res}} = f'_{0,\mathrm{res}} - f'_{0,0}, \tag{4.89}$$

where $f'_{0,\mathrm{res}}(\beta, \theta)$ is given precisely by (4.14). This follows from (4.23), (4.88), and the identity N [Eq. (6.33)].

According to (4.88), the substitution of $f'_{0,\mathrm{res}}$ by $\tilde{f}'_{0,\mathrm{res}}$ amounts precisely to subtracting out from (4.82) the residue series in $\zeta^+_{1,0}$, which would diverge for $\theta < \theta_t$. The first term in the remaining residue series $\tilde{f}'_{0,\mathrm{res}}$ then corresponds to the angle $\zeta^+_{1,1}$, as it should, according to Fig. 11(b). Thus, the residue series $\tilde{f}'_{0,\mathrm{res}}$ is rapidly convergent for all $\theta < \theta_t$.

The saddle-point evaluation of (4.87) is entirely similar to that which led to (4.35), except that, in (4.29), we have to make the substitution

$$(\alpha^2 - \lambda^2)^{\frac{1}{2}} \to -i(\lambda^2 - \alpha^2)^{\frac{1}{2}}. \tag{4.90}$$

Correspondingly, (4.35) is replaced by

$$\tilde{f}_{0,g}(\beta,\theta) = -\frac{1}{2}\left(\frac{[\cos^2(\theta/2)-N^2]^{\frac{1}{2}} - i\sin(\theta/2)}{[\cos^2(\theta/2)-N^2]^{\frac{1}{2}} + i\sin(\theta/2)}\right)\exp(-2i\beta\sin(\theta/2))$$
$$\times\left\{1+\frac{i}{2\beta}\left[\frac{1}{\sin^3(\theta/2)} + i\frac{(2N^2-\cos^2(\theta/2))}{(\cos^2(\theta/2)-N^2)^{\frac{3}{2}}}\right] + \mathcal{O}(\beta^{-2})\right\},$$
$$N<1, \quad \theta_t-\theta \gg N^{\frac{1}{3}}\gamma^2/M', \quad \theta \gg \gamma, \quad (4.91)$$

where the restriction on $\theta_t - \theta$ arises in the same way as (4.79). As ought to be expected, we find the unimodular Fresnel reflection coefficient associated with total reflection [cf. Eq. (4.36)].

On the other hand, nothing changes in the residue series associated with the poles λ_n, so that we finally obtain [cf. (4.41)]

$$f_0(\beta,\theta) \approx -\frac{1}{2}\left(\frac{[\cos^2(\theta/2)-N^2]^{\frac{1}{2}} - i\sin(\theta/2)}{[\cos^2(\theta/2)-N^2]^{\frac{1}{2}} + i\sin(\theta/2)}\right)\exp(-2i\beta\sin(\theta/2))$$
$$\times\left\{1+\frac{i}{2\beta}\left[\frac{1}{\sin^3(\theta/2)} + i\frac{(2N^2-\cos^2(\theta/2))}{(\cos^2(\theta/2)-N^2)^{\frac{3}{2}}}\right] + \mathcal{O}(\beta^{-2})\right\} + \tfrac{1}{2}e^{i\pi/12}\left(\frac{\gamma}{\pi\sin\theta}\right)^{\frac{1}{2}}$$
$$\times\left\{-i\sum_n (a_n')^{-2}\exp(i\lambda_n v_0^+) + \sum_{m=1}^{\infty}(-1)^m\sum_n (a_n')^{-2}[\exp(i\lambda_n v_m^-) - i\exp(i\lambda_n v_m^+)]\right\}$$
$$+ 2e^{-i\pi/4}\frac{N^{\frac{3}{2}}}{M'}\left(\frac{2\pi}{\beta\sin\theta}\right)^{\frac{1}{2}}\exp(-2iM'\beta)\sum_{m=1}^{\infty}(-1)^m\sum_n [\exp(-i\lambda_n'\zeta_{1,m}^+) + i\exp(-i\lambda_n'\zeta_{1,m}^-)],$$
$$N<1, \quad \theta_t-\theta \gg \gamma, \quad \theta \gg \gamma. \quad (4.92)$$

In the region $0 \leq \theta \lesssim \gamma$, where the forward diffraction peak is contained, $f_0(\beta,\theta)$ is still given by (4.70), provided that we make the substitution (3.30) and that (4.46) is replaced by (4.81) in the residue series at the poles λ_n'.

There remains only for us to consider the transition region (ii) in (4.77):

$$|\theta-\theta_t| \lesssim \gamma. \quad (4.93)$$

In this region, the approximation (4.29) for R_{22} is no longer valid within the range of the saddle point: the Debye asymptotic expansions have to be replaced by [cf. (3.33)]

$$[2\alpha] \approx e^{i\pi/3}\left(\frac{2}{\alpha}\right)^{\frac{1}{3}}\ln' \mathrm{Ai}(e^{-2i\pi/3}\zeta), \quad (4.94)$$

where

$$\zeta = (2/\alpha)^{\frac{1}{3}}(\lambda-\alpha). \quad (4.95)$$

The main contribution to the integral in (3.21) still comes from the neighborhood of the saddle point

$$\bar{\lambda} = \beta\cos(\theta/2) \approx \beta\cos(\theta_t/2) = N\beta = \alpha, \quad (4.96)$$

so that we may replace λ by α in slowly varying factors. Thus, (4.29) is replaced by

$$R_{22}(\lambda,\beta) \approx \frac{1+\kappa^2\ln' \mathrm{Ai}(e^{-2i\pi/3}\zeta)}{1-\kappa^2\ln' \mathrm{Ai}(e^{-2i\pi/3}\zeta)} \quad (4.97)$$

in first approximation, where

$$\kappa^2 = e^{-i\pi/6}N^{\frac{2}{3}}\gamma/M'; \quad |\kappa^2| \ll 1. \quad (4.98)$$

The remaining approximations employed in (4.31) are still valid.

As θ ranges through the transition region (4.93), the saddle-point path of integration sweeps across the poles, as shown in Fig. 10. Let us make the change of variable (4.30) and expand everything around the saddle point:

$$w-\theta/2 = e^{-i\pi/4}u[\beta\sin(\theta/2)]^{-\frac{1}{2}};$$
$$\zeta = \bar{\zeta} - \sqrt{2}\,e^{-i\pi/3}u/\kappa, \quad (4.99)$$

where

$$\bar{\zeta} \approx \frac{M'}{N^{\frac{1}{3}}}\frac{(\theta_t-\theta)}{\gamma^2}. \quad (4.100)$$

Then, we finally get

$$f_{0,g}(\beta,\theta) \approx \tfrac{1}{2}\exp(-2i\beta\sin(\theta/2))\left\{1+\frac{2\kappa^2}{\sqrt{\pi}}\int_{-\infty}^{\infty}\exp(-u^2)\frac{\ln' \mathrm{Ai}(e^{-2i\pi/3}\bar{\zeta}+\sqrt{2}\,u/\kappa)}{1-\kappa^2\ln' \mathrm{Ai}(e^{-2i\pi/3}\bar{\zeta}+\sqrt{2}\,u/\kappa)}\,du\right\}$$
$$-2e^{i\pi/4}\frac{N^{\frac{3}{2}}}{M'}\left(\frac{2\pi}{\beta\sin\theta}\right)^{\frac{1}{2}}\exp(-2iM'\beta)\sum_{n\geq n_0}\exp(-i\lambda_n'\zeta_{1,0}^+), \quad N<1, \quad |\theta-\theta_t| \lesssim \gamma \quad (4.101)$$

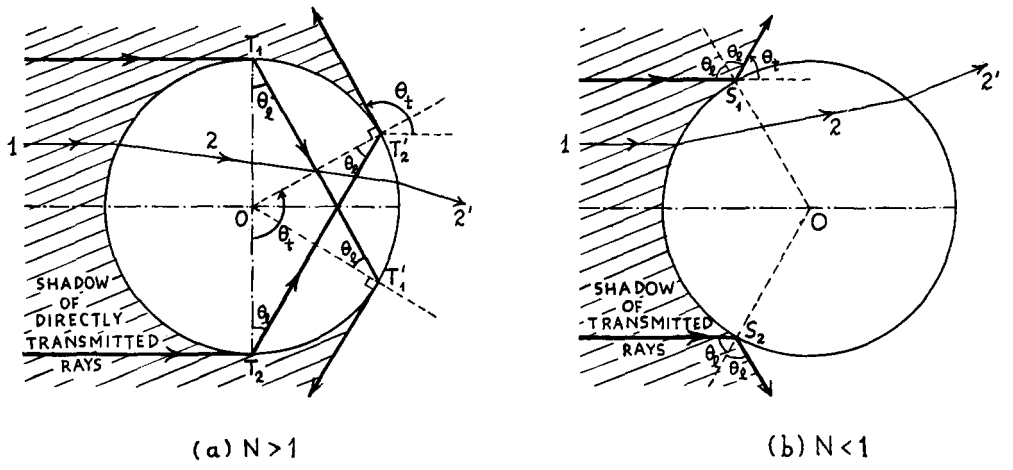

FIG. 13. Structure of the lit and shadow regions in the geometrical-optics approximation, for the second term of the Debye expansion, corresponding to directly transmitted rays, such as 2'. (a) $N > 1$; (b) $N < 1$. In both cases, the shadow boundary is $\theta_i = \pi - 2\theta_t$, where θ_t is the critical angle.

where n_0 is the last pole that has been swept by the path of integration. When all the poles have been swept (e.g., for $\theta < \theta_i$), their total contribution is given by (4.88), so that the terms in (4.82) that would be poorly converging are gradually subtracted out. Otherwise, (4.82) and the corresponding expression for $f_{0,\mathrm{res}}(\beta, \theta)$ remain valid.

The first term (unity) in the expression within curly brackets in (4.101) is the dominant one. The other term, according to (4.98), is a small correction, which contains the effects due to the poles not yet subtracted out, as well as the corrections to the reflection coefficient. In fact, within the present order of approximation, the poles correspond to the roots of the denominator in the integrand. For $\theta > \theta_i$, there may be several poles within the range of the saddle-point.

The asymptotic expansion of integrals containing poles in the neighborhood of a saddle point has been investigated by several authors (cf. e.g., Ref. 39). The transition term representing the effect of the poles can be expressed in terms of error functions with complex argument. We shall not carry out this procedure explicitly for (4.101).

As will be seen later, the structure of the transition region is actually quite complicated, because all higher-order terms in the Debye expansion lead to the same shadow boundary for $N < 1$, so that all their contributions should be taken into account.

This concludes the discussion of the asymptotic behavior of $f_0(\beta, \theta)$. We see that it can be determined for all values of θ, $0 \leq \theta \leq \pi$, both for $N > 1$ and for $N < 1$.

[39] B. L. van der Waerden, Appl. Sci. Res. B2, 33 (1950).

5. THE SECOND TERM OF THE DEBYE EXPANSION

A. Preliminary Considerations

The second term of the Debye expansion is given by either one of the equivalent representations (3.23) and (3.26), with $p = 1$. In the geometrical-optics approximation, it is associated with rays that are directly transmitted through the sphere, without any internal reflection, like the ray 2' in Fig. 5.

The structure of the lit and shadow regions for this class of rays is shown in Fig. 13(a) for $N > 1$ and in Fig. 13(b) for $N < 1$. In both cases, there is a shadow region (shown shaded in Fig. 13), which is inaccessible to directly transmitted rays. For $N > 1$, the shadow boundary corresponds to transmitted rays associated with tangentially incident rays at T_1 and T_2 [Fig. 13(a)]. According to geometrical optics, these rays are critically refracted and reemerge tangentially at T_1' and T_2', respectively. For $N < 1$, the shadow boundary is associated with the critically incident rays at S_1 and S_2, which are totally reflected; it is the same one already found for the first term of the Debye expansion and shown in Fig. 8(b).

The direction of the shadow boundary is given in both cases by [cf. Eq. (4.76)]

$$\theta_i = \pi - 2\theta_t, \tag{5.1}$$

where θ_t is the critical angle. Notice, however, that, while θ_t is given by (4.1) for $N < 1$, it is given by

$$\sin \theta_t = 1/N \tag{5.2}$$

for $N > 1$.

Thus, we expect to find three different regions, as in (4.77):

$$\begin{aligned} &\text{(i)} && \theta - \theta_t \gg \Delta\theta; \\ &\text{(ii)} && |\theta - \theta_t| \lesssim \Delta\theta; \\ &\text{(iii)} && \theta_t - \theta \gg \Delta\theta, \end{aligned} \tag{5.3}$$

where $\Delta\theta$ is the angular width of the transition domain (ii) between the shadow region (i) and the lit region (iii). We shall see that this is a normal transition, so that

$$\Delta\theta \sim \gamma. \tag{5.4}$$

In the shadow region (i), the amplitude can be reduced to a pure residue series. Since this region extends up to $\theta = \pi$, we employ the representation (3.26). Changing λ to $-\lambda$ in the sum from $m = -\infty$ to -1, and taking into account (3.10), we find that (3.26) becomes

$$f_1(\beta, \theta) = -\frac{1}{\beta}\sum_{m=0}^{\infty}(-1)^m \int_{-\infty}^{\infty} U(\lambda, \beta) P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[i(2m+1)\pi\lambda]\lambda\, d\lambda, \tag{5.5}$$

where $U(\lambda, \beta)$ is given by (3.24).

The asymptotic behavior of $U(\lambda, \beta)$ as $|\lambda| \to \infty$ in the upper half-plane is shown in Fig. 14. We see that

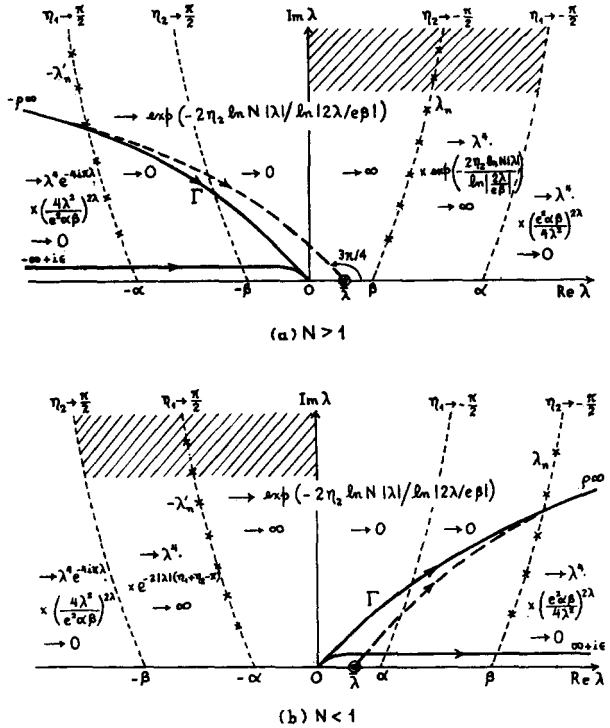

FIG. 14. Asymptotic behavior of $U(\lambda, \beta)$ [cf. Eq. (3.24)] as $|\lambda| \to \infty$ in different regions of the λ plane. (a) $N > 1$; (b) $N < 1$. $U \to \infty$ in the shaded regions and $U \to 0$ elsewhere (apart from the poles). The paths of integration in (5.11) and (5.15) are replaced by symmetric paths from $-\rho\infty$ to $\rho\infty$ prior to the saddle-point evaluation; one-half of these paths is shown. ×—poles; ⊙—saddle point; — — — steepest descent path.

$U \to 0$ everywhere, except in the shaded regions in the neighborhood of the imaginary axis, where it diverges like

$$\exp(c\,|\lambda|/\ln|\lambda|), \quad c = \text{const} > 0.$$

On the other hand, according to N [Eq. (C8)], $e^{i\pi\lambda}P_{\lambda-\frac{1}{2}}(-\cos\theta)$ behaves like $e^{i\lambda\theta}$ as $|\lambda| \to \infty$ in the upper half-plane, so that, for any $\theta > 0$, the path of integration in (5.5) can be closed at infinity, reducing the integrals to pure residue series:

$$f_1(\beta, \theta) = f_{1,\text{res}}(\beta, \theta) + f'_{1,\text{res}}(\beta, \theta), \tag{5.6}$$

where

$$f_{1,\text{res}}(\beta, \theta) = -\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m \sum_n \text{residue}\,\{\lambda U(\lambda, \beta) \times \exp[i(2m+1)\pi\lambda]P_{\lambda-\frac{1}{2}}(-\cos\theta)\}_{\lambda_n}, \tag{5.7}$$

$$f'_{1,\text{res}}(\beta, \theta) = -\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m \sum_n \text{residue}\,\{\lambda U(\lambda, \beta) \times \exp[i(2m+1)\pi\lambda]P_{\lambda-\frac{1}{2}}(-\cos\theta)\}_{-\lambda_n'}. \tag{5.8}$$

[Actually, of course, we have to consider a sequence of contours passing between the poles, as was done in N (Sec. IV). For a more careful discussion of this point, see Ref. 40.] This representation will be employed in the shadow region (i).

In the lit region (iii), we start from (5.5). We shift the path of integration to a straight line above the real axis (from $-\infty + i\epsilon$ to $\infty + i\epsilon$, $\epsilon > 0$), and we substitute the identity N [Eq. (C6)]:

$$P_{\lambda-\frac{1}{2}}(-\cos\theta) = -ie^{i\pi\lambda}P_{\lambda-\frac{1}{2}}(\cos\theta) + 2i\cos(\pi\lambda)Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta). \tag{5.9}$$

[This shift is necessary because of the singularities of $Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)$ on the negative real axis.] Taking into account also the identity

$$\sum_{m=0}^{\infty}(-1)^m \cos(\pi\lambda)\exp[i(2m+1)\pi\lambda] = \tfrac{1}{2}, \quad \text{Im}\,\lambda > 0, \tag{5.10}$$

valid over the new path of integration, we find

$$f_1(\beta, \theta) = -\frac{i}{\beta}\int_{-\infty+i\epsilon}^{\infty-i\epsilon} U(\lambda, \beta)Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda - \frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m \sum_n \text{residues}\,\{\lambda U(\lambda, \beta)P_{\lambda-\frac{1}{2}}(\cos\theta) \times \exp[2i(m+1)\pi\lambda]\}_{\lambda_n, -\lambda_n'}. \tag{5.11}$$

In (5.11), the integrals containing $P_{\lambda-\frac{1}{2}}(\cos\theta)$ have been reduced to residue series at the poles

[40] R. F. Goodrich and N. D. Kazarinoff, Proc. Cambridge Phil. Soc. **59**, 167 (1963).

λ_n, $-\lambda_n'$ by closing the path of integration at infinity in the upper half-plane. This is allowed, according to Fig. 14, due to the extra convergence factor $e^{i\pi\lambda}$ in the first term of (5.9). Furthermore, in the integral containing $Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)$, the path of integration has been shifted from $(-\infty + i\epsilon,\ \infty + i\epsilon)$ to a path symmetric about the origin $(-\infty + i\epsilon,\ \infty - i\epsilon)$, by crossing the *positive* real axis, which is allowed, because $Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)$ is regular there.

If we now split the path of integration at the origin and change λ to $-\lambda$ over one-half of it, making use of the identity

$$Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta) - Q^{(2)}_{-\lambda-\frac{1}{2}}(\cos\theta) = i\tan(\pi\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta), \tag{5.12}$$

which follows from (5.9), we find

$$-\frac{i}{\beta}\int_{-\infty+i\epsilon}^{\infty-i\epsilon} U(\lambda,\beta)Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda = \frac{1}{\beta}\int_0^{\infty-i\epsilon} U(\lambda,\beta)P_{\lambda-\frac{1}{2}}(\cos\theta)\tan(\pi\lambda)\lambda\,d\lambda. \tag{5.13}$$

Substituting this in (5.11), we see that the resulting expression is regular down to $\theta = 0$.

By an entirely similar procedure, but employing, instead of (5.9), the identity N [Eq. (C5)],

$$_{-\frac{1}{2}}(-\cos\theta) = ie^{-i\pi\lambda}P_{\lambda-\frac{1}{2}}(\cos\theta) - 2i\cos(\pi\lambda)Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta), \tag{5.14}$$

we find

$$f_1(\beta,\theta) = -\frac{i}{\beta}\int_{-\infty-i\epsilon}^{\infty+i\epsilon} U(\lambda,\beta)Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda + \frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residues}\{\lambda U(\lambda,\beta)P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[-2i(m+1)\pi\lambda]\}_{-\lambda_n,\lambda_n'}, \tag{5.15}$$

where the residues are now taken at the poles in the lower half-plane, $\lambda = -\lambda_n$, $\lambda = \lambda_n'$. Similarly to (5.13), we have

$$-\frac{i}{\beta}\int_{-\infty-i\epsilon}^{\infty+i\epsilon} U(\lambda,\beta)Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda = -\frac{1}{\beta}\int_0^{\infty+i\epsilon} U(\lambda,\beta)P_{\lambda-\frac{1}{2}}(\cos\theta)\tan(\pi\lambda)\lambda\,d\lambda. \tag{5.16}$$

The above expressions could also have been obtained by starting from (3.23) instead of (3.26).

We shall see that the representations (5.11) and (5.13) are appropriate in the lit region for $N > 1$, whereas (5.15) and (5.16) will be employed for $N < 1$. Let us start by considering the behavior of the amplitude in the shadow region for $N > 1$.

B. Behavior for $N > 1$ in the Shadow Region ($\theta - \theta_t \gg \gamma$)

In this region, we shall employ the representations (5.6)–(5.8). According to (5.7), (3.24), (3.5), and (3.8), we have

$$f_{1,\,\text{res}}(\beta,\theta) = \frac{32i}{\pi\beta^3}\sum_{m=1}^{\infty}(-1)^m\sum_n \text{residue}\left\{\frac{c_{1m}(\lambda,\beta,\theta)}{[d(\lambda,\beta)]^2}\right\}_{\lambda_n}, \tag{5.17}$$

where $d(\lambda,\beta)$ is given by (4.38) and

$$c_{1m}(\lambda,\beta,\theta) = \frac{\lambda\exp[i(2m+1)\pi\lambda]P_{\lambda-\frac{1}{2}}(-\cos\theta)}{[H^{(1)}_\lambda(\beta)H^{(2)}_\lambda(\alpha)]^2}. \tag{5.18}$$

A similar expression is valid for $f'_{1,\text{res}}(\beta,\theta)$, with λ_n replaced by $-\lambda_n'$. In both cases, the poles are double poles.

The residue of the expression within curly brackets in (5.17) at a double pole is given by (cf. Ref. 29, Appendix II)

$$\text{residue}\left\{\frac{c_{1m}(\lambda,\beta,\theta)}{[d(\lambda,\beta)]^2}\right\}_{\lambda_n} = \frac{c_{1m}}{\dot d^2}\left(\frac{\dot c_{1m}}{c_{1m}} - \frac{\ddot d}{\dot d}\right)_{\lambda_n}, \tag{5.19}$$

where the dots denote partial derivatives with respect to λ and all quantities in the second member are to be evaluated at the poles λ_n.

The evaluation can be carried out by employing the asymptotic expansions N, Eq. (A16) for $H^{(2)}_\lambda(\alpha)$, N, Eq. (C11) for $P_{\lambda-\frac{1}{2}}(-\cos\theta)$ and the expansions for $H^{(1)}_\lambda(\beta)$ and its derivatives given in Appendix A. Retaining only the dominant term in each of these expressions and neglecting corrections of order γ, we find the following final result. [The evaluation of the dominant term in the residue-series contribution at the poles λ_n for an arbitrary term of the Debye expansion will be carried out in Paper II (Appendix C).]

$$f_{1,\text{res}}(\beta,\theta) \approx 2i\frac{e^{i\pi/3}}{\gamma M}\left(\frac{\pi-\theta}{\sin\theta}\right)^{\frac{1}{2}}\exp(2iM\beta) \times \sum_{m=0}^{\infty}(-1)^m\sum_n (a_n')^{-2}\exp\{i\lambda_n[(2m+1)\pi - \theta_t]\} \times \{[(2m+1)\pi - \theta_t]J_0[\lambda_n(\pi-\theta)] + i(\pi-\theta)J_1[\lambda_n(\pi-\theta)]\},\quad \theta - \theta_t \gg \gamma,\quad \theta \le \pi, \tag{5.20}$$

where θ_t is given by (5.1), (5.2), i.e.,

$$\theta_t = 2\cos^{-1}(1/N). \tag{5.21}$$

In particular, for $\pi - \theta \gg \beta^{-1}$, this result can be simplified by inserting the asymptotic expansions for the Bessel functions, which lead to

$$f_{1,\mathrm{res}}(\beta, \theta) \approx -\frac{e^{i\pi/12}}{M}\left(\frac{\gamma}{\pi \sin\theta}\right)^{\frac{1}{2}} \times \exp(2iM\beta)\Big\{\sum_n (a_n')^{-2}\zeta_{1,0}^{+} \exp(i\lambda_n\zeta_{1,0}^{+}) + \sum_{m=1}^{\infty}(-1)^m \sum_n (a_n')^{-2}[\zeta_{1,m}^{+}\exp(i\lambda_n\zeta_{1,m}^{+}) + i\zeta_{1,m}^{-}\exp(i\lambda_n\zeta_{1,m}^{-})]\Big\}, \quad \theta - \theta_t \gg \gamma, \quad \pi - \theta \gg \beta^{-1}, \tag{5.22}$$

where

$$\zeta_{1,m}^{\pm} = 2m\pi - \theta_t \pm \theta, \tag{5.23}$$

as in (4.83) [but note that θ_t is now given by (5.21) instead of (4.76)!].

By analogy with (4.43), this result can be rewritten as follows (cf. also Ref. 29):

$$f_{1,\mathrm{res}}(\beta, \theta) = -\frac{i}{(\sin\theta)^{\frac{1}{2}}}\exp(2iM\beta)\Big\{-i\sum_n D_n^2 D_{21}D_{12} \times \int_0^{\zeta_{1,0}^{+}} \exp(i\lambda_n\zeta_{1,0}^{+})\,d\varphi + \sum_{m=1}^{\infty}(-1)^m \sum_n D_n^2 D_{21}D_{12} \times \Big[\int_0^{\zeta_{1,m}^{-}} \exp(i\lambda_n\zeta_{1,m}^{-})\,d\varphi - i\int_0^{\zeta_{1,m}^{+}} \exp(i\lambda_n\zeta_{1,m}^{+})\,d\varphi\Big]\Big\}, \tag{5.24}$$

where D_n^2 is given by (4.45) and

$$D_{21}D_{12} = 2/M. \tag{5.25}$$

The physical interpretation of these results in terms of diffracted rays is illustrated in Fig. 15. The incident rays tangential to the sphere at T_1 and T_2, after penetrating into the sphere at the critical angle θ_t, reemerge tangentially at T_1' and T_2', respectively, defining the shadow boundary. At the points of emergence, they launch surface waves, travelling from the shadow boundary into the shadow. A typical diffracted ray of this type is $T_2T_2'T_2''B$ in Fig. 15.

However, before penetrating into the sphere, a ray can also describe part of its path as a surface wave. Rays of this type are generated by diffracted rays associated with the first term of the Debye expansion (Fig. 9), which, after critical refraction into the sphere, reemerge as surface waves, to complete the remainder of their path along the surface, before leaving it tangentially in the direction of observation. A typical example is $T_2\hat{T}_2'\hat{T}_2''T_2''B$ in Fig. 14.

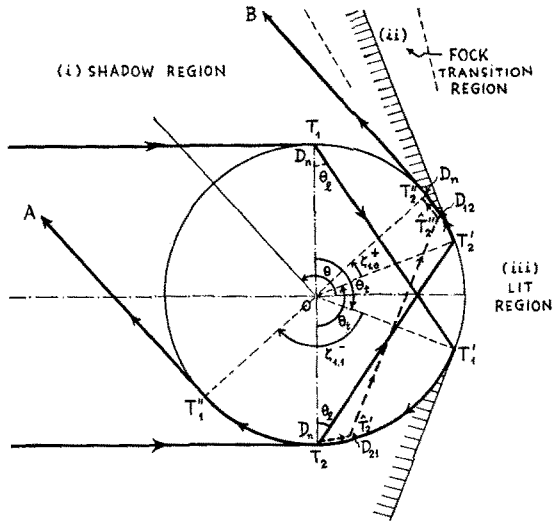

FIG. 15. Physical interpretation of (5.22) and (5.24). The limiting rays T_1T_1' and T_2T_2' that define the shadow boundaries excite surface waves propagating into the shadow, generating the diffracted rays $T_1T_1'T_1''A$ and $T_2T_2'T_2''B$ in the direction θ. The corresponding angles described along the surface are $\zeta_{1,1}^{-}$ and $\zeta_{1,0}^{+}$, respectively. There are infinitely many other possible paths for diffracted rays belonging to this class. One such path, $T_2\hat{T}_2'\hat{T}_2''T_2''B$, corresponding to the same angle $\zeta_{1,0}^{+}$, is shown in broken line. The subdivision into regions is also indicated.

Since the total angle $\zeta_{1,m}^{\pm}$ described along the surface can be broken up into two parts in an infinite number of ways, there is an infinite class of diffracted rays of this type, and the resultant amplitude is the sum of all their contributions. The contribution from all paths such that an angle between φ and $\varphi + d\varphi$ is described before critical refraction is proportional to $d\varphi$. Since the maximum value of φ is the total angle $\zeta_{1,m}^{\pm}$ described, this accounts for the integrals appearing in (5.24).

The factor D_n^2 arises from the excitation of the diffracted wave (e.g., at T_2) and its reconversion into a tangential ray (e.g., at T_2''). The factors D_{21} and D_{12} represent the transmission coefficients of surface waves into the sphere (e.g., at $\hat{T}_2'$) and out of the sphere (e.g., at $\hat{T}_2''$), respectively.

The factor $\exp(2iM\beta)$ represents the phase shift corresponding to the "shortcut" through the sphere (e.g., T_1T_1' or $\hat{T}_2'\hat{T}_2''$). The factor $-i$ corresponds to the phase decrease by $\pi/2$ experienced by a diffracted ray such as $T_1T_1'T_1''A$ as it passes through the pole T_2, which is a focal point for diffracted rays.

According to (5.8), $f_{1,\mathrm{res}}'(\beta, \theta)$ is given by an expression identical to (5.17)–(5.19), except that the residues are now to be evaluated at the poles $-\lambda_n'$. Employing the asymptotic expansion corresponding to (A1) for $H_\lambda^{(2)}(\alpha)$, the Debye asymptotic expansion given in N (Fig. 15), for $H_\lambda^{(1)}(\beta)$, and N [Eq. (C11)] for $P_{\lambda-\frac{1}{2}}(-\cos\theta)$, and keeping only the dominant terms,

we find, with the help of (3.33)–(3.35),

$$f'_{1,\mathrm{res}}(\beta,\theta) \approx 2e^{-i\pi/3}\frac{N^{\frac{7}{3}}}{\gamma M}\left(\frac{\pi-\theta}{\sin\theta}\right)^{\frac{1}{2}}\exp(2M\beta)\sum_{m=0}^{\infty}(-1)^m\sum_n(a'_n)^{-2} \times\exp\{-i\lambda'_n[(2m+1)\pi-2i\cosh^{-1}N]\} \times\{[(2m+1)\pi-2i\cosh^{-1}N]J_0[\lambda'_n(\pi-\theta)] - i(\pi-\theta)J_1[\lambda'_n(\pi-\theta)]\}, \quad \theta-\theta_t\gg\gamma,\quad \theta\le\pi. \tag{5.26}$$

In particular, for $\pi-\theta\gg\alpha^{-1}$, this becomes

$$f'_{1,\mathrm{res}}(\beta,\theta) \approx e^{-i\pi/3}\frac{N^{\frac{11}{6}}}{M}\left(\frac{\gamma}{\pi\sin\theta}\right)^{\frac{1}{2}} \times\exp(2M\beta)\Big\{\sum_n(a'_n)^{-2}(\theta-2i\cosh^{-1}N) \times\exp[-i\lambda'_n(\theta-2i\cosh^{-1}N)-i(\pi/4)] +\sum_{m=1}^{\infty}(-1)^m\sum_n(a'_n)^{-2}[(2m\pi+\theta-2i\cosh^{-1}N) \times\exp[-i\lambda'_n(2m\pi+\theta-2i\cosh^{-1}N)-i(\pi/4)] -(2m\pi-\theta-2i\cosh^{-1}N) \times\exp[-i\lambda'_n(2m\pi-\theta-2i\cosh^{-1}N)+i(\pi/4)]]\Big\}, \quad \theta-\theta_t\gg\gamma,\quad \pi-\theta\gg\alpha^{-1}. \tag{5.27}$$

By comparing these results with (5.20)–(5.22), we see again, as for (4.48), that $f'_{1,\mathrm{res}}(\beta,\theta)$ is exponentially small and may therefore be neglected. For $N<1$, we shall see that the situation is just the reverse; (5.26)–(5.27) represent the analytic continuation of the results for that case.

Finally, let us remark that the damping factor for the least strongly damped terms in (5.22) is proportional to [cf. Eq. (3.29)]:

$$\exp(-\mathrm{Im}\,\lambda_n\zeta^+_{1,0})\sim\exp[-(\sqrt{3}/2)x_n(\theta-\theta_t)/\gamma],$$

so that the residue series is rapidly convergent for $\theta-\theta_t\gg\gamma$.

C. Behavior for $N>1$ in the Lit Region ($\theta_t-\theta\gg\gamma$)

In this region, we employ the representation (5.11), where the integral is to be evaluated by the saddle-point method. For this purpose, the path of integration is first deformed from $(-\infty+i\epsilon,\ \infty-i\epsilon)$ into a new path Γ from $-\rho\infty$ to $\rho\infty$, symmetric about the origin, one half of which is shown in Fig. 14(a). This brings it closer to the steepest descent path, represented by the curve in broken line in Fig. 14(a), which will be discussed below. [The steepest descent path crosses the real axis between $\lambda=0$ and $\lambda=\beta$, at an angle of $-\pi/4$, as will be seen later. It must curve away from the imaginary axis as $|\lambda|\to\infty$, to get into the regions where the integrand goes to zero [cf. Fig. 14, where an additional factor $e^{i\lambda\theta}$ has to be introduced, corresponding to

$$Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)].$$

Its exact shape in the intermediate region is difficult to determine and need not be considered here.]

In this process, we sweep across poles λ'_n and $-\lambda'_n$ with the lower and upper halves of the contour, respectively, so that (5.11) becomes

$$f_1(\beta,\theta)=f_{1,g}(\beta,\theta)+\tilde{f}_{1,\mathrm{res}}(\beta,\theta)+\tilde{f}'_{1,\mathrm{res}}(\beta,\theta), \tag{5.28}$$

where

$$f_{1,g}(\beta,\theta)=-\frac{i}{\beta}\int_\Gamma U(\lambda,\beta)Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda, \tag{5.29}$$

$$\tilde{f}_{1,\mathrm{res}}(\beta,\theta)=-\frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n\text{residue} \times\{\lambda UP_{\lambda-\frac{1}{2}}(\cos\theta)\exp[2i(m+1)\pi\lambda]\}_{\lambda_n}, \tag{5.30}$$

$$\tilde{f}'_{1,\mathrm{res}}(\beta,\theta) =-\frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n\text{residue} \times\{\lambda UP_{\lambda-\frac{1}{2}}(\cos\theta)\exp[2i(m+1)\pi\lambda]\}_{-\lambda_n'} +\frac{2\pi i}{\beta}\sum_{n=1}^{n_0}\text{residue}\{\lambda UP_{\lambda-\frac{1}{2}}(\cos\theta)\tan(\pi\lambda)\}_{-\lambda_n'}, \tag{5.31}$$

where the last term in (5.31) is the sum of the contributions from the $2n_0$ poles swept by the upper and lower halves of the contour together, and we have made use of (5.12).

The residue series (5.30) differs from (5.7) only by the substitution

$$iP_{\lambda-\frac{1}{2}}(-\cos\theta)\to e^{i\pi\lambda}P_{\lambda-\frac{1}{2}}(\cos\theta).$$

Accordingly, (5.20) is replaced by

$$\tilde{f}'_{1,\mathrm{res}}(\beta,\theta) \approx\frac{2e^{i\pi/3}}{\gamma M}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\exp(2iM\beta)\sum_{m=0}^{\infty}(-1)^m\sum_n(a'_n)^{-2} \times\exp\{i\lambda_n[(2m+2)\pi-\theta_t]\} \times\{[(2m+2)\pi-\theta_t]J_0(\lambda_n\theta)+i\theta J_1(\lambda_n\theta)\}, \quad \theta_t-\theta\gg\gamma,\quad \theta\gtrsim 0. \tag{5.32}$$

In particular, for $\theta \gg \beta^{-1}$, this becomes

$$\tilde{f}_{1,\mathrm{res}}(\beta, \theta) \approx -\frac{e^{i\pi/3}}{M}\left(\frac{\gamma}{\pi \sin\theta}\right)^{\frac{1}{2}} \exp(2iM\beta) \cdot \times \sum_{m=1}^{\infty}(-1)^m \sum_n (a_n')^{-2}[\zeta_{1,m}^{+} \exp(i\lambda_n \zeta_{1,m}^{+} - i(\pi/4)) + \zeta_{1,m}^{-} \exp(i\lambda_n \zeta_{1,m}^{-} + i(\pi/4))], \quad \theta_t - \theta \gg \gamma, \quad \theta \gg \beta^{-1}. \quad (5.33)$$

This differs from (5.22) only by the omission of the series in $\zeta_{1,0}^{+}$, which would not converge rapidly in this region. Physically, this omission corresponds to the fact that, in order to reach a direction θ in the lit region, a surface wave excited at T_2' (Fig. 15) must describe an angle $\zeta_{1,1}^{+} = 2\pi - \zeta_{1,0}^{+}$, rather than $\zeta_{1,0}^{+}$.

In the last residue series of (5.31), we can apply the approximation

$$\tan(\pi\lambda) \approx i,$$

valid in the neighborhood of the poles $-\lambda_n'$. We then find

$$\tilde{f}_{1,\mathrm{res}}'(\beta, \theta) \approx -2e^{i\pi/6}\frac{N^{\frac{7}{3}}}{\gamma M}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}} \times \exp(2M\beta)\left\{\sum_{m=1}^{\infty}(-1)^m \sum_n (a_n')^{-2} \times \exp[-i\lambda_n'(2m\pi - 2i\cosh^{-1}N)] \times [(2m\pi - 2i\cosh^{-1}N)J_0(\lambda_n'\theta) - i\theta J_1(\lambda_n'\theta)] + i\sum_{n=1}^{n_0}(a_n')^{-2}\exp(-2\lambda_n'\cosh^{-1}N) \times [2\cosh^{-1}N J_0(\lambda_n'\theta) + \theta J_1(\lambda_n'\theta)], \quad \theta_t - \theta \gg \gamma, \quad \theta \geq 0, \quad (5.34)$$

which is again negligible as compared with $\tilde{f}_{1,\mathrm{res}}(\beta, \theta)$ [cf. Eq. (5.27)].

Finally, let us evaluate $f_{1,g}(\beta, \theta)$. The integral (5.29) has a saddle point on the real axis, between $\lambda = 0$ and $\lambda = \beta$, so that we may employ asymptotic expansions for the integrand similar to those employed in connection with (4.31). With the change of variables

$$\lambda = \beta \sin w_1 = \alpha \sin w_2, \quad (5.35)$$

we find

$$f_{1,g}(\beta, \theta) = -2e^{i\pi/4}N\left(\frac{2\beta}{\pi \sin\theta}\right)^{\frac{1}{2}} \int B(w_1, \beta, \theta) \times \exp[i\beta\delta(w_1, \theta)]\, dw_1, \quad (5.36)$$

where

$$\delta(w_1, \theta) = 2[N\cos w_2 - \cos w_1 + (w_2 - w_1 + \theta/2)\sin w_1], \quad (5.37)$$

$$B(w_1, \beta, \theta) = \frac{(\sin w_1)^{\frac{1}{2}}\cos^2 w_1 \cos w_2}{(N\cos w_2 + \cos w_1)^2} \times \left\{1 + \frac{i}{\beta}\left[\frac{1}{4\cos w_1}(1 + \tfrac{5}{3}\tan^2 w_1) - \frac{1}{4N\cos w_2}(1 + \tfrac{5}{3}\tan^2 w_2) - \frac{\tan^2 w_2}{\cos^2 w_1} \times (N\cos w_2 - \cos w_1) - \frac{\cot\theta}{8\sin w_1}\right] + O(\beta^{-2})\right\}, \quad (5.38)$$

and the path of integration is the image of Γ [Fig. 14(a)] in the w_1 plane.

Taking into account the relation

$$dw_2/dw_1 = \cos w_1/(N\cos w_2), \quad (5.39)$$

we find from (5.37) that the location of the saddle point is determined by

$$\bar{w}_1 = \theta_1, \quad \bar{w}_2 = \theta_2, \quad (5.40)$$

where

$$\theta_1 - \theta_2 = \theta/2, \quad \sin\theta_1 = N\sin\theta_2. \quad (5.41)$$

The corresponding saddle point in the λ plane is

$$\bar{\lambda} = kp = \beta\sin\theta_1, \quad (5.42)$$

where p is the impact parameter of the incident ray AB (Fig. 16) which, after two refractions (angles θ_1, θ_2) and no reflection, emerges in the direction θ, according to the laws of geometrical optics.

It is possible to solve (5.41) to express $\sin\theta_1$ directly in terms of θ:

$$\sin\theta_1 = (N/\tau)\sin(\theta/2), \quad (5.43)$$

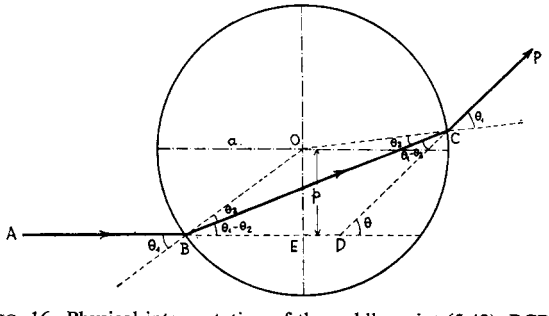

FIG. 16. Physical interpretation of the saddle point (5.42). BCP is the directly transmitted ray corresponding to the incident ray AB according to geometrical optics. The impact parameter associated with this ray is $\overline{OE} = p = \bar{\lambda}/k = a\sin\theta_1$, where $\theta = 2(\theta_1 - \theta_2)(N > 1)$.

where

$$\tau = (1 - 2N\cos(\theta/2) + N^2)^{\frac{1}{2}}. \qquad (5.44)$$

The steepest descent path crosses the real w_1 axis at an angle of $-\pi/4$. The corresponding path in the λ plane is represented by the curve in broken line in Fig. 14(a).

The saddle-point evaluation of (5.36) can now proceed by applying (4.34). A straightforward but rather lengthy calculation finally leads to the result

$$f_{1,g}(\beta,\theta) = -\left(\frac{\sin\theta_1}{\sin\theta}\right)^{\frac{1}{2}} \frac{(2N\cos\theta_1\cos\theta_2)^{\frac{3}{2}}}{(\cos\theta_1 + N\cos\theta_2)^2} \times \frac{\exp[2i\beta(N\cos\theta_2 - \cos\theta_1)]}{(N\cos\theta_2 - \cos\theta_1)^{\frac{1}{2}}} \times \left\{1 - \frac{i\mathcal{F}(\theta)}{16\beta\cos\theta_1} + \mathcal{O}(\beta^{-2})\right\}, \quad \theta_t - \theta \gg \gamma, \qquad (5.45)$$

where

$$\mathcal{F}(\theta) = 2\cot\theta_1\left[\cot\theta - \frac{\cot\theta_1}{2(1-\chi)}\right] - \frac{9}{1-\chi} + 15\chi - 6 + (\chi - 1)(8\chi^2 + 5\chi + 8)\tan^2\theta_1, \qquad (5.46)$$

and [cf. Eq. (5.39)]:

$$\chi = \cos\theta_1/(N\cos\theta_2). \qquad (5.47)$$

Let us now discuss the domain of validity of (5.45). It must clearly fail near the shadow boundary, $\theta \to \theta_t$, because the Debye asymptotic expansions for $H_\lambda^{(1,2)}(\beta)$ employed in (5.36)–(5.38) are then no longer valid. We must have $\beta - \tilde{\lambda} \gg \beta^{\frac{1}{3}}$. According to (5.41), this implies $\theta_t - \theta \gg \gamma$, which is the condition given in (5.45). The same condition is found from the requirement that the first correction term $\mathcal{F}(\theta)/\beta\cos\theta_1$ in (5.45) must remain small as θ_1 approaches $\pi/2$.

At the other extreme, near $\theta = 0$, the derivation of (5.45) is again unjustified, because the asymptotic expansion N, Eq. (C7), for $Q_{\lambda-\frac{1}{2}}^{(2)}(\cos\theta)$ in (5.29) is no longer valid. However, it is found that (5.45) approaches a finite limit as $\theta \to 0$, namely,

$$f_{1,g}(\beta,0) = -\frac{2N^2}{(N-1)(N+1)^2}\exp[2i(N-1)\beta] \times \left\{1 + \frac{i}{\beta}\left[1 - \frac{1}{N} + \frac{1}{2(N-1)}\right] + \mathcal{O}(\beta^{-2})\right\}. \qquad (5.48)$$

The proper way to evaluate $f_{1,g}(\beta,\theta)$ near $\theta = 0$ is to apply the transformation (5.13) to (5.29), to substitute $P_{\lambda-\frac{1}{2}}(\cos\theta)$ by N, Eq. (C9), expanding the integrand around $\lambda = 0$, from where the dominant contribution arises, and to employ the techniques developed in N (Sec. IX.C and Appendix F). The result for $\theta = 0$ is identical to (5.48), showing that (5.45) is, in fact, uniformly valid down to $\theta = 0$ [a similar situation was found for (4.35)].

The result (5.45) depends implicitly on θ through (5.41). The dependence can be made explicit with the help of (5.43). The final result is

$$\begin{aligned} f_{1,g}(\beta,\theta) &= -\frac{2N^2}{(N^2-1)^2} \times \frac{[(N\cos(\theta/2) - 1)(N - \cos(\theta/2))]^{\frac{3}{2}}}{(\cos(\theta/2))^{\frac{1}{2}}} \frac{\exp(2i\tau\beta)}{\tau^2} \\ &\times \left\{1 - \frac{i\tau}{16\beta(N\cos(\theta/2) - 1)}\left[\frac{2(N\cos(\theta/2) - 1)}{N\sin(\theta/2)}\right.\right. \\ &\times \left(\cot\theta - \frac{(N\cos(\theta/2) - 1)(N - \cos(\theta/2))}{2\tau^2\sin(\theta/2)}\right) \\ &\left.\left. - \frac{9}{1-\chi} + 15\chi - 6 + 8(\chi - 1) \times (\chi^2 + \tfrac{5}{8}\chi + 1)\frac{N^2\sin^2(\theta/2)}{(N\cos(\theta/2) - 1)^2}\right] + \mathcal{O}(\beta^{-2})\right\}, \\ &\theta_t - \theta \gg \gamma, \quad \theta \geq 0, \qquad (5.49) \end{aligned}$$

where τ is given by (5.44) and [cf. Eq. (5.47)]

$$\chi = \frac{N\cos(\theta/2) - 1}{N(N - \cos(\theta/2))}. \qquad (5.50)$$

The dominant term, represented by the factor outside of the curly brackets, agrees with the result found by Rubinow [Ref. 12, Eq. (53)]. As observed by Rubinow, the corresponding contribution to the differential scattering cross section,

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega}\right)_1 &= a^2|f_{1,g}(\beta,\theta)|^2 \\ &= \frac{4a^2N^4}{\cos(\theta/2)(N^2-1)^4} \times \frac{[(N\cos(\theta/2) - 1)(N - \cos(\theta/2))]^3}{(N^2 - 2N\cos(\theta/2) + 1)^2}, \qquad (5.51) \end{aligned}$$

differs from the prediction of classical mechanics for square-well scattering only by a factor

$$\begin{aligned} t &= (T_{21}T_{12})^2 \\ &= \left[\frac{2\cos\theta_1}{(\cos\theta_1 + N\cos\theta_2)}\frac{2N\cos\theta_2}{(\cos\theta_1 + N\cos\theta_2)}\right]^2 \\ &= \frac{16N^2}{(N^2-1)^4}[(N\cos(\theta/2) - 1)(N - \cos(\theta/2))]^2, \qquad (5.52) \end{aligned}$$

which represents the transmissivity of the well (T_{21} and T_{12} are given by the well-known Fresnel formulas).

However, it must be kept in mind that this is by no means the only quantum effect: there are other contributions to the differential cross section from the remaining terms of the Debye expansion (in particular, from the forward diffraction peak in f_0), as well as interference terms.

D. Behavior for $N > 1$ in the Penumbra Region ($|\theta - \theta_t| \lesssim \gamma$)

Let us now go over to the transition region (ii) of (5.3), $|\theta - \theta_t| \lesssim \gamma$ (penumbra). In this region, as was mentioned following (5.47), the above evaluation of $f_{1,g}(\beta, \theta)$ breaks down, because the Debye expansions for $H_\lambda^{(1,2)}(\beta)$ employed in (5.36)–(5.38) are no longer valid. With this single exception, all the results derived in Sec. 5C remain valid in the present region, so that we only need to consider $f_{1,g}$.

Since the dominant contribution to (5.29) in the penumbra region arises from the domain $|\lambda| - \beta = \mathcal{O}(\beta^{\frac{1}{3}})$, the appropriate expansions for $H_\lambda^{(1,2)}(\beta)$ in (3.24), as well as for $[1\,\beta]$ and $[2\,\beta]$ in $T_{21}T_{12}$, are those given in Appendix A and already employed in Sec. 4D. We shall keep only the dominant term in each expansion. For $H_\lambda^{(2)}(\beta)/H_\lambda^{(1)}(\beta)$, the result is given by (4.54); for T_{21}, by (3.5) and (4.58), and we find

$$T_{12} \approx 2. \tag{5.53}$$

Finally, we get

$$f_{1,g}(\beta, \theta) \approx -\frac{e^{5i\pi/12}\gamma}{\pi\beta M(2\pi \sin\theta)^{\frac{1}{2}}} \times \int \exp\left[2i((\alpha^2 - \lambda^2)^{\frac{1}{2}} - \lambda \cos^{-1}(\lambda/\alpha)) + i\lambda\theta\right] \frac{\sqrt{\lambda}\, d\lambda}{A^2(\zeta)}, \tag{5.54}$$

where ζ and $A(\zeta)$ are given by (4.55) and (4.56), respectively. The path of integration in the ζ plane is chosen to be the same as in (4.65)–(4.66), so that the dominant contribution arises from $|\zeta| \lesssim 1$. Accordingly, the integrand may be expanded around $\lambda = \beta$. This leads to the final expression

$$f_{1,g}(\beta, \theta) \approx -2\frac{e^{i\pi/4}}{M} \frac{\exp\left[2iM\beta + i\beta(\theta - \theta_t)\right]}{(2\pi\beta \sin\theta)^{\frac{1}{2}}} f(s), \qquad |\theta - \theta_t| \lesssim \gamma, \tag{5.55}$$

where

$$s = (\theta - \theta_t)/\gamma \tag{5.56}$$

and

$$f(s) = \frac{e^{i\pi/6}}{2\pi} \int_\Gamma \frac{\exp(is\zeta)}{A^2(\zeta)}\, d\zeta \tag{5.57}$$

is the Fock function already defined in N [Eq. (8.23)]. The path Γ runs from $e^{2i\pi/3}\infty$ to 0 and from 0 to ∞ (cf. N, Fig. 10).

Thus, we find a normal (Fock-type) transition from light to shadow, described by $f(s)$. In the shadow region, $s \gg 1$, (5.55) becomes, according to N [Eq. (8.24)],

$$f_{1,g}(\beta, \theta) \approx -\frac{e^{i\pi/12}}{M}\left(\frac{\gamma}{\pi \sin\theta}\right)^{\frac{1}{2}} \exp(2iM\beta) \times \sum_n (a_n')^{-2}(\theta - \theta_t) \exp\left[i(\beta + e^{i\pi/3}x_n/\gamma)(\theta - \theta_t)\right], \qquad \theta - \theta_t \gg \gamma, \tag{5.58}$$

which, according to (3.29) and (5.23), corresponds to the residue series in $\zeta_{1,0}^+$ in (5.22) as it should [see the remarks following (5.33)].

On the other hand, for $s < 0$, $|s| \gg 1$, the Fock function (5.57) can be evaluated by the saddle-point method, with the following result:

$$f(s) \approx \sqrt{\pi}\, e^{-i\pi/4}|s|^{\frac{3}{2}} \exp\left[-(i/12)s^3\right], \qquad s < 0, \quad |s| \gg 1. \tag{5.59}$$

Substituting this in (5.55), we find, in the lit region,

$$f_{1,g}(\beta, \theta) \approx -\frac{(\theta_t - \theta)^{\frac{3}{2}}}{M(\sin\theta)^{\frac{1}{2}}} \times \exp\left\{2iM\beta - i\beta\left[(\theta_t - \theta) - \tfrac{1}{24}(\theta_t - \theta)^3\right]\right\}, \qquad \theta_t - \theta \gg \gamma. \tag{5.60}$$

Again, this agrees with the dominant term of (5.49), provided that, as in previous cases, we do not try to push the Fock-function representation too far into the lit region: its domain of validity is just sufficient to produce a smooth transition.

Finally, since $f(0) = 1$ [cf. N, Eq. (8.26)], we find, at the shadow boundary,

$$f_{1,g}(\beta, \theta_t) \approx -\frac{e^{i\pi/4}N}{(\pi\beta)^{\frac{1}{2}}M^{\frac{3}{2}}} \exp(2iM\beta). \tag{5.61}$$

This completes the evaluation of the second term of the Debye expansion for $N > 1$.

E. Behavior for $N < 1$

For $N < 1$, according to Fig. 13(b), we again have to consider three regions: shadow, penumbra, and lit region, defined precisely as in (5.3) [however, θ_t is now given by (4.76)!]. We shall see that the width of the penumbra region is given by

$$\Delta\theta \sim \gamma' = (2/\alpha)^{\frac{1}{3}} = \gamma/N^{\frac{1}{3}}. \tag{5.62}$$

Let us consider first the shadow region, $\theta - \theta_t \gg \gamma'$. The amplitude is again a pure residue series, given by (5.6)–(5.8), and the evaluation of the residues again proceeds according to (5.17)–(5.19). For $f_{1,\mathrm{res}}'(\beta, \theta)$, the main difference with respect to (5.26) is that $H_\lambda^{(1,2)}(\beta)$ is now given by N, Eq. (A16). Accordingly,

the result differs from (5.26) only by the substitutions [cf. Eqs. (4.46) and (4.81)]:

$$M \to -iM', \quad \cosh^{-1} N \to -i \cos^{-1} N = -i\theta_t/2. \tag{5.63}$$

Thus, we find

$$f'_{1,\mathrm{res}}(\beta, \theta) \approx 2e^{i\pi/6} \frac{N^2}{\gamma' M'} \left(\frac{\pi - \theta}{\sin \theta}\right)^{\frac{1}{2}} \exp(-2iM'\beta) \times \sum_{m=0}^{\infty} (-1)^m \sum_n (a'_n)^{-2} \exp\{-i\lambda'_n[(2m+1)\pi - \theta_t]\} \times \{[(2m+1)\pi - \theta_t] J_0[\lambda'_n(\pi - \theta)] - i(\pi - \theta) J_1[\lambda'_n(\pi - \theta)]\}, \quad \theta - \theta_t \gg \gamma', \quad \theta \leq \pi. \tag{5.64}$$

[The evaluation of the dominant term in the residue-series contribution at the poles λ'_n for an arbitrary term of the Debye expansion will be carried out in Paper II (Appendix D).]

In particular, for $\pi - \theta \gg \alpha^{-1}$, we find [cf. Eq. (5.27)]

$$f'_{1,\mathrm{res}}(\beta, \theta) \approx \frac{e^{-i\pi/12} N^2}{M'} \left(\frac{\gamma'}{\pi \sin \theta}\right)^{\frac{1}{2}} \exp(-2iM'\beta) \times \left\{ \sum_n (a'_n)^{-2} \zeta^+_{1,0} \exp(-i\lambda'_n \zeta^+_{1,0}) + \sum_{m=1}^{\infty} (-1)^m \sum_n (a'_n)^{-2} \times [\zeta^+_{1,m} \exp(-i\lambda'_n \zeta^+_{1,m}) - i\zeta^-_{1,m} \exp(-i\lambda'_n \zeta^-_{1,m})] \right\}, \quad \theta - \theta_t \gg \gamma', \quad \pi - \theta \gg \alpha^{-1}. \tag{5.65}$$

By comparing this result with (4.82), we see that it can be rewritten as follows:

$$f'_{1,\mathrm{res}}(\beta, \theta) \approx 2e^{i\pi/4} \frac{N^2}{M'} \left(\frac{2\pi}{N\beta \sin \theta}\right)^{\frac{1}{2}} \exp(-2iM'\beta) \times \left\{ \sum_n \mathcal{D}_n \zeta^+_{1,0} \exp(-i\lambda'_n \zeta^+_{1,0}) + \sum_{m=1}^{\infty} (-1)^m \sum_n [\mathcal{D}_n \zeta^+_{1,m} \exp(-i\lambda'_n \zeta^+_{1,m}) - i\mathcal{D}_n \zeta^-_{1,m} \exp(-i\lambda'_n \zeta^-_{1,m})] \right\}, \quad \theta - \theta_t \gg \gamma', \quad \pi - \theta \gg \alpha^{-1}, \tag{5.66}$$

where

$$\mathcal{D}_n = e^{-i\pi/3}/2\pi a'^2_n \gamma'. \tag{5.67}$$

Each term in (5.66) differs from the corresponding term in (4.82) only by a factor

$$\mathcal{D}_n \zeta^{\pm}_{1,m} = \mathcal{D}_n \int_0^{\zeta_{1,m}^{\pm}} d\varphi. \tag{5.68}$$

This result can be physically interpreted as follows [Figs. 11(a) and 17]. The diffracted rays shown in Fig. 11(a) travel along the *inner* side of the surface, so that they cannot make any "shortcuts" such as those found for $N > 1$ (Fig. 15). Their only possible interaction with the surface is to produce a ray in the exterior region leaving the surface at the critical angle,

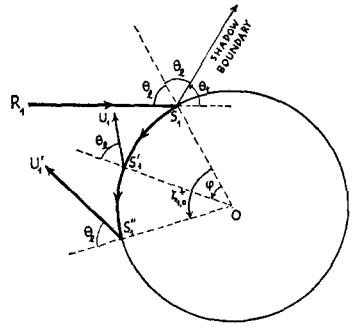

FIG. 17. Physical interpretation of the diffracted rays in (5.66); $S_1S'_1S''_1U'_1$ is a typical diffracted ray of this class.

such as S'_1U_1 in Figs. 11(a) and 17. Each time a surface wave associated with the first term of the Debye expansion does this, it excites further surface waves by a kind of "internal diffraction," and these are precisely the contributions found in (5.66). They have had one additional interaction with the surface as compared with (4.82), in agreement with the general physical interpretation of the Debye expansion given in Sec. 3A. We see that $\mathcal{D}_n$ represents the *internal diffraction coefficient.*

A typical diffracted ray of this class is $S_1S'_1S''_1U'_1$ in Fig. 17. The angle φ described by the "parent" surface wave up to the point of excitation S'_1 can take any value between 0 and $\zeta^{\pm}_{1,m}$, so that we again have an infinity of possible paths and must sum all their contributions. This leads to the integral in (5.68) [cf. the similar discussion for (5.24)].

To obtain the contribution from the residue series at the poles λ_n, it suffices to analytically continue (5.22) to $N < 1$, by making the substitutions

$$M \to -iM', \quad \cos^{-1}\frac{1}{N} \to -i \cosh^{-1}\frac{1}{N}. \tag{5.69}$$

This leads to

$$f_{1,\mathrm{res}}(\beta, \theta) \approx -\frac{e^{i\pi/3}}{M'} \left(\frac{\gamma}{\pi \sin \theta}\right)^{\frac{1}{2}} \exp(2M'\beta) \times \left(\sum_n (a'_n)^{-2} (\theta + 2i \cosh^{-1}(1/N)) \times \exp[i\lambda_n(\theta + 2i \cosh^{-1}(1/N))] + \sum_{m=1}^{\infty} (-1)^m \sum_n (a'_n)^{-2} \left\{ (2m\pi + \theta + 2i \cosh^{-1}(1/N)) \times \exp[i\lambda_n(2m\pi + \theta + 2i \cosh^{-1}(1/N))] + i(2m\pi - \theta + 2i \cosh^{-1}(1/N)) \times \exp[i\lambda_n(2m\pi - \theta + 2i \cosh^{-1}(1/N))] \right\} \right), \quad \theta - \theta^t \gg \gamma', \quad \pi - \theta \gg \alpha^{-1}. \tag{5.70}$$

These terms play the same role here that (5.27) played for $N > 1$. We can regard them as arising from

refraction of the surface waves excited by the tangentially incident rays (Fig. 9), which, as we have seen in Sec. 4E, are still given by (4.41) for $N < 1$. However, this is refraction with grazing angle of incidence, i.e., well beyond the critical angle, so that the corresponding angle of refraction is complex, corresponding to evanescent waves in the optically rare medium, as in total reflection. This gives rise to strong damping and makes (5.70) exponentially small, and therefore negligible, in comparison with (5.65), which, consequently, describes the total amplitude in the shadow region.

Thus, for the second term of the Debye expansion, the poles λ_n and λ'_n interchange their roles as we go over from $N > 1$ to $N < 1$. For $N > 1$ ($N < 1$), the contribution from the poles $\lambda_n(\lambda'_n)$ is dominant, and that from the other set of poles is exponentially small in comparison, although both contributions can be analytically continued in N from one case to the other. The two sets of poles play complementary roles, and λ'_n is just as important for $N < 1$ as λ_n is for $N > 1$.

Let us consider next the lit region, $\theta_t - \theta \gg \gamma'$. In this region, we must employ the representation (5.15)–(5.16) instead of (5.11)–(5.13). In order to apply the saddle-point method, the path of integration in (5.15) is first deformed into the path Γ shown in Fig. 14(b). In this process, it sweeps across poles λ_n and $-\lambda_n$ (say $2n_0$ of them), so that we get [cf. Eq. (5.28)]

$$f_1(\beta, \theta) = f_{1,g}(\beta, \theta) + \tilde{f}_{1,\text{res}}(\beta, \theta) + \tilde{f}'_{1,\text{res}}(\beta, \theta), \quad (5.71)$$

with

$$f_{1,g}(\beta, \theta) = -\frac{i}{\beta}\int_\Gamma U(\lambda, \beta) Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda, \quad (5.72)$$

$$\tilde{f}_{1,\text{res}}(\beta, \theta) = \frac{2\pi}{\beta}\left\{-i\sum_{n=1}^{n_0}\text{residue}\,[\lambda U P_{\lambda-\frac{1}{2}}(\cos\theta)\tan(\pi\lambda)]_{\lambda_n} + \sum_{m=0}^{\infty}(-1)^m\sum_n \text{residue}\,[\lambda U P_{\lambda-\frac{1}{2}}(\cos\theta)e^{2i(m+1)\pi\lambda}]_{\lambda_n}\right\}, \quad (5.73)$$

$$\tilde{f}'_{1,\text{res}}(\beta, \theta) = \frac{2\pi}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residue} \times \{\lambda U P_{\lambda-\frac{1}{2}}(\cos\theta)\exp[2i(m+1)\pi\lambda]\}_{-\lambda_n'}. \quad (5.74)$$

We now find

$$\tilde{f}'_{1,\text{res}}(\beta, \theta) \approx 2e^{i\pi/6}\frac{N^2}{\gamma' M'}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\exp(-2iM'\beta) \times \sum_{m=0}^{\infty}(-1)^m\sum_n (a'_n)^{-2}\exp\{-i\lambda'_n[2(m+1)\pi - \theta_t]\} \times \{i[2(m+1)\pi - \theta_t]J_0(\lambda'_n\theta) + \theta J_1(\lambda'_n\theta)\}, \quad \theta_t - \theta \gg \gamma', \quad \theta \geq 0. \quad (5.75)$$

In particular, for $\theta \gg \alpha^{-1}$,

$$\tilde{f}'_{1,\text{res}}(\beta, \theta) \approx \frac{e^{-i\pi/12}N^2}{M'}\left(\frac{\gamma'}{\pi\sin\theta}\right)^{\frac{1}{2}}\exp(-2iM'\beta) \times \sum_{m=1}^{\infty}(-1)^m\sum_n (a'_n)^{-2}[\zeta^+_{1,m}\exp(-i\lambda'_n\zeta^+_{1,m}) - i\zeta^-_{1,m}\exp(-i\lambda'_n\zeta^-_{1,m})], \quad \theta_t - \theta \gg \gamma', \quad \theta \gg \alpha^{-1}, \quad (5.76)$$

which differs from (5.65) only by the omission of the series in $\zeta^+_{1,0}$, as it should [see the comments following (5.33)].

On the other hand,

$$\tilde{f}_{1,\text{res}}(\beta, \theta) \approx \frac{2e^{i\pi/12}}{\gamma M'}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}}\exp(2M'\beta) \times \left\{\sum_{n=1}^{n_0}(a'_n)^{-2}\exp(-2\lambda_n\cosh^{-1}(1/N)) \times [2\cosh^{-1}(1/N)J_0(\lambda_n\theta) + \theta J_1(\lambda_n\theta)] + \sum_{m=1}^{\infty}(-1)^m\sum_n (a'_n)^{-2} \times \exp(2im\pi\lambda_n - 2\lambda_n\cosh^{-1}(1/N)) \times [(2im\pi - 2\cosh^{-1}(1/N))J_0(\lambda_n\theta) - \theta J_1(\lambda_n\theta)]\right\}, \quad \theta_t - \theta \gg \gamma', \quad \theta \geq 0, \quad (5.77)$$

which is negligible in comparison with $\tilde{f}'_{1,\text{res}}(\beta, \theta)$.

Finally, let us consider the "geometrical-optic" contribution $f_{1,g}(\beta, \theta)$, given by (5.72). This differs from (5.29) by having $Q^{(1)}_{\lambda-\frac{1}{2}}$ instead of $Q^{(2)}_{\lambda-\frac{1}{2}}$ and by the different path of integration. With the same change of variables (5.35), the saddle point is found to be determined by [cf. Eqs. (5.40) and (5.41)]:

$$\bar{w}_1 = \theta_1, \quad \bar{w}_2 = \theta_2, \quad (5.78)$$

where

$$\theta_2 - \theta_1 = \frac{\theta}{2}, \quad \sin\theta_1 = N\sin\theta_2. \quad (5.79)$$

This agrees with the laws of geometrical optics for $N < 1$ ($\theta_1 < \theta_2$), and it is the reason why it was necessary to employ the representation (5.15) instead of (5.11).

The steepest descent path now crosses the real axis at an angle of $\pi/4$ [Fig. 14(b)]. Thus, we have to employ N, Eq. (6.12), rather than N, Eq. (6.21). Making appropriate changes in the calculation that led to (5.45), we finally obtain

$$f_{1,g}(\beta, \theta) = \left(\frac{\sin\theta_1}{\sin\theta}\right)^{\frac{1}{2}}\frac{(2N\cos\theta_1\cos\theta_2)^{\frac{3}{2}}}{(\cos\theta_1 + N\cos\theta_2)^2} \times \frac{\exp[-2i\beta(\cos\theta_1 - N\cos\theta_2)]}{(\cos\theta_1 - N\cos\theta_2)^{\frac{1}{2}}} \times \left\{1 - \frac{i\mathcal{F}(\theta)}{16\beta\cos\theta_1} + \mathcal{O}(\beta^{-2})\right\}, \quad (5.80)$$

where

$$\mathcal{F}(\theta) = 2\cot\theta_1\left[\frac{\cot\theta_1}{2(\chi-1)} - \cot\theta\right] + \frac{9}{\chi-1} + 15\chi - 6 + 8(\chi-1)(\chi^2 + \tfrac{5}{8}\chi + 1)\tan^2\theta_1, \qquad (5.81)$$

and χ is still given by (5.47).

With the help of (5.43), this result can also be expressed directly in terms of the angle θ. We find

$$f_{1,g}(\beta,\theta) = \frac{2N^2}{(1-N^2)^2}\frac{[(1-N\cos(\theta/2))(\cos(\theta/2)-N)]^{\frac{3}{2}}}{(\cos(\theta/2))^{\frac{1}{2}}}\frac{\exp(-2i\tau\beta)}{\tau^2}$$
$$\times\left(1 - \frac{i\tau}{16\beta(1-N\cos(\theta/2))}\left\{\frac{2(1-N\cos(\theta/2))}{N\sin(\theta/2)}\left[\frac{(1-N\cos(\theta/2))(\cos(\theta/2)-N)}{2\tau^2\sin(\theta/2)} - \cot\theta\right]\right.\right.$$
$$\left.\left. + \frac{9}{\chi-1} + 15\chi - 6 + 8(\chi-1)(\chi^2+\tfrac{5}{8}\chi+1)\frac{N^2\sin^2(\theta/2)}{(1-N\cos(\theta/2))^2}\right\} + \mathcal{O}(\beta^{-2})\right),$$
$$\theta_t - \theta \gg \gamma', \quad \theta \geq 0, \qquad (5.82)$$

where τ and χ are again given by (5.44) and (5.50), respectively. The result is also uniformly valid down to $\theta = 0$. It differs from (5.49) only by the over-all sign factor and by the replacement $\tau \to -\tau$. This gives the correct continuation for $N < 1$, as can be verified by checking that, for $\theta = 0$, Eq. (5.82) becomes identical to (5.48).

The last region that remains to be considered is the penumbra region, $|\theta - \theta_t| \lesssim \gamma'$. In this region, we must employ the expansions of Appendix A for $H_\lambda^{(1,2)}(\alpha)$. By a procedure entirely similar to that which led to (5.55), we find

$$f_{1,g}(\beta,\theta) \approx 2e^{-i\pi/4}\frac{N^{\frac{3}{2}}}{M'} \times \frac{\exp[-2iM'\beta - iN\beta(\theta-\theta_t)]}{(2\pi\beta\sin\theta)^{\frac{1}{2}}}\bar{f}(s'), \quad |\theta-\theta_t| \lesssim \gamma', \qquad (5.83)$$

where

$$s' = (\alpha/2)^{\frac{1}{3}}(\theta-\theta_t) = (\theta-\theta_t)/\gamma' \qquad (5.84)$$

and

$$\bar{f}(s) = \frac{e^{-i\pi/6}}{2\pi}\int_{\bar{\Gamma}}\frac{\exp(-is\zeta)}{\bar{A}^2(\zeta)}\,d\zeta, \qquad (5.85)$$

where $\bar{A}(\zeta)$ is defined by (4.56) and the path $\bar{\Gamma}$ consists of a straight line from $e^{-2i\pi/3}\infty$ to 0 and the real axis from 0 to ∞. By comparing (5.85) with (5.57), we find that they are complex conjugate:

$$\bar{f}(s) = [f(s)]^* \qquad (5.86)$$

The behavior of $\bar{f}(s)$ for $|s| \gg 1$ therefore follows immediately from the corresponding behavior of $f(s)$. In this way, we also find that (5.83) gives rise to a smooth transition between shadow and lit region. Note that it is a normal (Fock-type) transition, similar to that found for $N > 1$. This behavior differs from that found in the same region for the first term of the Debye expansion [cf. Eq. (4.101)]. As has already been mentioned, all terms in the Debye expansion give rise to the same transition region for $N < 1$, so that the behavior of the complete amplitude within this region is quite complicated.

This concludes the discussion of the behavior of the second term in the Debye expansion. We see that the modified Watson transformation indeed enables us to determine the high-frequency behavior of the first two terms in any direction θ, both for $N > 1$ and for $N < 1$. The behavior of the remaining terms will be discussed in Paper II.

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APPENDIX A: ASYMPTOTIC EXPANSIONS FOR THE POLES AND AUXILIARY FORMULAS FOR THE COMPUTATION OF RESIDUES

The following asymptotic expansions for $H_\lambda^{(1)}(x)$, $H_\lambda'^{(1)}(x)$, valid when $|\lambda - x| = \mathcal{O}(x^{\frac{1}{3}})$, $x \gg 1$, have been derived by Schöbe[41]:

$$H_\lambda^{(1)}(x) = 2e^{-i\pi/3}\left(\frac{2}{x}\right)^{\frac{1}{3}}\sum_{n=0}^{\infty}(-1)^n\left(\frac{2}{x}\right)^{2n/3}[P_n(\xi)\,\mathrm{Ai}(-\xi) - e^{-i\pi/3}Q_n(\xi)\,\mathrm{Ai}'(-\xi)], \qquad (A1)$$

$$H_\lambda'^{(1)}(x) = -2e^{-i\pi/3}\left(\frac{2}{x}\right)^{\frac{2}{3}}\sum_{n=0}^{\infty}(-1)^n\left(\frac{2}{x}\right)^{2n/3}[\bar{P}_n(\xi)\,\mathrm{Ai}(-\xi) - e^{-i\pi/3}\bar{Q}_n(\xi)\,\mathrm{Ai}'(-\xi)], \qquad (A2)$$

[41] W. Schöbe, Acta Math. **92**, 265 (1954).

where

$$\xi = e^{-i\pi/3}\left(\frac{2}{x}\right)^{\frac{1}{3}}(\lambda - x), \tag{A3}$$

and

$$\begin{aligned} P_0(\xi) &= 1, & Q_0(\xi) &= 0, \\ P_1(\xi) &= e^{i\pi/3}\frac{\xi}{15}, & Q_1(\xi) &= -e^{-i\pi/3}\frac{\xi^2}{60}, \\ P_2(\xi) &= e^{-i\pi/3}\left(\frac{\xi^5}{7200} - \frac{13\xi^2}{1260}\right), & Q_2(\xi) &= -\frac{\xi^3}{420} + \frac{1}{140}, \end{aligned} \tag{A4}$$

$$\begin{aligned} \bar{P}_0(\xi) &= 0, & \bar{Q}_0(\xi) &= 1, \\ \bar{P}_1(\xi) &= -\frac{\xi^3}{60} - \frac{1}{10}, & \bar{Q}_1(\xi) &= -e^{i\pi/3}\frac{\xi}{15}, \\ \bar{P}_2(\xi) &= -e^{i\pi/3}\left(\frac{\xi^4}{3360} + \frac{\xi}{60}\right), & \bar{Q}_2(\xi) &= e^{-i\pi/3}\left(\frac{\xi^5}{7200} + \frac{19\xi^2}{2520}\right). \end{aligned} \tag{A5}$$

The corresponding expansions for $H_\lambda^{(2)}(x)$, $H_\lambda'^{(2)}(x)$ are obtained by changing the sign of i everywhere in the above expressions.

By employing a slightly different version of these results, Streifer and Kodis[28] found the following improved asymptotic expansion for the poles (3.29):

$$\lambda_n = \beta + e^{i\pi/3}\xi_n/\gamma, \tag{A6}$$

where $\gamma \ll 1$ [cf. Eq. (2.49)] is the expansion parameter, and

$$\xi_n = x_n - \delta_n, \tag{A7}$$

with x_n defined by (2.54) [nth zero of Ai $(-x)$], and

$$\begin{aligned} \delta_n = {} & -e^{i\pi/3}\frac{x_n^2}{60}\gamma^2 - e^{-i\pi/3}\left(\frac{x_n^3}{1400} - \frac{1}{140}\right)\gamma^4 - \left(\frac{281x_n^4}{4536000} - \frac{29x_n}{12600}\right)\gamma^6 \\ & + e^{i\pi/6}\frac{\gamma}{M}\Bigg[1 + e^{i\pi/3}\frac{x_n}{6}\left(1 + \frac{1}{M^2}\right)\gamma^2 - e^{-i\pi/3}\frac{x_n^2}{20} \\ & \times \left(\frac{3}{2M^4} + \frac{13}{9M^2} - \frac{1}{18}\right)\gamma^4 - \frac{e^{-i\pi/6}}{M}\frac{x_n}{36}\left(\frac{1}{M^4} + \frac{2}{M^2} + 1\right)\gamma^5\Bigg] + \mathcal{O}(\gamma^7), \end{aligned} \tag{A8}$$

where $M = (N^2 - 1)^{\frac{1}{2}}$, as in (2.53). The corresponding result for $N < 1$ (which was actually the case considered in Ref. 28) is obtained by the substitution (3.30): $M = -iM' = -i(1 - N^2)^{\frac{1}{2}}$. Notice that $\delta_n = \mathcal{O}(\gamma)$, so that $|\delta_n| \ll 1$.

The first three terms of (A8), which do not depend on N, correspond to the Regge poles [N, Eq. (3.5)] for an impenetrable sphere, i.e., the roots of $H_\lambda^{(1)}(\beta) = 0$. They can formally be obtained by letting $N \to i\infty$, corresponding to an infinitely high potential barrier. The remaining terms in (A8) represent the effect of a finite refractive index.

For the evaluation of the residue series appearing in the first three terms of the Debye expansion, the values of $H_\lambda^{(1)}(\beta)$, $H_\lambda'^{(1)}(\beta)$ and their derivatives up to third order with respect to λ, taken at the poles λ_n, are required. The corresponding asymptotic expansions may be obtained from (A1)–(A5) with the help of the following formulas, which follow from (A3):

$$\dot{\xi} = e^{-i\pi/3}\gamma, \quad \dot{A} = -e^{-i\pi/3}\gamma A', \quad \dot{A}' = e^{-i\pi/3}\gamma\xi A, \tag{A9}$$

where the dots denote partial derivatives with respect to λ and we have introduced the abbreviations

$$A = \mathrm{Ai}\,(-\xi), \quad A' = \mathrm{Ai}'\,(-\xi), \quad \xi = e^{-i\pi/3}\gamma(\lambda - \beta). \tag{A10}$$

We then find the following results:

$$H_\lambda^{(1)}(\beta) = 2e^{-i\pi/3}\gamma\left\{A + \frac{\gamma^2}{15}e^{i\pi/3}\left(\frac{\xi^2}{4}A' - \xi A\right) + \frac{\gamma^4}{20}e^{-i\pi/3}\left[\frac{1}{7}\left(\frac{\xi^3}{3} - 1\right)A' + \frac{\xi^2}{9}\left(\frac{\xi^3}{40} - \frac{13}{7}\right)A\right] + O(\gamma^6)\right\}, \quad \text{(A11)}$$

$$H_\lambda'^{(1)}(\beta) = -2e^{i\pi/3}\gamma^2\left\{A' + \frac{\gamma^2}{15}e^{i\pi/3}\left[\xi A' - \left(\frac{\xi^3}{4} + \frac{3}{2}\right)A\right] + \frac{\gamma^4}{60}e^{-i\pi/3}\left[\frac{\xi^2}{6}\left(\frac{\xi^3}{20} + \frac{19}{7}\right)A' - \xi\left(\frac{\xi^3}{56} + 1\right)A\right] + O(\gamma^6)\right\}, \quad \text{(A12)}$$

$$\dot{H}_\lambda^{(1)}(\beta) = 2e^{i\pi/3}\gamma^2\left\{A' - \frac{\gamma^2}{15}e^{i\pi/3}\left[\frac{3\xi}{2}A' + \left(\frac{\xi^3}{4} - 1\right)A\right] - \frac{\gamma^4}{180}e^{-i\pi/3}\left[\xi^2\left(\frac{22}{7} - \frac{\xi^3}{40}\right)A' + \xi\left(\frac{31}{56}\xi^3 - 5\right)A\right] + O(\gamma^6)\right\}, \quad \text{(A13)}$$

$$\dot{H}_\lambda'^{(1)}(\beta) = -2\gamma^3\left\{\xi A + \frac{\gamma^2}{30}e^{i\pi/3}\left[\left(\frac{\xi^3}{2} + 5\right)A' + \frac{\xi^2}{2}A\right] + \frac{\gamma^4}{60}e^{-i\pi/3}\left[\frac{10}{21}\xi\left(\frac{\xi^3}{8} + 4\right)A' + \left(\frac{\xi^6}{120} + \frac{8}{21}\xi^3 - 1\right)A\right] + O(\gamma^6)\right\}, \quad \text{(A14)}$$

$$\ddot{H}_\lambda^{(1)}(\beta) = 2\gamma^3\left\{\xi A + \frac{\gamma^2}{30}e^{i\pi/3}\left[\left(\frac{\xi^3}{2} - 5\right)A' - \frac{9}{2}\xi^2 A\right] - \frac{\gamma^4}{180}e^{-i\pi/3}\left[\frac{\xi}{7}\left(79 - \frac{19}{4}\xi^3\right)A' - \left(\frac{\xi^6}{40} - \frac{75}{14}\xi^3 + 5\right)A\right] + O(\gamma^6)\right\}, \quad \text{(A15)}$$

$$\ddot{H}_\lambda'^{(1)}(\beta) = 2\gamma^4 e^{-i\pi/3}\left\{\xi A' - A - \frac{\gamma^2}{30}e^{i\pi/3}\left[\xi^2 A' + \xi\left(\frac{\xi^3}{2} + 6\right)A\right] + O(\gamma^4)\right\}, \quad \text{(A16)}$$

$$\dddot{H}_\lambda^{(1)}(\beta) = -2\gamma^4 e^{-i\pi/3}\left\{\xi A' - A - \frac{\gamma^2}{30}e^{i\pi/3}\left[6\xi^2 A' - \xi\left(14 - \frac{\xi^3}{2}\right)A\right] + O(\gamma^4)\right\}, \quad \text{(A17)}$$

$$\dddot{H}_\lambda'^{(1)}(\beta) = -2\gamma^5 e^{i\pi/3}\left\{2A' + \xi^2 A + \frac{\gamma^2}{30}e^{i\pi/3}\left[\xi\left(\frac{\xi^3}{2} + 4\right)A' - 3(\xi^3 + 2)A\right] + O(\gamma^4)\right\}. \quad \text{(A18)}$$

To evaluate these expressions at the pole λ_n, it suffices to replace ξ by ξ_n, which is given by (A7)–(A8). Since $|\delta_n| \ll 1$, the Taylor expansion of the Airy functions around $\xi = x_n$ may be employed, with the results

$$A_n = \mathrm{Ai}(-\xi_n) = \delta_n a_n'\left(1 - \frac{x_n}{6}\delta_n^2 + \tfrac{1}{12}\delta_n^3 + \frac{x_n^2}{120}\delta_n^4 - \frac{x_n}{120}\delta_n^5 + \cdots\right), \quad \text{(A19)}$$

$$A_n' = \mathrm{Ai}'(-\xi_n) = a_n'\left(1 - \frac{x_n}{2}\delta_n^2 + \tfrac{1}{8}\delta_n^3 + \frac{x_n^2}{24}\delta_n^4 - \frac{x_n}{20}\delta_n^5 + \cdots\right), \quad \text{(A20)}$$

where $a_n' = \mathrm{Ai}'(-x_n)$, as in (4.40), and we have employed the differential equation of the Airy functions,

$$\mathrm{Ai}''(z) = z\,\mathrm{Ai}(z). \quad \text{(A21)}$$

The denominator that gives rise to the poles is [cf. Eq. (4.38)]:

$$d(\lambda, \beta) = [1\ \beta] - N[2\ \alpha] \quad \text{(A22)}$$

and the value of its partial derivatives with respect to λ, up to third order, at the poles λ_n is also required for the evaluation of residues.

In the neighborhood of the poles, we have, by N, Eq. (A16):

$$[2\ \alpha] = -i\frac{(N^2 - \omega^2)^{\frac{1}{2}}}{N} - \frac{N\gamma^3}{4(N^2 - \omega^2)} + O(\gamma^6), \quad \text{(A23)}$$

where

$$\omega = \lambda/\beta. \tag{A24}$$

The partial derivatives of [2 α] with respect to λ can be readily evaluated from this expression. Those of [1 β], on the other hand, can be expressed in terms of (A11)–(A18) by means of the following formulas:

$$[1\dot{\beta}] = \frac{1}{H_\lambda^{(1)}(\beta)}\{\dot{H}_\lambda^{\prime(1)}(\beta) - [1\ \beta]H_\lambda^{(1)}(\beta)\}, \tag{A25}$$

$$[1\ddot{\beta}] = \frac{1}{H_\lambda^{(1)}(\beta)}\{\ddot{H}_\lambda^{\prime(1)}(\beta) - [1\ \beta]\dot{H}_\lambda^{(1)}(\beta)\} - 2\frac{\dot{H}_\lambda^{(1)}(\beta)}{H_\lambda^{(1)}(\beta)}[1\dot{\beta}], \tag{A26}$$

$$[1\dddot{\beta}] = \frac{1}{H_\lambda^{(1)}(\beta)}\{\dddot{H}_\lambda^{\prime(1)}(\beta) - [1\ \beta]\ddot{H}_\lambda^{(1)}(\beta)\} - 3\frac{\dot{H}_\lambda^{(1)}(\beta)}{H_\lambda^{(1)}(\beta)}[1\ddot{\beta}] - 3\frac{\ddot{H}_\lambda^{(1)}(\beta)}{H_\lambda^{(1)}(\beta)}[1\dot{\beta}], \tag{A27}$$

where, at the poles, [1 β] can be computed from (3.27) and (A23):

$$[1\ \beta]_{\lambda_n} = N[2\ \alpha]_{\lambda_n}. \tag{A28}$$

APPENDIX B: ASYMPTOTIC BEHAVIOR OF THE SPHERICAL REFLECTION AND TRANSMISSION COEFFICIENTS

We collect in this appendix the main results required in the text about the asymptotic behavior of $S(\lambda, \beta)$ and of the spherical reflection and transmission coefficients (3.4)–(3.8) as $|\lambda| \to \infty$. The derivation is omitted: it is based upon the formulas for the asymptotic behavior of cylindrical functions given in N (Appendix A).

The results are presented graphically in Figs. 18–21. The expression given in each region of the λ plane represents the asymptotic behavior of the corresponding function in that region. Inessential factors, such as constants, are omitted.

The notation is the same as in N (Appendix A): when $|\lambda| \to \infty$ along directions approaching the positive or negative imaginary axis, we take, respectively,

$$\lambda = \pm\sigma|\lambda|, \quad \sigma = \exp[i(\pi/2 + \epsilon)], \tag{B1}$$

and we define

$$\eta_1 = \epsilon \ln\left|\frac{2\lambda}{e\alpha}\right|, \quad \eta_2 = \epsilon \ln\left|\frac{2\lambda}{e\beta}\right|. \tag{B2}$$

The asymptotic behavior of $S(\lambda, \beta)$ is given in Fig. 18, and that of all the spherical reflection and transmission coefficients can be obtained from Figs. 19 and 20. Finally, Fig. 21 shows the asymptotic behavior of $\rho = R_{11}H_\lambda^{(1)}(\alpha)/H_\lambda^{(2)}(\alpha)$, the expansion parameter in the Debye expansion [cf. Eq. (3.15)].

All the results shown refer to the case $N > 1$. However, it is not difficult to adapt them to the case $N < 1$.

APPENDIX C: REDUCTION TO GENERALIZED FOCK FUNCTIONS

To reduce the first two integrals in (4.64) to the generalized Fock functions (4.67), we first note that, by (4.63),

$$(1 + \tfrac{1}{2}\zeta\gamma^2)J_0 = \frac{\gamma}{\theta}\frac{d}{d\zeta}[(1 + \tfrac{1}{2}\zeta\gamma^2)J_1], \tag{C1}$$

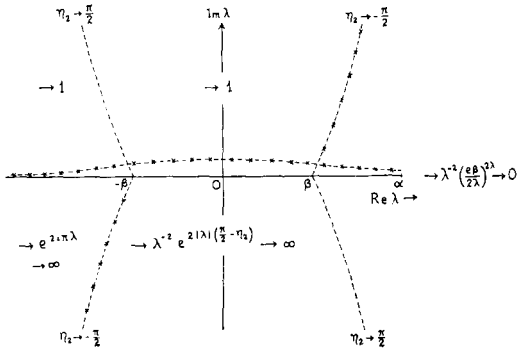

FIG. 18. Asymptotic behavior of $1 - S(\lambda, \beta)$ as $|\lambda| \to \infty$ in different regions of the λ plane. ×—poles ($N > 1$).

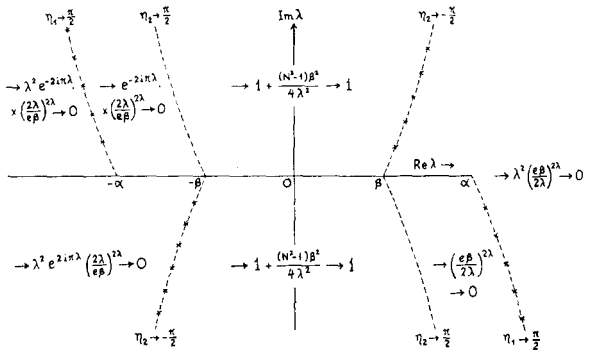

FIG. 19. Asymptotic behavior of $T_{21}(\lambda, \beta) = 1 + R_{22}(\lambda, \beta)$ as $|\lambda| \to \infty$ in different regions of the λ plane. ×—poles ($N > 1$).

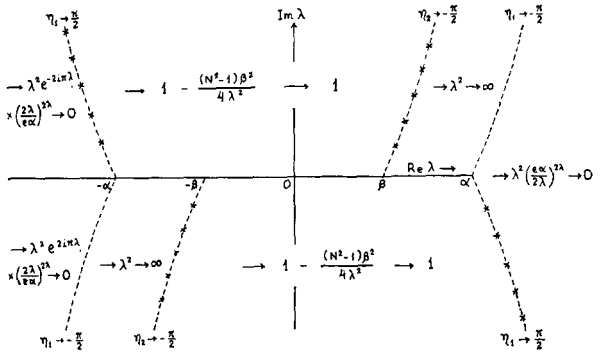

FIG. 20. Asymptotic behavior of $T_{12}(\lambda, \beta) = 1 + R_{11}(\lambda, \beta)$ as $|\lambda| \to \infty$ in different regions of the λ plane. ×—poles ($N > 1$).

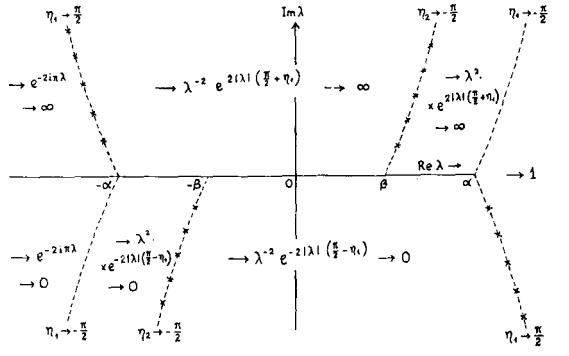

FIG. 21. Asymptotic behavior of $\rho(\lambda, \beta) = R_{11}(\lambda, \beta)H_\lambda^{(1)}(\alpha)/H_\lambda^{(2)}(\alpha)$ as $|\lambda| \to \infty$ in different regions of the λ plane. Note that $|\rho| < 1$ along the real axis. ×—poles ($N > 1$).

where, unless otherwise indicated, the argument of the Bessel functions is always the same as in (4.63). We then find, by partial integration,

$$e^{2i\pi/3}\int_{\sigma_1\infty}^{0}(1 + \tfrac{1}{2}\zeta\gamma^2)J_0\frac{\bar{A}}{A}\,d\zeta$$
$$= e^{2i\pi/3}\frac{\gamma}{\theta}J_1(\beta\theta) + \frac{e^{i\pi/6}}{2\pi}\frac{\gamma}{\theta}\int_{\sigma_1\infty}^{0}(1 + \tfrac{1}{2}\zeta\gamma^2)\frac{J_1}{A^2}\,d\zeta, \quad \text{(C2)}$$

where the Wronskian relation (4.57) has been employed.

A similar transformation can be performed for the second integral in (4.64), with the help of the Wronskian relation [N, Eq. (D2)]. Putting together the results, we obtain

$$e^{2i\pi/3}\int_{\sigma_1\infty}^{0}(1 + \tfrac{1}{2}\zeta\gamma^2)J_0\frac{\bar{A}}{A}\,d\zeta$$
$$+ e^{i\pi/3}\int_0^{\infty}(1 + \tfrac{1}{2}\zeta\gamma^2)J_0\frac{\mathrm{Ai}(\zeta)}{A}\,d\zeta$$
$$= -\frac{\gamma}{\theta}J_1(\beta\theta) + \frac{\gamma}{\theta}[F_{0,1}(\beta, \theta) + \tfrac{1}{2}\gamma^2F_{1,1}(\beta, \theta)], \quad \text{(C3)}$$

where $F_{m,n}$ is defined by (4.67).

Similarly, by partial integration, we find

$$\frac{e^{-i\pi/6}}{2\pi}\int_\Gamma\frac{A'}{A^3}J_0\,d\zeta = \frac{\theta}{2\gamma}F_{0,1}(\beta, \theta). \quad \text{(C4)}$$

It follows from the differential equation (A21) of the Airy functions that

$$\frac{A'^2}{A^4} = \tfrac{1}{3}e^{2i\pi/3}\frac{\zeta}{A^2} - \frac{1}{3}\frac{d}{d\zeta}\left(\frac{A'}{A^3}\right). \quad \text{(C5)}$$

Thus, by partial integration, we get

$$\frac{1}{2\pi}\int_\Gamma\frac{A'^2}{A^4}J_0\,d\zeta$$
$$= \frac{i}{3}F_{1,0}(\beta, \theta) + e^{i\pi/6}\frac{\theta^2}{12\gamma^2}[F_{0,0}(\beta, \theta) - F_{0,2}(\beta, \theta)], \quad \text{(C6)}$$

where we have employed the relation

$$J_1' = \tfrac{1}{2}(J_0 - J_2).$$

Finally, we have

$$\frac{1}{2\pi}\int_\Gamma\zeta^2\frac{A'}{A^3}J_0\,d\zeta = -e^{i\pi/6}\left[F_{1,0}(\beta, \theta) - \frac{\theta}{2\gamma}F_{2,1}(\beta, \theta)\right]. \quad \text{(C7)}$$

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High-Frequency Scattering by a Transparent Sphere. II. Theory of the Rainbow and the Glory

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The treatment, initiated in Paper I [J. Math. Phys. **10**, 82 (1969)], of the high-frequency scattering of a scalar plane wave by a transparent sphere is continued. The main results here are an improved theory of the rainbow and a theory of the glory. The modified Watson transformation is applied to the third term of the Debye expansion of the scattering amplitude in terms of multiple reflections. Only the range $1 < N < \sqrt{2}$, where N is the refractive index, is considered. In the geometrical-optic approximation, this term is associated with rays transmitted after one internal reflection, and there are three angular regions, corresponding to one ray, two rays, or no ray (shadow) passing through each direction. Together with transition regions, this leads to six different angular domains. In the 1-ray and 2-ray regions, geometrical-optic terms are dominant. Correction terms corresponding to the 2nd-order WKB approximation are also evaluated. In the 0-ray region, the amplitude is dominated by complex rays and surface waves. The 1-ray/2-ray transition is a Fock-type region. The rainbow appears in the 2-ray/0-ray transition region. The extension of the method of steepest descents due to Chester, Friedman and Ursell is applied. The result is a uniform asymptotic expansion for the scattering amplitude. It reduces to Airy's theory in the lowest-order approximation, but its domain of validity is considerably greater, both with regard to size parameter and to angles. The glory is an example of strong "Regge-pole dominance" of the near-backward scattering amplitude. Van de Hulst's conjecture that surface waves are responsible for the glory is confirmed. However, besides surface waves taking two shortcuts through the sphere, higher-order terms in the Debye expansion must also be taken into account. By considering also the effect of higher-order surface-wave contributions, all the features observed in the glory (apart from the polarization) are explained. Resonance effects associated with nearly-closed paths of diffracted rays lead to large, rapid, quasiperiodic intensity fluctuations. The same effects are responsible for the ripple in the total cross-section. Similar fluctuations appear in any direction, but their amplitude increases with the scattering angle, becoming a maximum near the backward direction, where they are dominant. They can also be interpreted as a collective effect due to many nearly-resonant partial waves in the edge domain. The dominant surface-wave contributions can also be summed to all orders for $N < 1$, leading to a renormalization of the propagation constants of surface waves.

1. INTRODUCTION

In Paper I of this work[1] the high-frequency asymptotic behavior of the scattering amplitude for a scalar plane wave incident on a transparent sphere was investigated, with the help of techniques developed in an earlier paper.[2] It was assumed that

$$\beta^{\frac{1}{3}} \gg 1, \quad |N-1|^{\frac{1}{2}}\beta^{\frac{1}{3}} \gg 1, \tag{1.1}$$

where $\beta = ka$, k is the wavenumber, a is the radius of the sphere, and N is the refractive index.

The Debye expansion of the scattering amplitude, in terms of an infinite series of multiple internal reflections, was employed. In Paper I, the first two terms of this series, corresponding to direct reflection from the surface and to direct transmission through the sphere, were evaluated. Both $N > 1$ and $N < 1$ were treated.

In the present paper, the third term of the Debye expansion is evaluated and the effect of higher-order terms is discussed. In many cases of practical importance, higher-order terms may be neglected, although their contributions have to be taken into account in the neighborhood of certain special directions, as will be seen later. Any such contribution may be evaluated, in principle, by methods similar to those developed here.

In contrast with the first two terms, it is not possible to give a uniform treatment of the third term, valid for all $N > 1$. As is shown in Sec. 2, there are five different ranges of the refractive index, each of them requiring a separate treatment. This subdivision arises already at the level of geometrical optics. It is due to the fact that, for different ranges of N, there are different subdivisions into angular regions, each angular region being characterized by the number of rays going through a given direction within that region. This number may vary between zero and three.

Here we shall be concerned mostly with the range

$$1 < N < \sqrt{2}, \tag{1.2}$$

[1] H. M. Nussenzveig, J. Math. Phys. **10**, 82 (1969) (preceding paper; referred to as I).
[2] H. M. Nussenzveig, Ann. Phys. (N.Y.) **34**, 23 (1965) (referred to as N).

because we have in mind the application to light scattering by water droplets, and the refractive index of water, $N = 1.33$, falls within this range. Although several interesting phenomena occur in other ranges, especially near the transition points, our attention in the present work is focused mainly on the range (1.2). In this range, according to geometrical optics, there are three different angular regions: a 0-ray (shadow) region near the forward direction, a 1-ray region near the backward direction, and a 2-ray region in between. Taking into account, also, the corresponding transition regions, we find a total of six different angular regions to be considered.

The structure of the third term differs from that of the previous ones in many respects. Physically, this difference is due to the fact that it contains two new features, associated with two very beautiful natural phenomena: the rainbow and the glory. They are contained, respectively, in the 2-ray/0-ray transition region and in the region near the backward direction.

The remaining four regions, which we call "normal," are discussed first (Sec. 3). In the 1-ray region, in addition to the geometrical-optic contribution, we find surface waves, excited at the 1-ray/2-ray shadow boundary, corresponding to diffracted rays that take two "shortcuts" across the sphere. The 1-ray/2-ray transition region corresponds to a normal (Fock-type) transition. In the 2-ray region, there are two real saddle points, corresponding to the two rays passing through each direction within this region. These saddle points become complex in the shadow (0-ray) region, and, due to their presence, the amplitude cannot be reduced to a pure residue series in this region.

The rainbow (Sec. 4) corresponds to a new type of light-shadow transition, associated with the confluence of a pair of geometrical rays (real saddle points) and their transformation into complex rays (saddle points). The corresponding mathematical problem is the asymptotic expansion of an integral having two saddle points that move towards (or away from) each other. This problem has only recently been solved by Chester, Friedman, and Ursell.[3,4] By applying their method, we find a uniform asymptotic expansion of the amplitude, valid throughout the rainbow region and matching smoothly with the results in neighboring regions. Airy's classical theory of the rainbow,[5] the best approximate treatment known so far, corresponds to the lowest-order approximation in this expansion. The assumptions upon which Airy's theory is based, are known to have only a very limited range of applicability; the present theory is valid over a considerably extended range.

The glory corresponds to a strong enhancement in near-backward scattering. A more complete description of this effect and of some of the attempts to explain it is given in Sec. 5. The order of magnitude of the intensity predicted by geometrical optics is far too small to account for the effect. It was conjectured by Van de Hulst (Ref. 6; Ref. 7, p. 373) that the glory is due to surface waves of the kind discussed in Sec. 3, that make two shortcuts across the sphere. However, no quantitative treatment of the problem has been given. The modified Watson transformation enables us to treat the neighborhood of the backward direction and to evaluate the residue-series contributions. As is shown in Sec. 5, they are indeed of the right order of magnitude to account for the enhancement in the backward intensity. Physically, this arises from the focusing of the diffracted rays on the axis, which compensates for the exponential damping along the sphere surface. This confirms the basic correctness of Van de Hulst's conjecture. It also provides an impressive example of "Regge-pole dominance" of the scattering amplitude.

However, as is seen in Sec. 5, the residue-series contribution to the third term of the Debye expansion is unable to account for the detailed behavior of the backward-scattered intensity as a function of β. This behavior has recently been studied by Bryant and Cox,[8] by numerical summation of the partial-wave series. They found a very complicated fine structure, showing a quasiperiodic pattern with very prominent and irregular peaks. This behavior must be due to contributions from higher-order terms in the Debye expansion.

The effects produced by higher-order terms are investigated in Sec. 6, which deals almost entirely with the particular cases of forward and backward scattering. The geometrical-optic contribution to all orders is evaluated in these cases and it turns out to be quite small, as expected. The dominant term of the residue-series contribution for an arbitrary order in the Debye expansion is also evaluated. For $N > 1$, the result agrees with that obtained by Chen[9] from the geometrical theory of diffraction, in the case of a circular

[3] C. Chester, B. Friedman, and F. Ursell, Proc. Cambridge Phil. Soc. **53**, 599 (1957).
[4] F. Ursell, Proc. Cambridge Phil. Soc. **61**, 113 (1965).
[5] G. B. Airy, Trans. Cambridge Phil. Soc. **6**, 379 (1938).
[6] H. C. Van de Hulst, J. Opt. Soc. Am. **37**, 16 (1947).
[7] H. C. Van de Hulst, *Light Scattering by Small Particles* (John Wiley & Sons, New York, 1957).
[8] H. C. Bryant and A. J. Cox, J. Opt. Soc. Am. **56**, 1529 (1966).
[9] Y. M. Chen, J. Math. Phys. **5**, 820 (1964).

cylinder. For $N < 1$, it agrees with the physical interpretation given in Paper I, in terms of internal diffraction of surface waves excited by the critically incident rays. As was found in Paper I, the sense of propagation of these surface waves disagrees with the prediction of the geometrical theory of diffraction.

The rate of convergence of the Debye expansion for the residue-series contributions is also discussed in Sec. 6. It is found that they converge much more slowly than "geometrical-optic" contributions. However, for $N < 1$, when all terms have a common shadow boundary, the dominant terms can be summed to all orders, giving rise to a "renormalization" effect of the phase velocities and damping constants of surface waves. For $N > 1$, the summation to all orders is more difficult, due to the different shadow boundaries appearing in all terms. Nevertheless, with certain simplifying assumptions, the summation can still be performed, allowing us to estimate the resultant effect of all surface-wave contributions. It is found that the higher-order contributions account for the quasi-periodic fine structure found by Bryant and Cox, giving rise also to resonance effects. The main features observed in the glory, apart from polarization, are thereby explained.

Furthermore, the same effects are shown to be responsible also for the "ripple" in the total cross section for $N > 1$ (Ref. 7, p. 177). This also agrees with the explanation suggested by Van de Hulst. It is pointed out that the ripple is a very general phenomenon, affecting the intensity in any direction, but with variable amplitude, attaining its maximum at 180°. The corresponding fluctuations in other directions have been observed in numerical calculations by Penndorf.[10]

The conclusions pertaining to both Papers I and II are summed up in Sec. 7, where possible extensions and applications to nuclear physics are also discussed.

The treatment in Papers I and II deals only with a scalar field and, therefore, cannot be directly applied to light scattering. However, the whole treatment can be extended to electromagnetic scattering. The extension will be given in a subsequent paper.[11]

2. THE THIRD TERM OF THE DEBYE EXPANSION

A. Preliminary Considerations

The notation employed is everywhere the same as in Paper I, to which we refer for the definitions of all symbols that appear in the analysis.

[10] R. B. Penndorf, J. Opt. Soc. Am. **52**, 402 (1962).
[11] H. M. Nussenzveig, to be published.

The third term of the Debye expansion is given by [cf. Paper I, (3.23)]

$$f_2(\beta,\theta) = -\frac{i}{\beta}\sum_{m=-\infty}^{\infty}(-1)^m \times\int_0^{\infty}\rho(\lambda,\beta)U(\lambda,\beta)P_{\lambda-\frac{1}{2}}(\cos\theta) \times\exp(2im\pi\lambda)\lambda\,d\lambda, \quad (2.1)$$

where ρ and U are defined in Paper I, Eqs. (3.15) and (3.24), respectively. Changing λ to $-\lambda$ in the sum from $m = -\infty$ to 0, and noting that

$$\rho(-\lambda,\beta) = e^{2i\pi\lambda}\rho(\lambda,\beta), \quad U(-\lambda,\beta) = U(\lambda,\beta), \quad (2.2)$$

we can rewrite (2.1) as

$$f_2(\beta,\theta) = \frac{i}{\beta}\sum_{m=0}^{\infty}(-1)^m\int_{-\infty}^{\infty}\rho(\lambda,\beta)U(\lambda,\beta)P_{\lambda-\frac{1}{2}}(\cos\theta) \times\exp[2i(m+1)\pi\lambda]\lambda\,d\lambda. \quad (2.3)$$

With the help of Paper I, (2.12), this can also be rewritten as

$$f_2(\beta,\theta) = \frac{i}{2\beta}\int_{-\infty+i\epsilon}^{\infty+i\epsilon}\rho U P_{\lambda-\frac{1}{2}}(\cos\theta)e^{i\pi\lambda}\frac{\lambda\,d\lambda}{\cos(\pi\lambda)} = -\frac{i}{2\beta}\int_{-\infty-i\epsilon}^{\infty-i\epsilon}\rho U P_{\lambda-\frac{1}{2}}(\cos\theta)e^{i\pi\lambda}\frac{\lambda\,d\lambda}{\cos(\pi\lambda)}, \quad \epsilon > 0, \quad (2.4)$$

where the path of integration in the first integral has been shifted above the real axis. The last equality follows from the fact that the integrand is odd [cf. (2.2)].

It follows from N, (C3)–(C6), that

$$P_{\lambda-\frac{1}{2}}(\cos\theta) = e^{-i\pi\lambda}[iP_{\lambda-\frac{1}{2}}(-\cos\theta) + 2\cos(\pi\lambda)Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]. \quad (2.5)$$

Substituting this identity in (2.4), we find

$$f_2(\beta,\theta) = f^{+}_{2,0} + f_{2,r} = f^{-}_{2,0} - f_{2,r}, \quad (2.6)$$

where

$$f^{\pm}_{2,0}(\beta,\theta) = \pm\frac{i}{\beta}\int_{-\infty\pm i\epsilon}^{\infty\mp i\epsilon}\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda, \quad (2.7)$$

and

$$f_{2,r}(\beta,\theta) = -\frac{1}{2\beta}\int_{-\infty+i\epsilon}^{\infty+i\epsilon}\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta)\frac{\lambda\,d\lambda}{\cos(\pi\lambda)} = -\frac{1}{2\beta}\int_{-\infty-i\epsilon}^{\infty-i\epsilon}\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta)\frac{\lambda\,d\lambda}{\cos(\pi\lambda)} = \frac{1}{2\beta}\int_{-\infty+i\epsilon}^{\infty+i\epsilon}\rho U e^{2i\pi\lambda}\frac{\lambda\,d\lambda}{\cos(\pi\lambda)}. \quad (2.8)$$

In (2.7), the path of integration was made to cross the positive real axis (which is free of singularities) so that it becomes symmetric about the origin. The equality between the second and third integrals in (2.8) follows from the change of variable $\lambda \to -\lambda$, with the help of (2.2). The equality between the first and third integrals follows from the identity

$$\frac{e^{2i\pi\lambda}}{\cos(\pi\lambda)} = 2e^{i\pi\lambda} - \frac{1}{\cos(\pi\lambda)}, \tag{2.9}$$

where the first term gives no contribution because the corresponding path of integration can be shifted to the real axis and the integrand is odd.

Substituting in (2.7) the identity [N, (C2), (C5)]

$$Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta) = e^{2i\pi\lambda}Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta) - ie^{i\pi\lambda}P_{\lambda-\frac{1}{2}}(-\cos\theta), \tag{2.10}$$

we find once more that the second term leads to an odd integrand, so that

$$f^{\pm}_{2,0}(\beta,\theta) = \pm\frac{i}{\beta}\int_{-\infty\pm i\epsilon}^{\infty\mp i\epsilon}\rho U Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta)e^{2i\pi\lambda}\lambda\, d\lambda. \tag{2.11}$$

Again, splitting up the integral at the origin and making $\lambda \to -\lambda$ in the integral from $-\infty \pm i\epsilon$ to 0, we find, with the help of N, (6.25),

$$f^{\pm}_{2,0}(\beta,\theta) = \mp\frac{i}{\beta}\int_0^{\infty\mp i\epsilon}\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) \times e^{i\pi\lambda}\tan(\pi\lambda)\lambda\, d\lambda. \tag{2.12}$$

On the other hand, expanding the integrand in the last member of (2.8), we find

$$f_{2,r}(\beta,\theta) = \frac{1}{\beta}\sum_{m=0}^{\infty}(-1)^m\int_{-\infty}^{\infty}\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[i(2m+3)\pi\lambda]\lambda\, d\lambda. \tag{2.13}$$

All of the above representations are exact. The choice of an appropriate one among the manifold possibilities is determined by the ranges of values of the refractive index and by the direction under consideration, as will be seen later.

The asymptotic behavior of $e^{i\pi\lambda}\rho U$ as $|\lambda| \to \infty$ follows from Paper I, Figs. 14 and 21. Since it is an even function of λ, it suffices to consider its asymptotic behavior in the upper half-plane, which is shown in Fig. 1. We see that it tends to zero everywhere, except in the shaded regions in the neighborhood of the imaginary axis, where its maximum degree of divergence (neglecting factors such as powers of λ) is given by

$$e^{i\pi\lambda}\rho U = \mathcal{O}(e^{\pi|\lambda|}). \tag{2.14}$$

On the other hand, $e^{2i\pi\lambda}P_{\lambda-\frac{1}{2}}(-\cos\theta)$ behaves like $e^{i\lambda(\pi+\theta)}$ in the upper half-plane, so that we can always close the contour in (2.13) and reduce it to a residue series:

$$f_{2,r}(\beta,\theta) = \tilde{f}_{2,\mathrm{res}}(\beta,\theta) + \tilde{f}'_{2,\mathrm{res}}(\beta,\theta) = \frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residues}\,\{\lambda\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[i(2m+3)\pi\lambda]\}_{\lambda_n,-\lambda_{n'}}, \tag{2.15}$$

where $\tilde{f}_{2,\mathrm{res}}$ corresponds to the sum of the residues at the poles λ_n and $\tilde{f}'_{2,\mathrm{res}}$ to those at the poles $-\lambda'_n$.

However, since [cf. N, (C7)]:

$$e^{-i\pi\lambda}Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta) = \mathcal{O}[e^{-i\lambda(\pi-\theta)}] \quad (|\lambda| \to \infty), \tag{2.16}$$

$$e^{i\pi\lambda}Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta) = \mathcal{O}[e^{i\lambda(\pi-\theta)}] \quad (|\lambda| \to \infty), \tag{2.17}$$

it follows from (2.14) that, for any value of θ, there is always some neighborhood of the imaginary axis where the integrand of (2.7) or (2.11) diverges at infinity [note that (2.16) improves the convergence in the lower half-plane and (2.17) in the upper one]. Thus, *there is no domain of values of θ in which $f^{\pm}_{2,0}$ [and, consequently, $f_2(\beta,\theta)$] can be reduced to a pure residue series.*

This already shows that the structure of the shadow region for the third term of the Debye expansion is quite different from that found for the previous two. We shall see that this is related with the existence of complex saddle points in the present case. Our next task is to study the location of the saddle points for (2.7) and (2.11).

B. Ray Behavior According to Geometrical Optics

In the geometrical-optics approximation, the third term of the Debye expansion is associated with rays transmitted through the sphere after one internal reflection, like the ray 3′ in Paper I, Fig. 5. Three possible types of ray trajectories, leading to three different relations between the scattering angle θ and the angle of incidence θ_1 and angle of refraction θ_2,

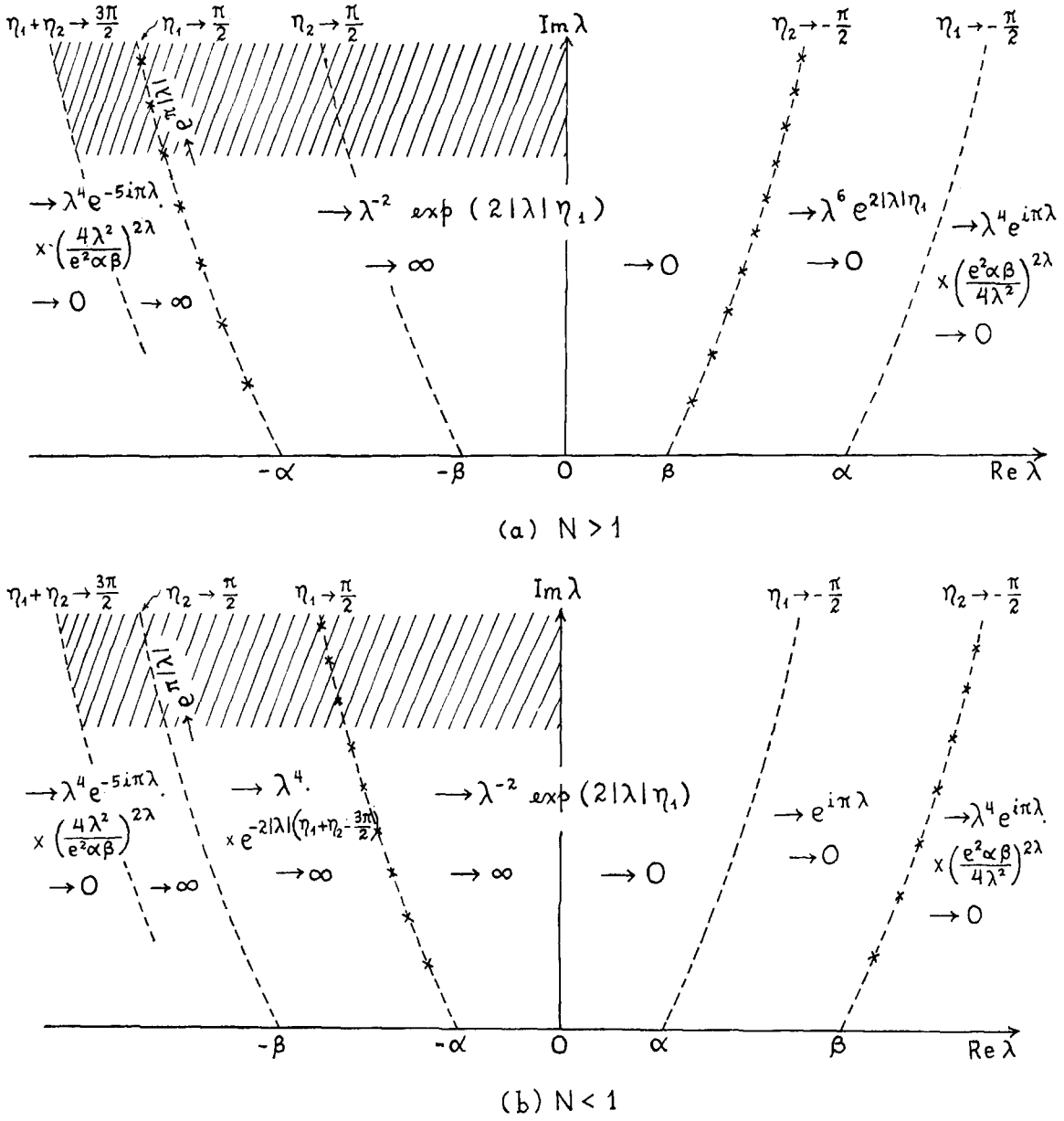


FIG. 1. Asymptotic behavior of $e^{i\pi\lambda}\rho(\lambda,\beta)U(\lambda,\beta)$ as $|\lambda|\to\infty$ in different regions of the λ plane. (a) $N>1$; (b) $N<1$. ×—poles. The function diverges at infinity in the shaded regions and tends to zero elsewhere. The notation is the same as in I, Fig. 14.

are shown in Fig. 2. We have, of course,

$$\sin\theta_1 = N\sin\theta_2,\quad 0\le\frac{\theta_1}{\theta_2}\le\frac{\pi}{2},\quad 0\le\theta\le\pi. \tag{2.18}$$

The three possible relations are

$$\theta = 2(2\theta_2-\theta_1)-\pi, \tag{2.19}$$

$$\theta = \pi-2(2\theta_2-\theta_1), \tag{2.20}$$

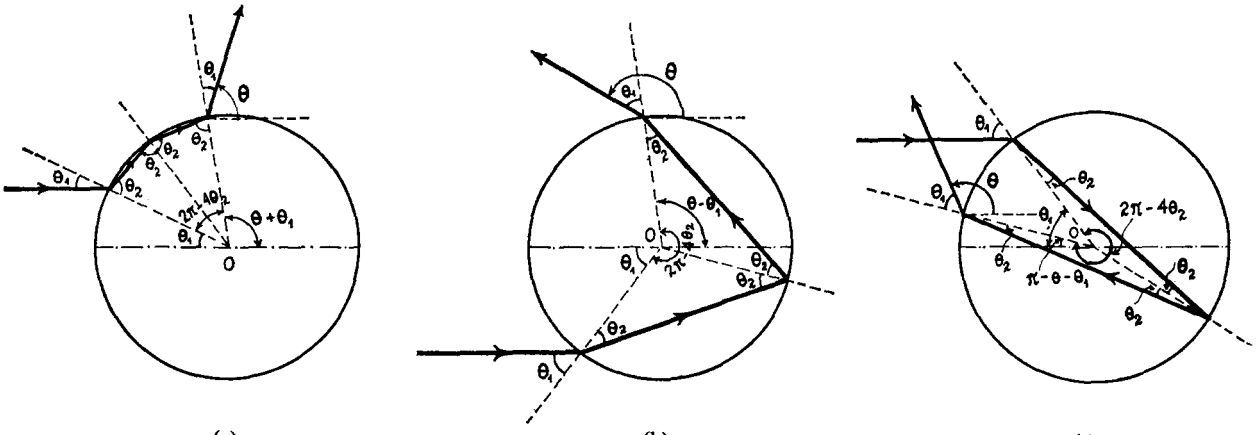
$$\theta = \pi+2(2\theta_2-\theta_1). \tag{2.21}$$

It is readily verified that any possible ray trajectory leads to one of these three relations. Relation (2.19) holds for $2(2\theta_2-\theta_1)>\pi$, i.e., $\theta_1>\theta_{1,c}$, where

$$\sin\theta_{1,c} = \sin\left(2\theta_{2,c}-\frac{\pi}{2}\right) = \frac{N^2}{4}\left[1+\left(1+\frac{8}{N^2}\right)^{\frac{1}{2}}\right], \tag{2.22}$$

which is only possible for $N<1$ [Fig. 2(a)].

If $N<1$ and $\theta_1<\theta_{1,c}$, we have to employ (2.20). This relation also holds for $N>1$, provided that



(a) (b) (c)

FIG. 2. Three possible ray trajectories according to geometrical optics and the corresponding relations among θ, θ_1, and θ_2. All possible trajectories for this class of rays lead to one of these three relations. (a) $N < 1$, $2(2\theta_2 - \theta_1) > \pi$, $\theta = 2(2\theta_2 - \theta_1) - \pi$; (b) $1 < N < 2$, $0 < 2(2\theta_2 - \theta_1) < \pi$, $\theta = \pi - 2(2\theta_2 - \theta_1)$; (c) $N > 2$, $2(2\theta_2 - \theta_1) < 0$, $\theta = \pi + 2(2\theta_2 - \theta_1)$.

$2\theta_2 - \theta_1 > 0$. The angle θ_{1A} such that

$$2\theta_{2A} - \theta_{1A} = 0 \tag{2.23}$$

is characterized by

$$\cos\theta_{1A} = \tfrac{1}{2}(N^2 - 2), \tag{2.24}$$

so that such an angle exists only for

$$\sqrt{2} \leq N \leq 2. \tag{2.25}$$

Thus, if

$$1 < N < \sqrt{2}, \tag{2.26}$$

we have $0 < 2(2\theta_2 - \theta_1) < \pi$, and (2.20) is the only valid relation. On the other hand, if N is in the range (2.25), we must employ (2.20) for $\theta_1 < \theta_{1A}$ and (2.21) for $\theta_1 > \theta_{1A}$. Finally, if $N > 2$, we have $2\theta_2 - \theta_1 < 0$, so that (2.21) is the only valid relation [Fig. 2(c)].

In all cases, $\theta_1 = 0$ yields $\theta = \pi$, corresponding to the central ray that is reflected backwards after transmission. For $N < 1$, the limiting incident ray that is transmitted corresponds to the critical angle,

$$\theta_1 = \theta_i = \sin^{-1} N, \quad \theta_2 = \pi/2 \quad (N < 1), \tag{2.27}$$

and, according to (2.19), the corresponding scattering angle is $\theta = \theta_t$, where

$$\theta_t = \pi - 2\theta_i = 2\cos^{-1} N \quad (N < 1). \tag{2.28}$$

This is the same shadow boundary angle already found in Paper I, Fig. 8(b) and Paper I, Fig. 13(b).

For $N > 1$, the limiting incident ray is

$$\theta_1 = \frac{\pi}{2}, \quad \theta_2 = \theta_i = \sin^{-1}\frac{1}{N} \quad (N > 1). \tag{2.29}$$

In the range (2.26), according to (2.20), the corresponding scattering angle is $\theta = \theta_L$, where

$$\theta_L = 4\left(\frac{\pi}{2} - \theta_i\right) = 2\theta_t = 4\cos^{-1}\frac{1}{N} \quad (1 < N < \sqrt{2}), \tag{2.30}$$

whereas, for $N > \sqrt{2}$, we have to employ (2.21) and we find for the limiting scattering angle

$$\theta_L = 4\theta_i \quad (N > \sqrt{2}). \tag{2.31}$$

Let

$$y = \sin\frac{\theta}{2} = \pm\cos(2\theta_2 - \theta_1), \tag{2.32}$$

where the + sign corresponds to the relations (2.20) and (2.21), and the − sign to (2.19). Taking into account (2.18), we find

$$\frac{dy}{d\theta_1} = \mp\frac{\sin(2\theta_2 - \theta_1)}{N\cos\theta_2}(2\cos\theta_1 - N\cos\theta_2). \tag{2.33}$$

The sign of $dy/d\theta_1$ tells us whether the scattering angle is an increasing or decreasing function of the angle of incidence. The change from − to + sign in (2.33) occurs only for $N < 1$, at $\theta_1 = \theta_{1c}$ [cf. (2.22)], which, by (2.19), corresponds to $\theta = 0$. Otherwise, $dy/d\theta_1$ changes sign only at $\theta_1 = \theta_{1A}$ [cf. (2.23)], which occurs only in the range (2.25) and corresponds to $\theta = \pi$, and for $\theta_1 = \theta_{1R}$, where

$$2\cos\theta_{1R} = N\cos\theta_{2R}, \tag{2.34}$$

which leads to

$$\sin\theta_{1R} = s = \left(\frac{4 - N^2}{3}\right)^{\frac{1}{2}},$$
$$\cos\theta_{1R} = c = \left(\frac{N^2 - 1}{3}\right)^{\frac{1}{2}}. \tag{2.35}$$

This is only possible for $1 < N < 2$. The corresponding scattering angle is $\theta = \theta_R$, where

$$y_R = \sin\frac{\theta_R}{2} = \frac{(8 + N^2)c}{3N^2}, \quad \cos\frac{\theta_R}{2} = \frac{s^3}{N^2}. \tag{2.36}$$

As will be seen later, θ_R is the *rainbow angle*.

According to (2.30) or (2.31), we have

$$y_L = \sin\frac{\theta_L}{2} = \sin(2\theta_l) = \frac{2M}{N^2}, \tag{2.37}$$

where [cf. Paper I, (2.53)]

$$M = (N^2 - 1)^{\frac{1}{2}} \quad (N > 1). \tag{2.38}$$

Thus, in the range (2.26), θ_R is always smaller than the limiting angle θ_L. However, in the range (2.25), we have

$$\theta_R < \theta_L \quad (N < N_0), \quad \theta_R > \theta_L \quad (N > N_0), \tag{2.39}$$

where

$$N_0 = (6\sqrt{3} - 8)^{\frac{1}{2}} \approx 1.547. \tag{2.40}$$

The above discussion enables us to give a complete description of the behavior of θ as a function of θ_1, for all ranges of the refractive index. The results are graphically displayed in Fig. 3.

Let us start from $\theta = \pi$ at $\theta_1 = 0$. Fig. 3(a) shows that for $N < 1$, θ first decreases from π to 0 as θ_1 increases from 0 to θ_{1c} [cf. (2.22)], and then increases again from 0 to θ_t [cf. (2.28)] as θ_1 increases from θ_{1c} to θ_l. Thus the domain $0 \leq \theta \leq \theta_t$ is covered twice: once by rays arising from (2.19) and once more by those from (2.20); there are two rays passing through

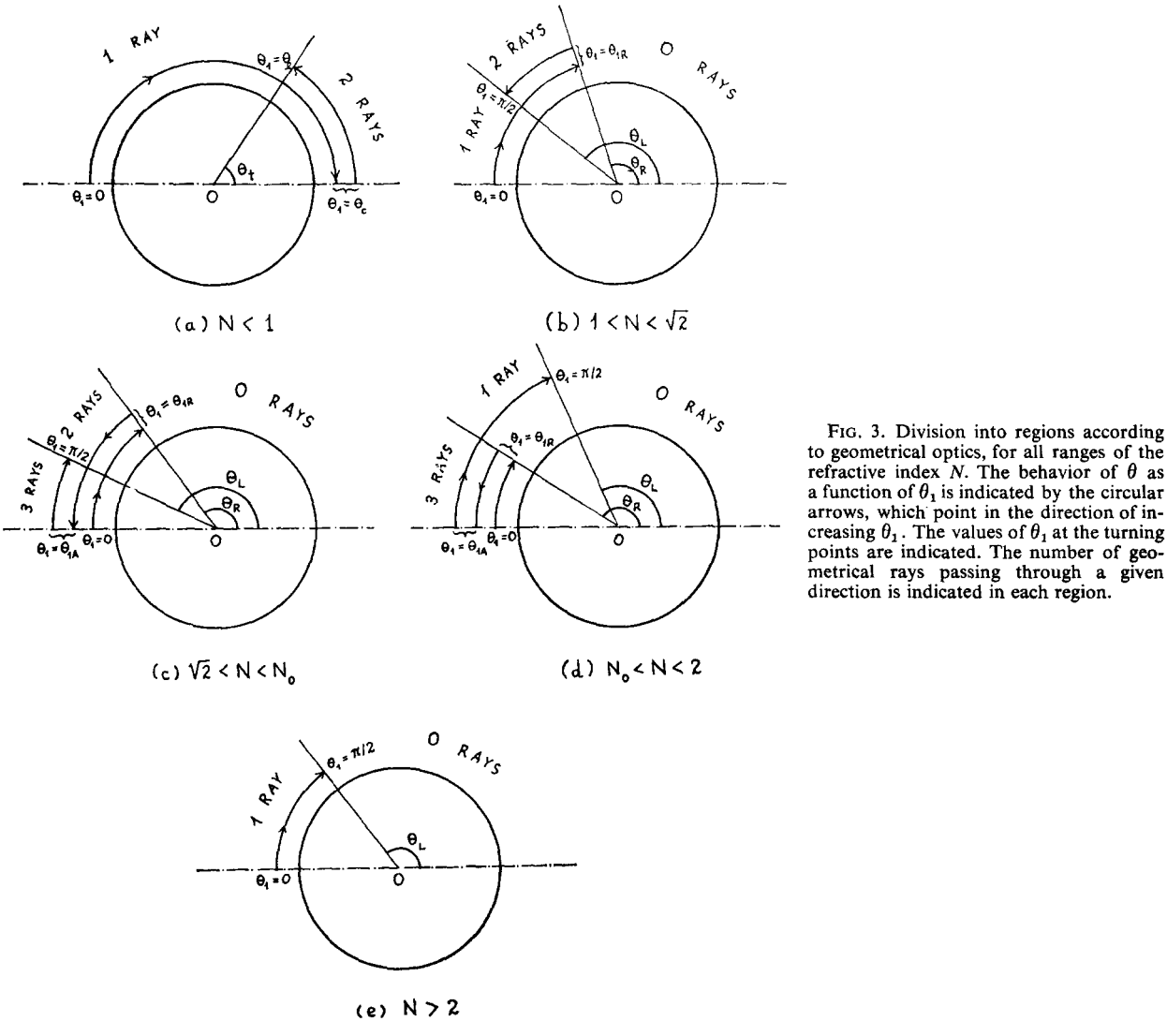


FIG. 3. Division into regions according to geometrical optics, for all ranges of the refractive index N. The behavior of θ as a function of θ_1 is indicated by the circular arrows, which point in the direction of increasing θ_1. The values of θ_1 at the turning points are indicated. The number of geometrical rays passing through a given direction is indicated in each region.

each direction in this region. There is no geometrical shadow (0-ray) region for $N < 1$: there is only a 1-ray/2-ray shadow boundary.

For $1 < N < \sqrt{2}$ [Fig. 3(b)], we have a turning point at $\theta_1 = \theta_{1R}$; the corresponding scattering angle θ_R is the angle of minimum deviation. The rainbow appears around this angle, which is a 2-ray/0-ray shadow boundary. The angle θ_L is a 1-ray/2-ray shadow boundary.

For $\sqrt{2} < N < 2$, there is, in addition to $\theta_1 = \theta_{1R}$, another turning point at $\theta_1 = \theta_{1A}$ [cf. (2.24)], beyond which (2.20) is replaced by (2.21). For $\theta_1 > \theta_{1A}$, θ decreases from π to θ_L [cf. (2.31)], where, by (2.39), $\theta_L > \theta_R$ for $N < N_0$ [Fig. 3(c)] and $\theta_L < \theta_R$ for $N > N_0$ [Fig. 3(d)]. Thus, for $N < N_0$, the rainbow occurs at a 2-ray/0-ray boundary, whereas for $N > N_0$ it occurs at a 3-ray/1-ray boundary, which should make it more difficult to observe. In the whole domain $\sqrt{2} < N < 2$, the neighborhood of the backward direction is covered by three rays.

Finally, for $N > 2$ [Fig. 3(e)], there are no turning points: we find only a 1-ray and a 0-ray region, just as for the previous terms of the Debye expansion.

C. The Saddle Points for $1 < N < \sqrt{2}$

From now on we shall deal mainly with the range $1 < N < \sqrt{2}$, for which the ray directions are determined by (2.20). The appropriate representation for $f^{\pm}_{2,0}(\beta, \theta)$ in this range is given by (2.7). In fact, as will now be seen, the saddle points on the real axis for the integrand of (2.7) are associated with the rays (2.20).

To determine the saddle points, let us consider the behavior of the integrand in the neighborhood of the real axis, between $\lambda = 0$ and $\lambda = \beta$, where the real saddle points must lie. The integrand differs from the corresponding one in Paper I, (5.29) only by a factor $-\rho(\lambda, \beta)$, so that we can employ approximations similar to those leading to Paper I, (5.36). With the change of variables [Paper I, (5.35)],

$$\lambda = \beta \sin w_1 = \alpha \sin w_2, \tag{2.41}$$

we find [cf. Paper I, (3.15)]

$$\begin{aligned}\rho(\lambda, \beta) = i&\left(\frac{\cos w_1 - N \cos w_2}{\cos w_1 + N \cos w_2}\right) \\ &\times \exp\left\{2i\beta\left[N \cos w_2 + \left(w_2 - \frac{\pi}{2}\right) \sin w_2\right]\right\} \\ &\times \left\{1 - \frac{i}{4\alpha \cos w_2}(1 + \tfrac{5}{3}\tan^2 w_2)\right. \\ &\left. - \frac{i \tan^2 w_1}{\alpha \cos w_2} + \mathcal{O}(\beta^{-2})\right\}.\end{aligned} \tag{2.42}$$

Taking into account Paper I, (5.36)–(5.38), this leads to

$$\begin{aligned}&\frac{i}{\beta}\int \rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda \, d\lambda \\ &\quad \approx -2e^{-i\pi/4} N \left(\frac{2\beta}{\pi \sin\theta}\right)^{\frac{1}{2}} \\ &\qquad \times \int C(w_1, \beta, \theta) \exp\left[i\beta\omega(w_1, \theta)\right] dw_1,\end{aligned} \tag{2.43}$$

where

$$\begin{aligned}\omega(w_1, \theta) = 2\Big[&2N \cos w_2 - \cos w_1 \\ &+ \left(2w_2 - w_1 - \frac{\pi - \theta}{2}\right) \sin w_1\Big],\end{aligned} \tag{2.44}$$

$$\begin{aligned}&C(w_1, \beta, \theta) \\ &\quad = (\sin w_1)^{\frac{1}{2}} \cos^2 w_1 \cos w_2 \frac{(\cos w_1 - N \cos w_2)}{(\cos w_1 + N \cos w_2)^3} \\ &\qquad \times \left\{1 + \frac{i}{\beta}\left[\frac{1}{4 \cos w_1}(1 + \tfrac{5}{3}\tan^2 w_1)\right.\right. \\ &\qquad - \frac{1}{2N \cos w_2}(1 + \tfrac{5}{3}\tan^2 w_2) - \frac{2 \tan^2 w_1}{N \cos w_2} \\ &\qquad \left.\left. + \frac{\tan^2 w_2}{\cos w_1} - \frac{\cot\theta}{8 \sin w_1}\right] + \mathcal{O}(\beta^{-2})\right\}.\end{aligned} \tag{2.45}$$

In the derivation of these results, in addition to [N, Eq. (C7)], we have employed the Debye asymptotic expansions [Paper N, (A16)] for $H^{(1,2)}_{\lambda}(\beta)$. The domain of validity of these expansions in the λ plane[12] is represented in Fig. 4 by the oblong-shaped region bounded by the curves in broken line, from which the domain

$$|\lambda| - \beta = \mathcal{O}(\beta^{\frac{1}{3}}) \tag{2.46}$$

also has to be excluded. Thus, we can employ (2.43)–(2.45) to locate not only real, but also complex saddle points (if any) contained within this region.

Taking into account Paper I, Eq. (5.39), we find

$$\partial\omega/\partial w_1 = 2 \cos w_1 [2w_2 - w_1 - \tfrac{1}{2}(\pi - \theta)], \tag{2.47}$$

so that the saddle points are determined by

$$\bar{w}_1 = \theta_1, \quad \bar{w}_2 = \theta_2, \quad \bar{\lambda} = \beta \sin\theta_1 = \alpha \sin\theta_2, \tag{2.48}$$

[12] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, London, 1962), 2nd ed., p. 265.

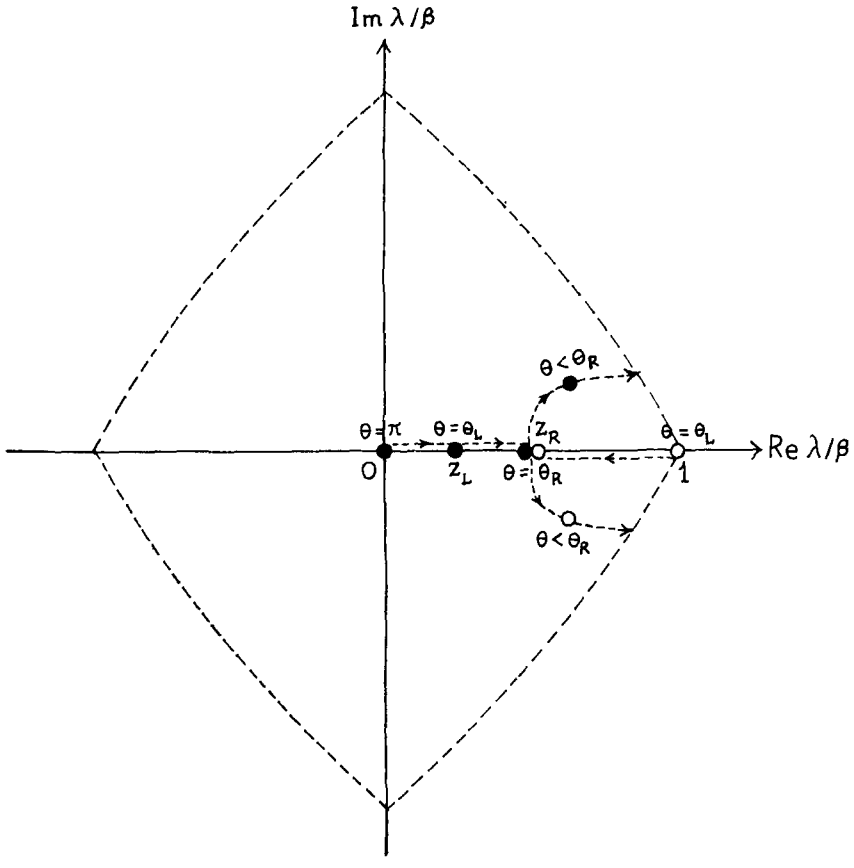


FIG. 4. Saddle-point trajectories in the λ plane as a function of θ for $1 < N < \sqrt{2}$. ●—z''; ○—z', where $z = \bar{\lambda}/\beta$ [cf. (A7)]. The limiting angle θ_L is given by (2.30) and the rainbow angle θ_R by (2.36). The two saddle points coalesce at $\theta = \theta_R$. For $\theta < \theta_R$, they move apart in complex conjugate directions. The oblong-shaped region is the domain of validity of the asymptotic expansions employed in (2.43)–(2.45).

where θ_1 and θ_2 are related to θ by (2.20). This justifies our choice of the representation (2.7). [As is readily seen with the help of [I, Eq. (C7)], had we chosen, instead, the representation (2.11), the resulting saddle points would correspond to (2.21). Thus, this would be the appropriate choice for $N > 2$.]

In order to determine the saddle points, we have to find the real and complex roots of (2.48), (2.20) that lie within the domain under consideration. This is done in Appendix A. The results are graphically displayed in Fig. 4, which shows the trajectories described by the saddle points in the λ plane as θ changes.

For $\theta_L < \theta < \pi$, the 1-ray region in Fig. 3(b), there is only one saddle point, given by $\bar{\lambda}/\beta = \sin\theta_1 = z''$, where z'' is defined in (A7). This saddle point moves from the origin to the point z_L as θ decreases from π to θ_L.

At $\theta = \theta_L$ [cf. (2.30)], another saddle point z' [cf. (A7)] appears at $\bar{\lambda}/\beta = 1$ and, as θ decreases from θ_L to θ_R, the two saddle points move towards each other. [This is not quite correct, since the Debye expansions employed in (2.43)–(2.45) fail in the domain (2.46); we shall see in Sec. 3 how to treat the region $\theta \approx \theta_L$.] Their confluence takes place at the rainbow angle θ_R. Thus, for $\theta_R < \theta < \theta_L$, there are two real saddle points, corresponding to the 2-ray region in Fig. 3(b).

Finally, for $\theta < \theta_R$, the two saddle points become complex. They leave the real axis at right angles and describe complex-conjugate trajectories. This corresponds to the 0-ray region in Fig. 3(b). However, the saddlepoint positions are given by (A7) only as long as they fall within the oblong-shaped domain indicated in Fig. 4. Outside of this domain, i.e., deep within the geometrical shadow region, the results are no longer valid. To evaluate the complex saddle points under these conditions, we would have to substitute (2.43)–(2.45) by the appropriate representation, valid outside of the oblong-shaped region. However, as will be seen in Sec. 3C, the contribution from the complex saddle points no longer dominates the amplitude in the deep shadow region, so that the corresponding results will not be required.

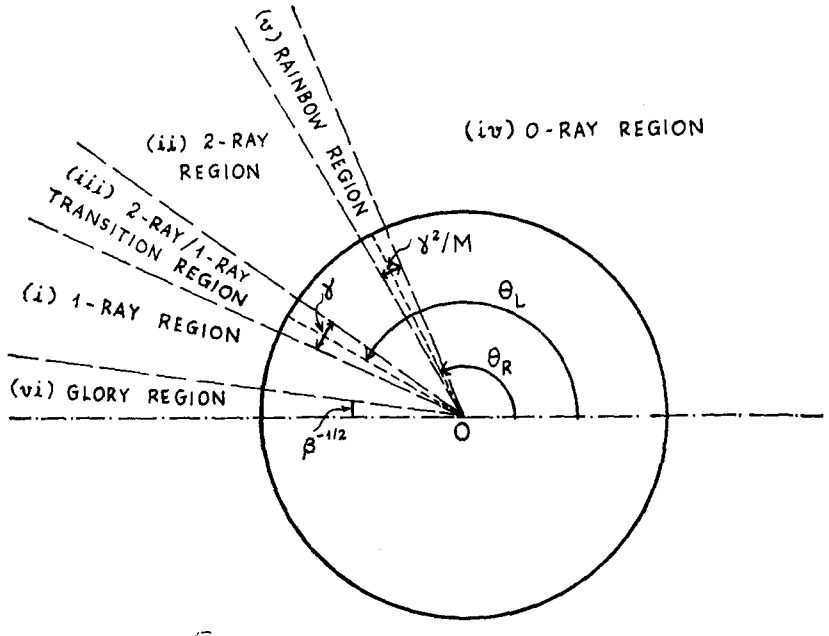


FIG. 5. Division into regions for $1 < N < \sqrt{2}$; θ_R = rainbow angle; θ_L = 2-ray/1-ray boundary angle. The angular width of the transition regions is also indicated.

3. BEHAVIOR IN THE NORMAL REGIONS

According to geometrical optics [cf. Fig. 3(b)], there are three different angular regions for $1 < N < \sqrt{2}$. They are distinguished by the number of geometrical rays passing through a given direction: 0-ray ($0 < \theta < \theta_R$), 2-ray ($\theta_R < \theta < \theta_L$) and 1-ray ($\theta_L < \theta < \pi$).

If we consider also the corresponding transition regions, including a transition region near the backward direction, we find six angular regions requiring separate treatments, as shown in Fig. 5. The width $\Delta\theta$ of each transition region will be derived later on.

Region (v), corresponding to the rainbow, and region (vi), where the glory is found, are treated in Secs. 4 and 5, respectively. The remaining regions, which will be called "normal" regions, are treated in the present Section.

A. The 1-Ray Region

This is the region

$$\theta - \theta_L \gg \gamma, \quad \pi - \theta \gg \beta^{-\frac{1}{2}}, \tag{3.1}$$

where θ_L is defined by (2.30) and $\gamma = (2/\beta)^{\frac{1}{3}}$, as in [I, Eq. (2.49)]. The restriction to $\pi - \theta \gg \beta^{-\frac{1}{2}}$ allows us to employ the asymptotic expansion [N, Eq. (C7)] for $Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)$ in (2.7), thus leading to the representation (2.43)–(2.45).

For $\theta > \theta_L$, we have seen that there is a single saddle point, given by

$$\bar{\lambda}/\beta = \sin\theta_1 = N \sin\theta_2 = z'', \tag{3.2}$$

where z'' is defined by (A7).

It follows from (2.47) that

$$\left(\frac{\partial^2\omega}{\partial w_1^2}\right)_{w_1=\theta_1} = \frac{2\cos\theta_1}{N\cos\theta_2}(2\cos\theta_1 - N\cos\theta_2). \tag{3.3}$$

Let

$$\cos\theta_1/\cos\theta_{1R} = \sqrt{3}\tan\phi \quad (0 < \phi < \pi/2),$$

where $\cos\theta_{1R}$ is given by (2.35). Then, (3.3) becomes

$$(4\cos\theta_1)^{-1}(\partial^2\omega)/(\partial w_1^2)_{w_1=\theta_1} = \sin\phi - \tfrac{1}{2},$$

so that

$$\left(\frac{\partial^2\omega}{\partial w_1^2}\right)_{\theta_1} > 0, \quad \text{for} \quad \theta_1 < \theta_{1R},$$

$$\left(\frac{\partial^2\omega}{\partial w_1^2}\right)_{\theta_1} < 0, \quad \text{for} \quad \theta_1 > \theta_{1R}. \tag{3.4}$$

In the present case (cf. Fig. 4), we have $\theta_1 < \theta_{1R}$, so that the steepest-descent path crosses the real axis at the saddle point at an angle of $\pi/4$. This leads us to choose $f^-_{2,0}$ (rather than $f^+_{2,0}$) in (2.7). The steepest-descent path is schematically represented by the curve in full line in Fig. 6. It must begin and end at

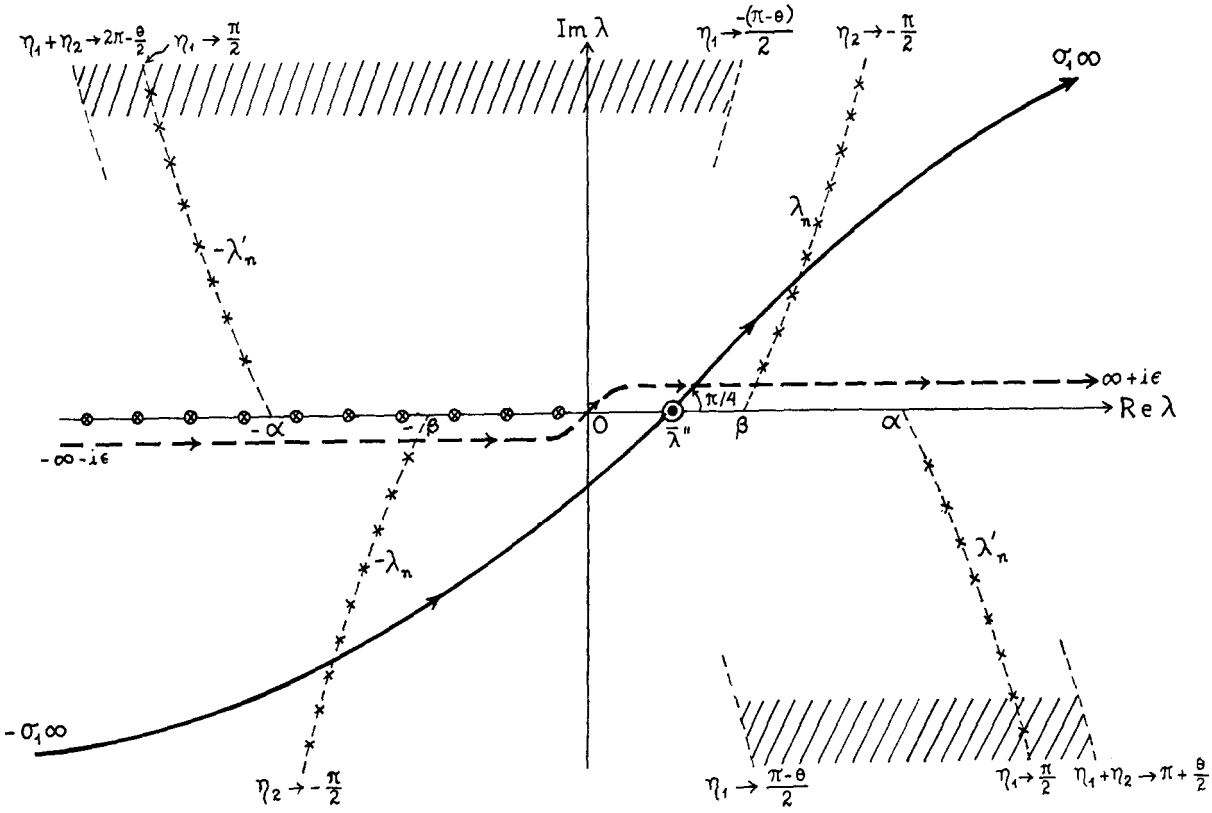


FIG. 6. Behavior of the integrand of (2.7) and the paths of integration in the λ plane ($\theta > \theta_L$). ×—poles of ρU; ⊗—poles of $Q^{(2)}_{\lambda-\frac{1}{2}}$ at the negative half-integers; ⊙—saddle point. The integrand diverges as $|\lambda| \to \infty$ within the shaded regions and tends to zero elsewhere (apart from the poles). The original path of integration, shown in broken line, must be deformed onto the steepest-descent path, shown in solid line; this gives rise to residues at the poles λ_n and $-\lambda_n$.

infinity outside of the shaded regions, where the integrand diverges [cf. Fig. 1 and (2.16)]. In order to deform the path of integration in (2.7) from $(-\infty - i\epsilon,\ \infty + i\epsilon)$ (curve in broken line in Fig. 6) to the steepest-descent path $(-\sigma_1\infty,\ \sigma_1\infty)$, we have to go across the poles λ_n and $-\lambda_n$, so that we find

$$f^{-}_{2,0}(\beta,\theta) = -\frac{i}{\beta}\int_{-\sigma_1\infty}^{\sigma_1\infty}\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda + \frac{2\pi}{\beta}\sum_n \{\text{residue } [\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{\lambda_n} - \text{residue } [\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{-\lambda_n}\}. \quad (3.5)$$

It is irrelevant for our purpose whether the number of poles crossed is finite or infinite. This depends on the shape of the path far away from the saddle point, which will not be investigated here. Actually, only poles close to the real axis give a significant contribution. For simplicity, the residues at all the poles have been included in (3.5) and subsequent relations, but only trivial changes are required if the number is finite.

Since $\lambda = -\lambda_n$ is a triple pole (cf. I, Sec. 3B), we have

$$\text{residue } [\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{-\lambda_n} = \frac{1}{2!}\frac{d^2}{d\lambda^2}[(\lambda+\lambda_n)^3\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{-\lambda_n}.$$

Changing $\lambda \to -\lambda$ on the right-hand side, and taking into account (2.2), we find

$$\text{residue } [\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{-\lambda_n} = \text{residue } [\lambda e^{2i\pi\lambda}\rho U Q^{(2)}_{-\lambda-\frac{1}{2}}(\cos\theta)]_{\lambda_n}. \quad (3.6)$$

It follows from N, Eq. (C5) and (C6), that

$$Q^{(2)}_{-\lambda-\frac{1}{2}}(\cos\theta) = Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta) - \frac{i}{\cos(\pi\lambda)}P_{\lambda-\frac{1}{2}}(-\cos\theta). \quad (3.7)$$

Substituting (3.6) and (3.7) in (3.5), and taking into account I, (2.12), we get

$$f_{2,0}^{-}(\beta,\theta) = -\frac{i}{\beta}\int_{-\sigma_1\infty}^{\sigma_1\infty}\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda + 2\bar{f}_{2,\mathrm{res}}(\beta,\theta) + \frac{2\pi}{\beta}\sum_n \text{residue}\,\{\lambda\rho U[Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta) - e^{2i\pi\lambda}Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta)]\}_{\lambda_n}, \tag{3.8}$$

where $\bar{f}_{2,\mathrm{res}}$ is the residue series at the poles λ_n defined in (2.15).

It follows from N, Eq. (C3)–(C4), that

$$Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta) - e^{2i\pi\lambda}Q^{(1)}_{\lambda-\frac{1}{2}}(\cos\theta) = -ie^{i\pi\lambda}P_{\lambda-\frac{1}{2}}(-\cos\theta). \tag{3.9}$$

Substituting the result in (3.8) and taking into account (2.15), we find that (2.6) finally becomes

$$f_2(\beta,\theta) = f_{2,g}(\beta,\theta) + f_{2,\mathrm{res}}(\beta,\theta) + f'_{2,\mathrm{res}}(\beta,\theta) \qquad (\theta_L < \theta < \pi), \tag{3.10}$$

where

$$f_{2,g}(\beta,\theta) = -\frac{i}{\beta}\int_{-\sigma_1\infty}^{\sigma_1\infty}\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda, \tag{3.11}$$

$$f_{2,\mathrm{res}}(\beta,\theta) = -\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m \times \sum_n \text{residue}\,\{\lambda\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[i(2m+1)\pi\lambda]\}_{\lambda_n}, \tag{3.12}$$

and

$$f'_{2,\mathrm{res}}(\beta,\theta) = \frac{2\pi i}{\beta}\sum_{m=1}^{\infty}(-1)^m \times \sum_n \text{residue}\,\{\lambda\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[i(2m+1)\pi\lambda]\}_{-\lambda_n}. \tag{3.13}$$

Let us consider first the "geometrical-optic" term $f_{2,g}(\beta,\theta)$. The expansion for the integrand in the vicinity of the saddle point follows from (2.43)–(2.45), and the saddle point is determined by (2.48) and (2.20). The path of integration is the image of that shown in Fig. 6 in the w_1-plane.

The saddlepoint evaluation of (3.11) now proceeds by applying the analog of N, Eq. (6.12), which differs from I, Eq. (4.34) only by the substitutions:

$$B \to C, \quad \delta \to \omega, \quad |\delta''| \to -\omega'', \quad |\delta''|^{\frac{1}{2}} \to -i(\omega'')^{\frac{1}{2}}. \tag{3.14}$$

A rather tedious calculation finally leads to the result

$$f_{2,g}(\beta,\theta) = -\left(\frac{\sin\theta_1}{\sin\theta}\right)^{\frac{1}{2}}\frac{(2N\cos\theta_1\cos\theta_2)^{\frac{3}{2}}}{(2\cos\theta_1 - N\cos\theta_2)^{\frac{1}{2}}} \times \frac{(N\cos\theta_2 - \cos\theta_1)}{(N\cos\theta_2 + \cos\theta_1)^3} \times \exp[2i\beta(2N\cos\theta_2 - \cos\theta_1)] \times \left\{1 - \frac{i\mathfrak{S}(\theta_1,\theta)}{64\beta\cos\theta_1} + \mathcal{O}(\beta^{-2})\right\}, \tag{3.15}$$

where

$$\mathfrak{S}(\theta_1,\theta) = 8\cot\theta_1\left[\cot\theta + \frac{\cot\theta_1}{2(2\chi-1)}\right] + 6(9\chi - 11) - \frac{15}{2\chi-1} - \frac{9}{(2\chi-1)^2} + \tan^2\theta_1\left[56\chi^3 - 3\chi^2 + \tfrac{39}{2}\chi - \frac{79}{2} - \frac{33}{2(2\chi-1)} - \frac{51}{4(2\chi-1)^2} - \frac{15}{4(2\chi-1)^3}\right], \tag{3.16}$$

and, as in I, (5.47),

$$\chi = \left(\frac{dw_2}{dw_1}\right)_{\bar{w}_1} = \frac{\cos\theta_1}{N\cos\theta_2}. \tag{3.17}$$

The relation between θ_1 and θ follows from (3.2) and Appendix A, so that, in principle, everything can be explicitly written as a function of θ, but the resulting expressions would be enormously complicated.

The result (3.15) should be compared with I, Eq. (5.45). It contains an additional factor corresponding to the internal Fresnel reflection coefficient, as well as the phase factor appropriate to the ray path shown in Fig. 2(b). The denominator $(2\cos\theta_1 - N\cos\theta_2)^{\frac{1}{2}}$ would vanish only at the rainbow angle (2.34), but this falls outside of the region (3.1).

Let us consider next the residue series at the poles λ_n, given by (3.12). Substituting ρ and U by their definitions I, Eq. (3.15) and I, Eq. (3.24), and taking

into account I, Eqs. (3.4)–(3.8), we find [cf. I, Eq. (5.17)]:

$$f_{2,\mathrm{res}}(\beta,\theta) = -\frac{32i}{\pi\beta^3}\sum_{m=0}^{\infty}(-1)^m \times \sum_n \text{residue}\left\{\frac{c_m(\lambda,\beta,\theta)}{[d(\lambda,\beta)]^3}\right\}_{\lambda_n}, \quad (3.18)$$

where, as in I, Eq. (4.38),

$$d(\lambda,\beta) = [1\ \beta] - N[2\ \alpha] \quad (3.19)$$

and

$$c_m(\lambda,\beta,\theta) = \lambda \exp[i(2m+1)\pi\lambda]\frac{H_\lambda^{(1)}(\alpha)}{[H_\lambda^{(1)}(\beta)]^2[H_\lambda^{(2)}(\alpha)]^3} \times ([1\ \beta] - N[1\ \alpha])P_{\lambda-\frac{1}{2}}(-\cos\theta). \quad (3.20)$$

The residue of the expression within curly brackets in (3.18) at a triple pole is given by (cf. Ref. 9, Appendix II):

$$\text{residue}\left\{\frac{c_m(\lambda,\beta,\theta)}{[d(\lambda,\beta)]^3}\right\}_{\lambda_n} = \frac{c_m}{2\dot{d}^3}\left[\frac{\ddot{c}_m}{c_m} - 3\frac{\dot{c}_m}{c_m}\frac{\ddot{d}}{\dot{d}} + 3\left(\frac{\ddot{d}}{\dot{d}}\right)^2 - \frac{\dddot{d}}{\dot{d}}\right]_{\lambda_n}, \quad (3.21)$$

where the dots denote partial derivatives with respect to λ and all quantities in the second member are to be evaluated at the pole λ_n.

Let us evaluate (3.21) to lowest order, just as we did for I, (5.22) [in Sec. 5C, we shall have to reevaluate (3.21) with much greater accuracy]. For this purpose, we employ the asymptotic expansions N, (A16) for $H_\lambda^{(1,2)}(\alpha)$ and N, (C11) for $P_{\lambda-\frac{1}{2}}(-\cos\theta)$ (this is allowed since $\pi - \theta \gg \beta^{-1}$), and the expansions given in I, Appendix A, for $H_\lambda^{(1)}(\beta)$ and its derivatives with respect to λ and β. Keeping only the dominant term in each expansion and neglecting corrections of order γ^2, we find the following final result:

$$\begin{aligned} f_{2,\mathrm{res}}(\beta,\theta) &\approx \frac{e^{i\pi/12}}{M^2}\left(\frac{\gamma}{\pi\sin\theta}\right)^{\frac{1}{2}}\exp(4iM\beta) \\ &\times \Big\{ i\sum_n (a_n')^{-2}[(\zeta_{2,0}^+)^2 + M\zeta_{2,0}^+]\exp(i\lambda_n\zeta_{2,0}^+) \\ &+ \sum_{m=1}^{\infty}(-1)^m\sum_n (a_n')^{-2}\{i[(\zeta_{2,m}^+)^2 + M\zeta_{2,m}^+] \\ &\times \exp(i\lambda_n\zeta_{2,m}^+) - [(\zeta_{2,m}^-)^2 + M\zeta_{2,m}^-] \\ &\times \exp(i\lambda_n\zeta_{2,m}^-)\}\Big\}, \end{aligned} \quad (3.22)$$

where [cf. (2.30)]

$$\zeta_{2,m}^{\pm} = 2m\pi - 2\theta_t \pm \theta = 2m\pi - \theta_L \pm \theta \quad (m = 0, 1, 2, \cdots). \quad (3.23)$$

For the general evaluation of the dominant term in the residue-series contribution at the poles λ_n, of which (3.22) is a particular case, see Appendix C.

Just as in Paper I [Eq. (5.24)], we can rewrite this result as follows:

$$\begin{aligned} f_{2,\mathrm{res}}(\beta,\theta) &\approx i(\sin\theta)^{-\frac{1}{2}}\exp(4iM\beta) \\ &\times \Big\{\sum_n D_n^2 D_{21}D_{12}[\tilde{R}_{11}\zeta_{2,0}^+ + \tfrac{1}{2}D_{21}D_{12}(\zeta_{2,0}^+)^2] \\ &\times \exp(i\lambda_n\zeta_{2,0}^+) + \sum_{m=1}^{\infty}(-1)^m\sum_n D_n^2 D_{21}D_{12} \\ &\times [(\tilde{R}_{11}\zeta_{2,m}^+ + \tfrac{1}{2}D_{21}D_{12}(\zeta_{2,m}^+)^2)\exp(i\lambda_n\zeta_{2,m}^+) \\ &+ i(\tilde{R}_{11}\zeta_{2,m}^- + \tfrac{1}{2}D_{21}D_{12}(\zeta_{2,m}^-)^2)\exp(i\lambda_n\zeta_{2,m}^-)]\Big\}, \end{aligned} \quad (3.24)$$

where, as in I, (4.45) and I,(5.25),

$$D_n^2 = \tfrac{1}{2}e^{i\pi/12}(\gamma/\pi)^{\frac{1}{2}}(a_n')^{-2}, \quad (3.25)$$

$$D_{21}D_{12} = 2/M, \quad (3.26)$$

with M given by (2.38) and

$$\tilde{R}_{11} = 1. \quad (3.27)$$

The physical interpretation of this result in terms of diffracted rays is similar to that of I, (5.24) (cf. also I, Fig. 15). As shown in Figs. 7(a) and 7(b), the tangentially incident rays at T_1 and T_2, after undergoing two critical refractions and one total internal reflection, reemerge tangentially to define the 2-ray/1-ray shadow boundary at the points T_1''' and T_2''', respectively. At these points, they excite surface waves propagating from the shadow boundary into the shadow (i.e., into the 1-ray region). This gives rise to the diffracted rays $T_2T_2'T_2''T_2'''B$ [Fig. 7(a)] and $T_1T_1'T_1''T_1'''A$ [Fig. 7(b)]. The corresponding angles described along the surface are $\zeta_{2,0}^+$ and $\zeta_{2,1}^-$, respectively, and after additional turns around the sphere, the angles are given by (3.23).

As in I, Sec. 5B, there are again infinitely many paths leading to the same direction of emergence for this class of diffracted rays. Their common feature is

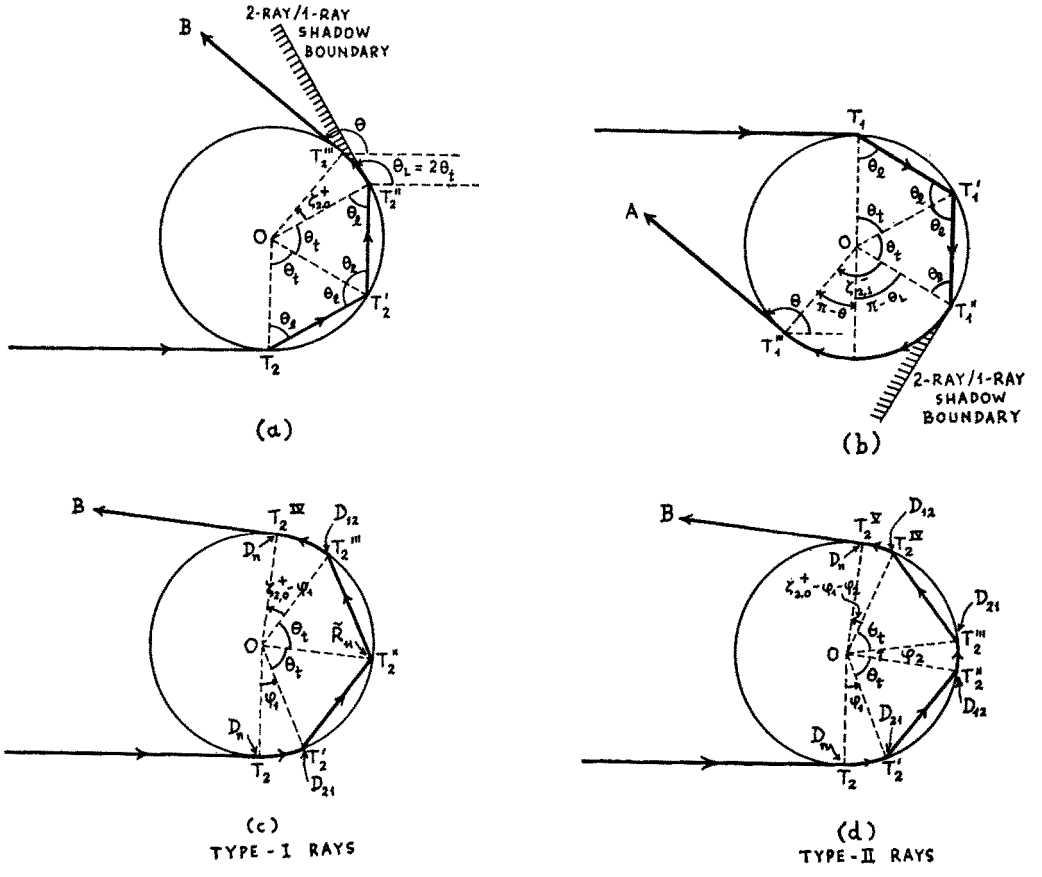


FIG. 7. Physical interpretation of (3.24). The limiting rays (a) $T_2T_2'T_2''$ and (b) $T_1T_1'T_1''$ which define the 2-ray/1-ray shadow boundary excite surface waves propagating into the shadow, generating the diffracted rays (a) $T_2T_2'T_2''T_2'''B$ and (b) $T_1T_1'T_1''T_1'''A$, in the direction θ. The corresponding angles described along the surface are $\zeta_{2,0}^+$ and $\zeta_{2,1}^-$, respectively. There are infinitely many possible paths for this class of diffracted rays: (c) type-I rays describe an angle ϕ_1 as surface waves before penetrating again into the sphere; (d) type-II rays describe two angles, ϕ_1 and ϕ_2, before emerging to describe the final angle $\zeta_{2,0}^+ - \phi_1 - \phi_2$.

that, for all of them, the diffracted rays take two "shortcuts" across the sphere. They can be subdivided into two types (cf. Ref. 9), as illustrated in Figs. 7(c) and 7(d) for $\zeta_{2,0}^+$.

Type-I rays [Fig. 7(c)] are those which, after excitation at T_2 (with diffraction coefficient D_n), describe an angle ϕ_1 ($0 \leq \phi_1 \leq \zeta_{2,0}^+$) as surface waves, are critically refracted into the sphere at T_2' (coefficient D_{21}), undergo total internal reflection at T_2'' (coefficient $\tilde{R}_{11}$), reemerge at T_2''' (coefficient D_{12}) to describe the final angle $\zeta_{2,0}^+ - \phi_1$, and finally leave the surface tangentially at T_2^{IV} (coefficient D_n). As in I, Sec. 5B, the contribution from those paths such that an angle between ϕ_1 and $\phi_1 + d\phi_1$ is described is proportional to $d\phi_1$, so that the total contribution from type-I rays is proportional to

$$D_n^2 D_{21} D_{12} \tilde{R}_{11} \int_0^{\zeta_{2,0}^+} d\phi_1 = D_n^2 D_{21} D_{12} \tilde{R}_{11} \zeta_{2,0}^+. \quad (3.28)$$

Type-II rays [Fig. 7(d)] differ from type-I only by the fact that, instead of undergoing total internal reflection at T_2'', they are critically refracted to the outside (coefficient D_{12}), deseribe another angle ϕ_2 ($0 \leq \phi_1 + \phi_2 \leq \zeta_{2,0}^+$) as surface waves, and are critically refracted to the inside at T_2'''; thereafter, they behave as type-I rays. The total contribution from type-II rays is therefore proportional to

$$D_n^2 (D_{21} D_{12})^2 \iint_{0 \leq \phi_1 + \phi_2 \leq \zeta_{2,0}^+} d\phi_1 \, d\phi_2$$

$$= D_n^2 (D_{21} D_{12})^2 \int_0^{\zeta_{2,0}^+} d\phi_1 \int_0^{\zeta_{2,0}^+ - \phi_1} d\phi_2$$

$$= \tfrac{1}{2} D_n^2 (D_{21} D_{12})^2 (\zeta_{2,0}^+)^2. \quad (3.29)$$

The phase factor $\exp(4iM\beta)$ in (3.24) accounts for the optical path difference associated with the two shortcuts. A similar discussion for a cylinder has been given by Chen.[9]

Finally, let us consider the residue series at the poles $-\lambda'_n$, given by (3.13). With the help of (3.6), we can rewrite (3.13) as

$$f'_{2,\mathrm{res}}(\beta,\theta) = \frac{2\pi i}{\beta}\sum_{m=1}^{\infty}(-1)^m \sum_n \text{residue} \times \{\lambda\rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) \times \exp[-i(2m-1)\pi\lambda]\}_{\lambda_{n'}}. \quad (3.30)$$

Except for the change in sign and the exclusion of $m = 0$, we can still apply (3.18)–(3.21), the main difference being that the residues are now to be evaluated at λ'_n, rather than λ_n.

The approximations employed for the evaluation of (3.30) are the same as for I, (5.27), except that (3.20) contains also $H_\lambda^{(1)}(\alpha)$. According to I, (3.35) and I, (A1), we have

$$H^{(1)}_{\lambda'_n}(\alpha) \approx 2\frac{e^{-i\pi/3}}{\gamma'}\,\mathrm{Ai}\,(e^{i\pi/3}x_n), \quad (3.31)$$

where $\gamma' = (2/\alpha)^{\frac{1}{3}}$, as in I, (5.62). It follows from the Wronskian relation N, (D3), that

$$\mathrm{Ai}\,(e^{i\pi/3}x_n) = -\frac{e^{i\pi/6}}{2\pi a'_n}. \quad (3.32)$$

Taking into account these results, we finally obtain

$$f'_{2,\mathrm{res}}(\beta,\theta) \approx \frac{e^{i\pi/12}N^2}{4\pi M}\frac{\exp(2M\beta)}{(\pi\gamma'\sin\theta)^{\frac{1}{2}}} \times \Big\{\sum_n (a'_n)^{-4}(\tilde\zeta^+_{2,0})^2\exp(-i\lambda'_n\tilde\zeta^+_{2,0}) + \sum_{m=1}^{\infty}(-1)^m\sum_n (a'_n)^{-4}[(\tilde\zeta^+_{2,m})^2 \times \exp(-i\lambda'_n\tilde\zeta^+_{2,m}) - i(\tilde\zeta^-_{2,m})^2 \times \exp(-i\lambda'_n\tilde\zeta^-_{2,m})]\Big\}, \quad (3.33)$$

where

$$\tilde\zeta^{\pm}_{2,m} = 2m\pi - 2i\cosh^{-1}N \pm \theta. \quad (3.34)$$

For $N < 1$, the general evaluation of the dominant term in the residue-series contribution at the poles λ'_n is given in Appendix D.

This result should be compared with I, (5.27). As in that case, $f'_{2,\mathrm{res}}$ is exponentially small as compared with $f_{2,\mathrm{res}}$, and can therefore be neglected. As will be seen in Sec. 7F the reverse is true for $N < 1$, and the analytic continuation of (3.33) to that case has a physical interpretation similar to that of I, (5.65).

The limitation to $\theta - \theta_L \gg \gamma$ in the domain of validity of the above results [cf. (3.1)] arises from (3.22): This is the domain where the least strongly damped series, involving $\exp(i\lambda_n\zeta^+_{2,0})$, is rapidly convergent.

B. The 2-Ray Region

This is the region

$$\theta_L - \theta \gg \gamma, \quad \theta - \theta_R \gg \gamma^2/M. \quad (3.35)$$

In this region, in addition to the real saddle point z'', with $\theta_1 < \theta_{1R}$, there is another real saddle point z', with $\theta_1 > \theta_{1R}$ (cf. Fig. 4 and Appendix A).

According to (3.4), the steepest-descent path at the new saddle point z' crosses the real axis at an angle of $-\pi/4$, so that the path of integration shown in Fig. 6 must be replaced by the new path shown in solid line in Fig. 8.

In order to deform the path of integration in (2.7) from $(-\infty - i\epsilon,\ \infty + i\epsilon)$ (curve in broken line in Fig. 8) to the new path $(-\sigma_1\infty,\ \sigma_2\infty)$, we have to go across the poles $-\lambda_n$ and λ'_n so that, instead of (3.10), we find

$$f_2(\beta,\theta) = \tilde f_{2,g}(\beta,\theta) + \tilde f_{2,\mathrm{res}}(\beta,\theta) + \tilde f'_{2,\mathrm{res}}(\beta,\theta), \quad (3.36)$$

where

$$\tilde f_{2,g}(\beta,\theta) = -\frac{i}{\beta}\int_{-\sigma_1\infty}^{\sigma_2\infty}\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,d\lambda, \quad (3.37)$$

$$\tilde f_{2,\mathrm{res}}(\beta,\theta) = f_{2,\mathrm{res}}(\beta,\theta) - \frac{2\pi}{\beta} \times \sum_n \text{residue}\,[\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{\lambda_n} \quad (3.38)$$

$$\tilde f'_{2,\mathrm{res}}(\beta,\theta) = f'_{2,\mathrm{res}}(\beta,\theta) - \frac{2\pi}{\beta} \times \sum_{n=1}^{n_0}\text{residue}\,[\lambda\rho U Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)]_{\lambda_{n'}}, \quad (3.39)$$

where $f_{2,\mathrm{res}}$ and $f'_{2,\mathrm{res}}$ are given by (3.12) and (3.13), respectively, and n_0 is the total number of poles λ'_n crossed by the contour. In order to determine the total number n_0 of poles λ'_n crossed, a detailed investigation of the shape of the steepest-descent path far away from the saddle points would be required. For our purposes, it is sufficient to know that the contribution from the poles λ'_n can be neglected.

The "geometrical-optic" term (3.37) now contains two contributions, one from each saddle point. The contribution from the left saddle point z'' is still given by (3.15)–(3.17); that from the right saddle point z' is similar, except that we must now employ I,

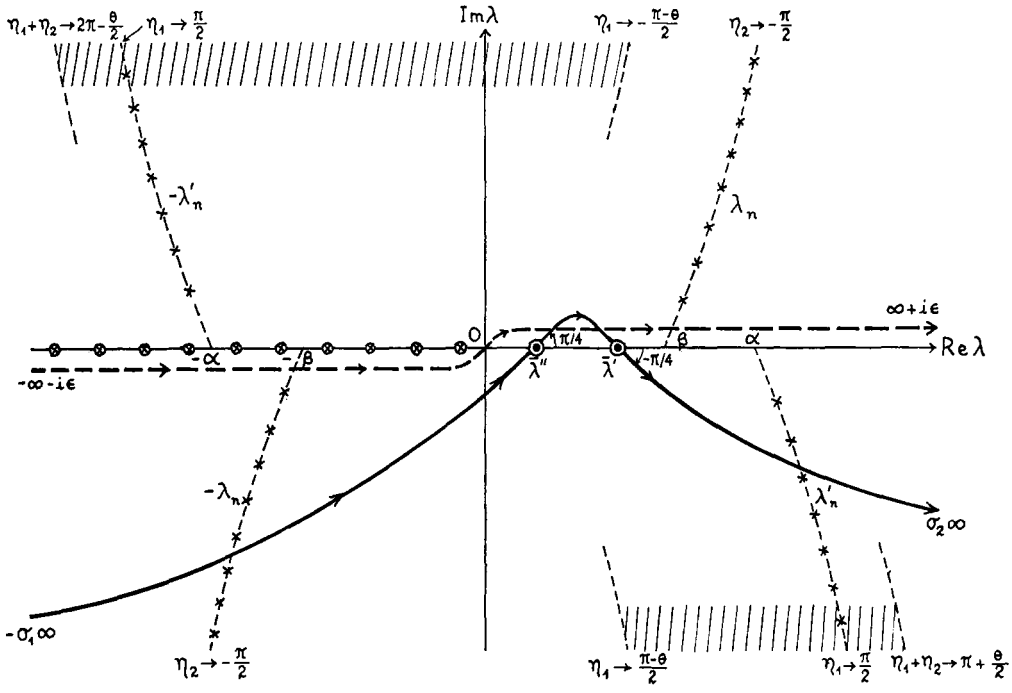


FIG. 8. Path of integration in (2.7) for $\theta_R < \theta < \theta_L$. ×—poles of ρU; ⊗—poles of $Q^{(2)}_{\lambda-\frac{1}{2}}$; ⊙—saddle points. The original path of integration, shown in broken line, must be deformed onto the path shown in solid line; this gives rise to residues at the poles $-\lambda_n$ and λ_n' (cf. Fig. 6).

(4.34), so that we find

$$\tilde{f}_{2,g}(\beta,\theta) = \tilde{f}'_{2,g}(\beta,\theta) + \tilde{f}''_{2,g}(\beta,\theta), \qquad (3.40)$$

where

$$\tilde{f}'_{2,g}(\beta,\theta) = i\left\{\left(\frac{\sin\theta_1}{\sin\theta}\right)^{\frac{1}{2}} \frac{(2N\cos\theta_1\cos\theta_2)^{\frac{3}{2}}}{(N\cos\theta_2 - 2\cos\theta_1)^{\frac{1}{2}}} \times \frac{(N\cos\theta_2 - \cos\theta_1)}{(N\cos\theta_2 + \cos\theta_1)^3} \times \exp\left[2i\beta(2N\cos\theta_2 - \cos\theta_1)\right] \times \left[1 - \frac{i\mathfrak{S}(\theta,\theta_1)}{64\beta\cos\theta_1}\right]\right\}_{\sin\theta_1 = z'}, \qquad (3.41)$$

$$\tilde{f}''_{2,g}(\beta,\theta) = -\left\{\left(\frac{\sin\theta_1}{\sin\theta}\right)^{\frac{1}{2}} \frac{(2N\cos\theta_1\cos\theta_2)^{\frac{3}{2}}}{(2\cos\theta_1 - N\cos\theta_2)^{\frac{1}{2}}} \times \frac{(N\cos\theta_2 - \cos\theta_1)}{(N\cos\theta_2 + \cos\theta_1)^3} \times \exp\left[2i\beta(2N\cos\theta_2 - \cos\theta_1)\right] \times \left[1 - \frac{i\mathfrak{S}(\theta,\theta_1)}{64\beta\cos\theta_1}\right]\right\}_{\sin\theta_1 = z''}, \qquad (3.42)$$

where $\mathfrak{S}(\theta,\theta_1)$ is still given by (3.16), and z', z'' are given by (A7).

In particular, near the rainbow angle, with

$$\theta = \theta_R + \epsilon, \qquad (3.43)$$

$$\gamma^2/M \ll \epsilon \ll \beta^{-\frac{1}{2}}, \qquad (3.44)$$

the saddle points are given by (A23), and we can also employ (A25)–(A26). Taking the slowly-varying factors outside the exponentials in (3.41)–(3.42) at the rainbow angle $\theta = \theta_R$, $\theta_1 = \theta_{1R}$, we then find

$$\tilde{f}_{2,g}(\beta,\theta_R+\epsilon) = -\frac{16}{27} e^{-i\pi/4} \frac{N^2}{(8+N^2)^{\frac{1}{2}}} \frac{c^{\frac{1}{2}}}{s^{\frac{3}{2}}} \times \exp\left[6ic\beta + is\beta\epsilon + \mathcal{O}(\beta\epsilon^2)\right] \times \sin\left[\frac{s\beta}{2}\left(\frac{4c}{3s}\epsilon\right)^{\frac{3}{2}} + \frac{\pi}{4}\right]\left(\frac{4c}{3s}\epsilon\right)^{-\frac{1}{4}} \times \left[1 + \mathcal{O}\left(\frac{1}{\beta\epsilon^{\frac{3}{2}}}\right)\right] \qquad (\gamma^2/M \ll \epsilon \ll \beta^{-\frac{1}{2}}), \qquad (3.45)$$

where c and s are defined by (2.35). This oscillatory behavior of the amplitude arises from interference between the two geometrical contributions (3.41) and (3.42), which have nearly equal amplitudes close to the rainbow angle.

To the same order of approximation employed in the derivation of (3.22), the residue series (3.38) differs from that result only by the omission of the terms in $\zeta^{+}_{2,0}$:

$$\tilde{f}_{2,\mathrm{res}}(\beta,\theta) \approx \frac{e^{i\pi/12}}{M^2}\left(\frac{\gamma}{\pi \sin\theta}\right)^{\frac{1}{2}} \times \exp(4iM\beta) \sum_{m=1}^{\infty}(-1)^m \sum_n (a'_n)^{-2} \times \{i[(\zeta^{+}_{2,m})^2 + M\zeta^{+}_{2,m}] \exp(i\lambda_n \zeta^{+}_{2,m}) - [(\zeta^{-}_{2,m})^2 + M\zeta^{-}_{2,m}] \exp(i\lambda_n \zeta^{-}_{2,m})\}. \tag{3.46}$$

This is just what we should get, since the surface wave excited at T''_2 [Fig. 7(a)] now has to describe an angle $2\pi - (\theta_L - \theta) = \zeta^{+}_{2,1} < 2\pi$ before emerging in the direction θ.

Similarly, the last term in (3.39) is equivalent to an additional contribution in $\tilde{\zeta}^{-}_{2,0}$ to (3.33), so that we get

$$\tilde{f}'_{2,\mathrm{res}}(\beta,\theta) \approx f'_{2,\mathrm{res}}(\beta,\theta) - i\frac{e^{i\pi/12}N^2}{4\pi M}\frac{\exp(2M\beta)}{(\pi\gamma' \sin\theta)^{\frac{1}{2}}}(\tilde{\zeta}^{-}_{2,0})^2 \times \sum_{n=1}^{n_0}(a'_n)^{-4}\exp(-i\lambda'_n\tilde{\zeta}^{-}_{2,0}), \tag{3.47}$$

where $f'_{2,\mathrm{res}}(\beta,\theta)$ is given by (3.33) and $\tilde{\zeta}^{-}_{2,0}$ by (3.34) with $m = 0$.

Let us now discuss the domain of validity of the above results. One restriction arises from the condition that the right saddle point $\bar{\lambda}'$, given by (A3) and (A7), must not lie too close to $\lambda = \beta$,

$$\beta - \bar{\lambda}' \gg \beta^{\frac{1}{3}}, \tag{3.48}$$

in order that the Debye asymptotic expansions be valid. One can verify that, in the neighborhood of $\theta = \theta_L$,

$$1 - \frac{\bar{\lambda}'}{\beta} = \mathcal{O}[(\theta_L - \theta)^2], \tag{3.49}$$

so that (3.48) leads to $\theta_L - \theta \gg \gamma$, the first condition in (3.35).

Further restrictions arise from the condition that the correction terms in $\mathcal{G}(\theta_1, \theta)$ in (3.41)–(3.42) be small. This condition is violated near the rainbow angle. According to (3.16), (3.41), and (3.42), the magnitude of the dominant correction terms near $\theta = \theta_R$ is

$$\frac{15\sin^2\theta_1}{256\beta\,|2\chi - 1|^3\cos^3\theta_1} \sim \{\beta[M(\theta - \theta_R)]^2\}^{-1}, \tag{3.50}$$

where we have employed (A22)–(A26). The requirement that (3.50) be much smaller than unity leads to the second condition in (3.35).

Another condition for the validity of the above results is that the integral (3.37) be reducible to the sum of two independent saddle point contributions. This approximation certainly fails in the neighborhood of the rainbow angle, when the two saddle points tend toward each other. A precise estimate of the error is difficult and will be postponed to Sec. 4. However, a necessary condition for the validity of this approximation is that the range of each saddle point be much smaller than the separation between the two saddle points. It can be verified that this leads precisely to the same condition already found, namely, $M(\theta - \theta_R) \gg \gamma^2$. For an explanation of the concept "range of a saddle point," see Ref. 13.

Finally, the domain of validity of (3.45) is much more restrictive. In addition to the above condition on $\theta - \theta_R$, it is necessary that the neglected terms in the exponent in (3.45) be small. This leads to the condition (3.44), so that (3.45) can be employed only in a very narrow angular domain near the rainbow angle.

C. The 0-Ray Region

This is the region

$$\theta_R - \theta \gg \gamma^2/M. \tag{3.51}$$

In this region the saddle points become complex. Their trajectories are partially shown in Fig. 4. Their behavior near the rainbow angle is given by (A23)–(A26).

Since the saddle points are complex conjugate, one of them would give rise to an increasing exponential, while the other one corresponds to the exponential decrease expected in the shadow. Thus, the path of integration in (3.37) must be taken only over the latter saddle point. With the help of Appendix A, one can verify that it is the lower saddle point that gives rise to the exponentially decreasing contribution. In Appendix A, this point is associated with the root z' (cf. Fig. 4), so that the "geometrical-optic" contribution in this region is given by (3.41) alone. This may be interpreted as a "complex ray".[14] The residue-series contributions are the same as in the 2-ray region.

[13] N. G. de Bruijn, *Asymptotic Methods in Analysis* (North-Holland Publishing Co., Amsterdam, 1958), p. 91.

[14] J. B. Keller, in *Calculus of Variations and its Applications*, Proc. Symp. Appl. Math., L. M. Graves, Ed. (McGraw-Hill Book Co., New York, 1958), Vol. 8, p. 27.

In particular, if θ is given by (3.43) with $\epsilon < 0$ and

$$\gamma^2/M \ll |\epsilon| \ll \beta^{-\frac{1}{2}}, \tag{3.52}$$

we can employ (A23)–(A26) and we find, similarly to (3.45),

$$\tilde{f}_{2,g}(\beta, \theta_R + \epsilon) \approx -\frac{8}{27} e^{-i\pi/4} \frac{N^2}{(8+N^2)^{\frac{1}{2}}} \frac{c^{\frac{1}{2}}}{s^{\frac{3}{2}}} \times \exp\left[6ic\beta - is\beta|\epsilon| + O(\beta\epsilon^2)\right] \times \exp\left[-\frac{s\beta}{2}\left(\frac{4c}{3s}|\epsilon|\right)^{\frac{3}{2}}\right]\left(\frac{4c}{3s}|\epsilon|\right)^{-\frac{1}{4}} \times \left\{1 + O\left(\frac{1}{\beta|\epsilon|^{\frac{3}{2}}}\right)\right\} \quad (\epsilon < 0,\ \gamma^2/M \ll |\epsilon| \ll \beta^{-\frac{1}{2}}). \tag{3.53}$$

Near the rainbow angle, the amplitude is dominated by this "complex-ray" contribution, which describes the exponential damping away from the 2-ray/0-ray shadow boundary. However, since the damping exponent is proportional to β, whereas it is proportional to $\beta^{\frac{1}{2}}$ for the residue-series contributions, the latter will eventually dominate the amplitude in the deep shadow region. Thus, the amplitude is more rapidly damped near the rainbow angle than far away from it.

D. The 1-Ray/2-Ray Transition Region

This is the region

$$|\theta - \theta_L| \lesssim \gamma. \tag{3.54}$$

In this region, we can use all the results derived for the 2-ray region, except for the contribution (3.41) from the right saddle point z', because it would now violate condition (3.48). The evaluation of this contribution is entirely similar to that in I, Sec. 5D. In fact, (3.37) differs from I, Eq. (5.29), only by a factor

$$\rho = R_{11} \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(2)}(\alpha)} \approx -i \exp\left\{2i\left[(\alpha^2 - \lambda^2)^{\frac{1}{2}} - \lambda \cos^{-1}\frac{\lambda}{\alpha}\right]\right\}, \tag{3.55}$$

so that we find, corresponding to I, (5.54),

$$\tilde{f}'_{2,g}(\beta, \theta) \approx -\frac{e^{-i\pi/12}[1 + O(\gamma)]}{\pi M(2\pi\beta \sin\theta)^{\frac{1}{2}}} \times \int \exp\left\{4i\left[(\alpha^2 - \lambda^2)^{\frac{1}{2}} - \lambda \cos^{-1}\frac{\lambda}{\alpha}\right] + i\lambda\theta\right\} \frac{d\zeta}{A^2(\zeta)}, \tag{3.56}$$

where the notation, as well as the path of integration, are the same as in I, (5.54).

Similarly to I, (5.55), we find from this

$$\tilde{f}'_{2,g}(\beta, \theta) = -\frac{2e^{-i\pi/4}}{M} \frac{\exp\left[4iM\beta + i\beta(\theta - \theta_L)\right]}{(2\pi\beta \sin\theta)^{\frac{1}{2}}} \times [1 + O(\gamma)] f\left(\frac{\theta - \theta_L}{\gamma}\right) \quad (|\theta - \theta_L| \lesssim \gamma), \tag{3.57}$$

where $f(s)$ is Fock's function, defined in I, (5.57). This expression now substitutes (3.41), whereas the remaining results obtained for the 2-ray region remain valid.

Thus, the 1-ray/2-ray transition corresponds to a normal (Fock-type) transition region. In particular, similarly to I, (5.58), we find

$$\tilde{f}'_{2,g}(\beta, \theta) \approx \frac{e^{i\pi/3}}{M}\left(\frac{\gamma}{\pi \sin\theta}\right)^{\frac{1}{2}} \exp(4iM\beta) \times \sum_n (a'_n)^{-2}[1 + O(\gamma)](\theta - \theta_L) \times \exp\left[i\left(\beta + e^{i\pi/3}\frac{x_n}{\gamma}\right)(\theta - \theta_L) + i\frac{\pi}{4}\right] \quad (\theta - \theta_L \gg \gamma). \tag{3.58}$$

Within the order of approximation to which this result is valid, i.e., $\theta - \theta_L \gg \gamma$ but still $\theta - \theta_L = O(\gamma)$, (3.58) is equivalent to the residue series in $\zeta_{2,0}^+$ by which (3.22) differs from (3.46) [in fact, the term $(\zeta_{2,0}^+)^2$ is then $O(\gamma)$ as compared with $M\zeta_{2,0}^+$].

Thus, as usual, the Fock amplitude interpolates smoothly between the 1-ray and 2-ray regions, but the corresponding representation (3.57) cannot be employed too far beyond the transition region.

4. THEORY OF THE RAINBOW

The present section deals mainly with the 2-ray/0-ray transition region (Fig. 5), i.e., the domain

$$|\theta - \theta_R| \lesssim \gamma^2/M, \tag{4.1}$$

where θ_R is the rainbow angle, given by (2.36). This is the region where the rainbow occurs.

A. The Rainbow

The mathematical problem with which we are confronted in the rainbow region is the asymptotic evaluation of the integral (3.37) in a domain where its two saddle points are very close to each other (cf. Fig. 4). As mentioned in Sec. 1, the extension of the saddle point method to this situation has only recently been given by Chester, Friedman, and Ursell.[3,4] The main features of their method are summarized in Appendix B. The present treatment is a direct application of this method.

According to (2.43)–(2.45), we may rewrite (3.37) in the form

$$f^{\infty}_{2,g}(\beta, \theta) = 2e^{-i\pi/4}N\left(\frac{2\beta}{\pi \sin\theta}\right)^{\frac{1}{2}} F(\kappa, \theta), \tag{4.2}$$

where

$$F(\kappa, \theta) = \int_{-\bar{\sigma}_1\infty}^{\bar{\sigma}_2\infty} g(w_1) \exp\left[\kappa f(w_1, \theta)\right] dw_1, \tag{4.3}$$

with

$$\kappa = 2\beta, \tag{4.4}$$

$$f(w_1, \theta) = i\Big[2N\cos w_2 - \cos w_1 + \left(2w_2 - w_1 - \frac{\pi - \theta}{2}\right)\sin w_1\Big], \tag{4.5}$$

$$g(w_1) = (\sin w_1)^{\frac{1}{2}} \cos^2 w_1 \cos w_2 \times \frac{(\cos w_1 - N\cos w_2)}{(\cos w_1 + N\cos w_2)^3}\left[1 + \mathcal{O}(\beta^{-1})\right], \tag{4.6}$$

where $-\bar{\sigma}_1\infty$ and $\bar{\sigma}_2\infty$ are the images of $-\sigma_1\infty$ and $\sigma_2\infty$ in the w_1-plane, respectively [cf. (3.37)]. For the sake of simplicity, the corrections of order β^{-1} will not be evaluated; their evaluation by the method given in Appendix B is straightforward, but rather cumbersome.

The two saddle points are given by

$$\bar{w}_1 = \theta_1', \theta_1'', \quad \text{with} \quad z' = \sin\theta_1', z'' = \sin\theta_1'', \tag{4.7}$$

where z' and z'' are given by (A7). In the domain (4.1), we have

$$\theta = \theta_R + \epsilon, \quad |\epsilon| \ll 1, \tag{4.8}$$

so that the expansions (A19)–(A26) can be employed. For definiteness, let us assume, to begin with, that $\epsilon > 0$, so that the two saddle points are real.

The integral (4.3) is of the form discussed in Appendix B. Let us make the change of variables (B2),

$$f(w_1, \theta) = \tfrac{1}{3}\mu^3 - \zeta(\epsilon)\mu + A(\epsilon). \tag{4.9}$$

According to (B4), (4.5), and (A1), the parameters $\zeta(\epsilon)$ and $A(\epsilon)$ are given by

$$A(\epsilon) = i[N(\cos\theta_2' + \cos\theta_2'') - \tfrac{1}{2}(\cos\theta_1' + \cos\theta_1'')], \tag{4.10}$$

$$\tfrac{2}{3}[\zeta(\epsilon)]^{\frac{3}{2}} = i[N(\cos\theta_2' - \cos\theta_2'') - \tfrac{1}{2}(\cos\theta_1' - \cos\theta_1'')], \tag{4.11}$$

where θ_2', θ_2'' are the values of θ_2 corresponding to (4.7), and we have made the association [cf. (B3)]:

$$\theta_1' \to -\zeta^{\frac{1}{2}}(\epsilon), \quad \theta_1'' \to \zeta^{\frac{1}{2}}(\epsilon). \tag{4.12}$$

In particular, for $|\epsilon| \ll 1$, we can employ the approximations (A19)–(A27), with the following results:

$$A(\epsilon) = i\left[3c + \tfrac{1}{2}s\epsilon + \frac{c(11c^2 - 15)}{72s^2}\epsilon^2 + \mathcal{O}(\epsilon^3)\right], \tag{4.13}$$

$$\frac{2}{3}[\zeta(\epsilon)]^{\frac{3}{2}} = \frac{2}{3}i\frac{(c\epsilon)^{\frac{3}{2}}}{(3s)^{\frac{1}{2}}} \times \left[1 + \frac{(875c^6 - 1257c^4 + 657c^2 + 45)}{5760(cs)^3}\epsilon + \mathcal{O}(\epsilon^2)\right], \tag{4.14}$$

where s and c are defined by (2.35).

The main contribution to the integral (4.3) arises from the neighborhood of the saddle points, where, for small enough ϵ, (4.5) may be expanded in powers of

$$\omega = w_1 - \theta_{1R}, \tag{4.15}$$

with the following result:

$$f(w_1, \theta) = i\Big[3c + \frac{s}{2}\epsilon + \frac{c}{2}\epsilon\omega - \frac{s}{4}\epsilon\omega^2 - \left(\frac{s}{8} + \frac{c\epsilon}{12}\right)\omega^3 + \mathcal{O}(\omega^4)\Big]. \tag{4.16}$$

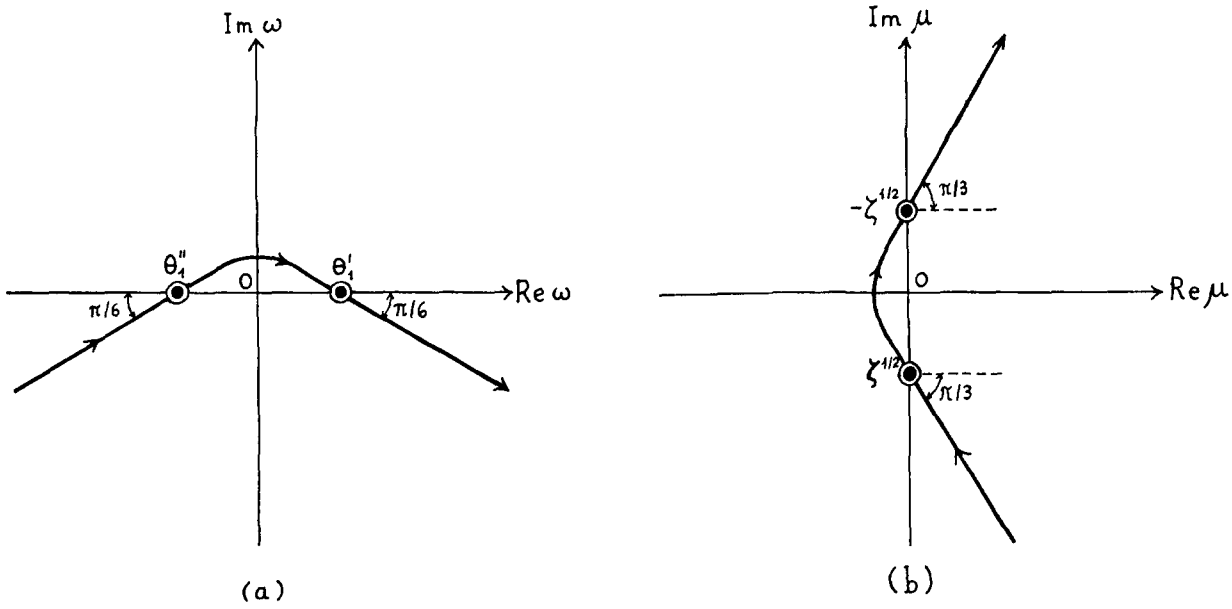


FIG. 9. The mapping of the ω plane onto the μ plane in the neighborhood of the origin.

For small enough ϵ, it also follows from (4.13)–(4.16) that, in the relevant portion of the path of integration, the transformation (4.9) is approximately given by

$$\mu^3/3 \approx -is\omega^3/8. \tag{4.17}$$

In solving (4.14) and (4.17) to determine $\zeta(\epsilon)$ and $\omega(\mu)$, care must be taken to choose the appropriate phase factors corresponding to the regular branch of the transformation. This branch is characterized by the condition that (4.12) holds on it (cf. Appendix B). The correct choice is

$$\omega \approx -2i\mu/(3s)^{\frac{1}{3}}, \tag{4.18}$$

$$\zeta(\epsilon) = e^{-i\pi}\frac{c\epsilon}{(3s)^{\frac{1}{3}}} \times \left[1 + \frac{(875c^6 - 1257c^4 + 657c^2 + 45)}{8640(sc)^3}\epsilon + \mathcal{O}(\epsilon^2)\right]. \tag{4.19}$$

In fact, if we set $\mu = -\zeta^{\frac{1}{2}}$ ($\mu = \zeta^{\frac{1}{2}}$) in (4.18), substituting ζ by (4.19), we find, respectively, $\omega = \delta'$ ($\omega = \delta''$), where δ' and δ'' are given by (A21), in agreement with (4.12).

According to (4.18), the mapping of the ω plane onto the μ plane in the relevant portion of the path of integration is as shown in Fig. 9. The path through the saddle points in Fig. 9(a) has been chosen in such a way that the transformed path in the μ-plane runs from $e^{-i\pi/3}\infty$ to $e^{i\pi/3}\infty$, as shown in Fig. 9(b).

Following (B5), we now expand

$$G(w_1, \epsilon) = g(w_1)\frac{dw_1}{d\mu} = \sum_m p_m(\epsilon)(\mu^2 - \zeta)^m + \sum_m q_m(\epsilon)\mu(\mu^2 - \zeta)^m, \tag{4.20}$$

where the coefficients $p_m(\epsilon)$, $q_m(\epsilon)$ are obtained by repeated differentiation of (4.20), setting $w_1 = \theta_1'$, $\mu = -\zeta^{\frac{1}{2}}$ and $w_1 = \theta_1''$, $\mu = \zeta^{\frac{1}{2}}$. Thus,

$$p_0(\epsilon) = \tfrac{1}{2}[G(\theta_1'', \epsilon) + G(\theta_1', \epsilon)], \tag{4.21}$$

$$q_0(\epsilon) = \tfrac{1}{2}\zeta^{-\frac{1}{2}}[G(\theta_1'', \epsilon) - G(\theta_1', \epsilon)], \tag{4.22}$$

$$p_1(\epsilon) = \tfrac{1}{4}\zeta^{-\frac{1}{2}}\left[\frac{dG}{d\mu}(\theta_1'', \epsilon) - \frac{dG}{d\mu}(\theta_1', \epsilon)\right], \tag{4.23}$$

$$q_1(\epsilon) = \tfrac{1}{4}\zeta^{-1}\left[\frac{dG}{d\mu}(\theta_1'', \epsilon) + \frac{dG}{d\mu}(\theta_1', \epsilon) - 2q_0(\epsilon)\right], \tag{4.24}$$

and so on. We shall compute explicitly only the coefficients p_0 and q_0.

Differentiating (4.5) twice with respect to μ and setting $\mu = -\zeta^{\frac{1}{2}}$, $w_1 = \theta_1'$, we get, taking into account (A1),

$$-2\zeta^{\frac{1}{2}} = i\frac{\cos\theta_1'}{N\cos\theta_2'}(2\cos\theta_1' - N\cos\theta_2')\left(\frac{dw_1}{d\mu}\right)^2_{\theta_1} \tag{4.25}$$

and, similarly for θ_1'', with $-\zeta^{\frac{1}{2}} \to \zeta^{\frac{1}{2}}$, $\theta_1' \to \theta_1''$. It follows that

$$\left(\frac{dw_1}{d\mu}\right)_{\theta_1'} = e^{-i\pi/4}\left[\frac{2N\cos\theta_2'}{\cos\theta_1'(N\cos\theta_2' - 2\cos\theta_1')}\right]^{\frac{1}{2}}\zeta^{\frac{1}{4}}, \tag{4.26}$$

$$\left(\frac{dw_1}{d\mu}\right)_{\theta_1''} = e^{-i\pi/4}\left[\frac{2N\cos\theta_2''}{\cos\theta_1''(2\cos\theta_1'' - N\cos\theta_2'')}\right]^{\frac{1}{2}}\zeta^{\frac{1}{4}}, \tag{4.27}$$

where the phase factors have been determined by the requirement that, for $|\epsilon| \ll 1$ [cf. (4.18)],

$$\left(\frac{dw_1}{d\mu}\right)_{\theta_1'} \approx \left(\frac{dw_1}{d\mu}\right)_{\theta_1''} \approx -\frac{2i}{(3s)^{\frac{1}{3}}}. \tag{4.28}$$

Employing the approximations (A23)–(A26) and (4.19) in (4.26)–(4.27), we find that (4.28) is indeed verified.

Substituting (4.26), (4.27), and (4.6) in (4.21)–(4.22), we find

$$\begin{Bmatrix} p_0 \\ q_0 \end{Bmatrix} = \frac{e^{-i\pi/4}}{4N}\zeta^{\pm\frac{1}{4}}\left[\left(\frac{\sin\theta_1''}{2\cos\theta_1'' - N\cos\theta_2''}\right)^{\frac{1}{2}}\right.$$
$$\times (2N\cos\theta_1''\cos\theta_2'')^{\frac{3}{2}}\frac{(\cos\theta_1'' - N\cos\theta_2'')}{(\cos\theta_1'' + N\cos\theta_2'')^3}$$
$$\pm\left(\frac{\sin\theta_1'}{N\cos\theta_2' - 2\cos\theta_1'}\right)^{\frac{1}{2}}(2N\cos\theta_1'\cos\theta_2')^{\frac{3}{2}}$$
$$\left.\times\frac{(\cos\theta_1' - N\cos\theta_2')}{(\cos\theta_1' + N\cos\theta_2')^3}\right][1 + \mathcal{O}(\beta^{-1})], \tag{4.29}$$

where upper and lower signs correspond to p_0 and q_0, respectively, ζ is given by (4.11) and θ_1', θ_1'' by (4.7).

In particular, for $|\epsilon| \ll 1$, we may employ (A23)–(A26) and (4.19), so that (4.29) becomes

$$p_0(\epsilon) = \frac{4i(3s)^{\frac{1}{6}}c}{27\sqrt{3}\,N}[1 + \mathcal{O}(\epsilon)], \tag{4.30}$$

$$q_0(\epsilon) = -\frac{(28 - 31s^2)}{27\sqrt{3}\,N(3s)^{\frac{7}{6}}}[1 + \mathcal{O}(\epsilon^{\frac{1}{2}})]. \tag{4.31}$$

If we now substitute (4.9) and (4.20) into (4.3), we find, by (B6),

$$F(\kappa, \theta) = 2\pi i\exp[\kappa A(\epsilon)]\left[\sum_m p_m(\epsilon)F_m(\zeta, \kappa, C_1)\right.$$
$$\left. + \sum_m q_m(\epsilon)G_m(\zeta, \kappa, C_1)\right], \tag{4.32}$$

where F_m and G_m are defined by (B7)–(B8) and the contour C_1 by (B9) (cf. Fig. 9).

Taking into account (B10) and (B12), we finally obtain

$$F(\kappa, \theta) = 2\pi i\kappa^{-\frac{1}{3}}\exp[\kappa A(\epsilon)]$$
$$\times\{[p_0(\epsilon) + \mathcal{O}(\kappa^{-1})]\,\mathrm{Ai}\,(\kappa^{\frac{2}{3}}\zeta)$$
$$- \kappa^{-\frac{1}{3}}[q_0(\epsilon) + \mathcal{O}(\kappa^{-1})]\,\mathrm{Ai}'\,(\kappa^{\frac{2}{3}}\zeta)\}, \tag{4.33}$$

where Ai (z) is the Airy function. Thus, taking into account (4.4), (4.2) finally becomes

$$\tilde{f}_{2,g}(\beta, \theta) = 4e^{i\pi/4}N\left(\frac{\pi}{\sin\theta}\right)^{\frac{1}{2}}(2\beta)^{\frac{1}{6}}\exp[2\beta A(\epsilon)]$$
$$\times\left\{p_0(\epsilon)\,\mathrm{Ai}\,[(2\beta)^{\frac{2}{3}}\zeta(\epsilon)]\right.$$
$$\left. - \frac{q_0(\epsilon)}{(2\beta)^{\frac{1}{3}}}\,\mathrm{Ai}'\,[(2\beta)^{\frac{2}{3}}\zeta(\epsilon)]\right\}[1 + \mathcal{O}(\beta^{-1})], \tag{4.34}$$

where $A(\epsilon)$, $\zeta(\epsilon)$ are given by (4.10)–(4.11), $p_0(\epsilon)$ and $q_0(\epsilon)$ by (4.29), and θ_1', θ_1'' by (4.7).

Higher-order terms in the Chester–Friedman–Ursell uniform asymptotic expansion of the scattering amplitude may be obtained, if required, by means of the procedure indicated in Appendix B. Here we shall restrict our consideration to the first two terms, given by (4.34).

In particular, for $|\epsilon| \ll 1$, we may employ (4.13), (4.19), (4.30), and (4.31), so that (4.34) becomes

$$\tilde{f}_{2,g}(\beta, \theta) = -\frac{16e^{-i\pi/4}}{27\sqrt{3}}\left(\frac{\pi}{\sin\theta}\right)^{\frac{1}{2}}c(6s\beta)^{\frac{1}{6}}$$
$$\times\exp[6ic\beta + is\beta\epsilon + i\mathcal{A}\beta\epsilon^2 + \mathcal{O}(\beta\epsilon^3)]$$
$$\times\left\{[1 + \mathcal{O}(\epsilon) + \mathcal{O}(\beta^{-1})]\right.$$
$$\times\,\mathrm{Ai}\left[-\frac{c(2\beta)^{\frac{2}{3}}\epsilon}{(3s)^{\frac{1}{3}}}(1 + \mathcal{B}\epsilon + \mathcal{O}(\epsilon^2))\right]$$
$$-\frac{i\mathcal{C}}{(2\beta)^{\frac{1}{3}}}[1 + \mathcal{O}(\epsilon^{\frac{1}{2}}) + \mathcal{O}(\beta^{-1})]$$
$$\left.\times\,\mathrm{Ai}'\left[-\frac{c(2\beta)^{\frac{2}{3}}\epsilon}{(3s)^{\frac{1}{3}}}(1 + \mathcal{B}\epsilon + \mathcal{O}(\epsilon^2))\right]\right\}, \tag{4.35}$$

where

$$\mathcal{A} = \frac{c(11c^2 - 15)}{36s^2}, \tag{4.36}$$

$$\mathcal{B} = \frac{875c^6 - 1257c^4 + 657c^2 + 45}{8640(sc)^3}, \tag{4.37}$$

$$\mathcal{C} = \frac{28 - 31s^2}{4c(3s)^{\frac{4}{3}}}. \tag{4.38}$$

The result (4.35) is a good approximation throughout the domain where the indicated error terms are small, i.e., for

$$|\epsilon| \ll \gamma. \tag{4.39}$$

This is true, in particular, within the rainbow region (4.1).

We can still employ (4.35) over part of the domain (3.44), in the 2-ray region, where the Airy functions may be replaced by their asymptotic expansions (B15)–(B16). With the help of (2.36), it is found that the result is equivalent to (3.45). The corresponding oscillations, arising from interference between the two geometrical ray contributions, give rise to the "supernumerary bows" sometimes seen on the inner side of the main rainbow.

For still larger scattering angles in the 2-ray region, we can no longer employ (4.35), but (4.34) remains valid. Again with the help of (B15)–(B16), taking into account (4.29), we find

$$\begin{aligned} \tilde{f}_{2,g}(\beta, \theta) = {} & \left(\frac{1}{\sin\theta}\right)^{\frac{1}{2}} \left(\frac{\sin\theta_1''}{2\cos\theta_1'' - N\cos\theta_2''}\right)^{\frac{1}{2}} \\ & \times (2N\cos\theta_1''\cos\theta_2'')^{\frac{1}{3}} \frac{(\cos\theta_1'' - N\cos\theta_2'')}{(\cos\theta_1'' + N\cos\theta_2'')^3} \\ & \times \exp\left[2\beta A(\epsilon) - \tfrac{4}{3}\beta\zeta^{\frac{3}{2}}(\epsilon)\right] \\ & - i\left(\frac{\sin\theta_1'}{N\cos\theta_2' - 2\cos\theta_1'}\right)^{\frac{1}{2}} \\ & \times (2N\cos\theta_1'\cos\theta_2')^{\frac{1}{3}} \frac{(\cos\theta_1' - N\cos\theta_2')}{(\cos\theta_1' + N\cos\theta_2')^3} \\ & \times \exp\left[2\beta A(\epsilon) + \tfrac{4}{3}\beta\zeta^{\frac{3}{2}}(\epsilon)\right]\Big)[1 + \mathcal{O}(\beta^{-1})]. \end{aligned} \tag{4.40}$$

In view of (4.10)–(4.11), this coincides exactly with the result (3.40)–(3.42) of the saddle-point method. Thus, the Chester–Friedman–Ursell method leads indeed to a uniform asymptotic expansion, matching smoothly the result obtained by the saddle-point method in the region where the latter is valid.

In the 0-ray region, within the domain (3.52), we may again employ (4.35), but now, since $\epsilon < 0$, we must employ the asymptotic expansions (B13)–(B14) for the Airy functions. The result is identical to (3.53), corresponding to the exponential damping on the shadow side of the rainbow (dark band between primary and secondary bows).

For still larger scattering angles in the 0-ray region, the Chester–Friedman–Ursell method would apparently have to be extended in order to match smoothly with the saddle-point method, since the coefficients (4.29) depend symmetrically on both saddle points, whereas, according to Sec. 3C, only the lower saddle point contributes to the steepest-descent result (cf. note A in Ref. 4, p. 126).

B. Comparison with Earlier Theories

An excellent review of the development of the theory of the rainbow has been given by Van de Hulst (Ref. 7, p. 240). A more detailed historical account may be found in Ref. 15.

Airy's theory[5] still remains the best approximation so far available, other than numerical summation of the partial-wave series. It is based on the application of Huygens' principle to the cubic wave front near the ray of minimum deviation. Van der Pol and Bremmer[16] applied Watson's transformation to the electromagnetic problem, but the expression thus obtained was finally reduced to Airy's approximation. The same is true for Rubinow's treatment[17] of the scalar problem. Bucerius[18] attempted to improve Airy's approximation by including terms up to the fifth order in a Taylor series expansion of the phase around the rainbow point [similar to (4.16)]. However, this does not lead to a uniform asymptotic expansion.

Airy's approximation may be obtained from (4.35) by retaining only the lowest-order term in all expansions, including those that appear in the argument of the exponential and Airy functions. This corresponds to setting

$$\mathcal{A} = \mathcal{B} = \mathcal{C} = 0. \tag{4.41}$$

Substituting also $\sin\theta$ by $\sin\theta_R$ and c and s by their values [cf. (2.35)–(2.36)], we find

$$\begin{aligned} \tilde{f}_{2,g}^{(\mathrm{Airy})}(\beta, \theta) = {} & -\frac{16}{27}\frac{3^{\frac{7}{12}}}{2^{\frac{1}{3}}} e^{-i\pi/4} \frac{N^2(N^2-1)^{\frac{1}{4}}}{(8+N^2)^{\frac{1}{2}}(4-N^2)^{\frac{3}{4}}} \beta^{\frac{1}{6}} \\ & \times \exp\left\{\frac{i\beta}{\sqrt{3}}\left[6(N^2-1)^{\frac{1}{2}} + (4-N^2)^{\frac{1}{2}}(\theta - \theta_R)\right]\right\} \\ & \times \mathrm{Ai}\left[-\frac{(N^2-1)^{\frac{1}{2}}}{(4-N^2)^{\frac{1}{4}}}\left(\frac{2\beta}{3}\right)^{\frac{2}{3}}(\theta - \theta_R)\right], \end{aligned} \tag{4.42}$$

which is Airy's approximation. The factor in front of

[15] C. B. Boyer, *The Rainbow* (Thomas Yoseloff, New York, 1959).
[16] B. van der Pol and H. Bremmer, Phil. Mag. **24**, 141, 825 (1937).
[17] S. I. Rubinow, Ann. Phys. (N.Y.) **14**, 305 (1961).
[18] H. Bucerius, Optik **1**, 188 (1946).

the Airy function agrees with that given in Ref. 17, Eq. (68), except for the sign. The argument of the Airy function is incorrectly given in Ref. 17, but the correct value appears in Ref. 7.

According to Van de Hulst (Ref. 7, pp. 246–249), Airy's approximation is a useful quantitative theory only for $\beta > 5000$ and $|\epsilon| < 0.5° \sim 0.01r$; Huygens's principle may still be applied for $\beta > 2000$, but "a quantitative theory of the rainbow for the entire gap $30 < \beta < 2000$ is lacking."

As we have seen, the result of the present theory, contained in the uniform asymptotic expansion (4.34), is valid even for large deviations from the rainbow angle, matching smoothly with the results obtained within the domain of validity of the saddle-point method. While it remains to be seen whether it can be applied to values of β as low as 30, values a few times bigger should be accessible. Thus, a considerable portion of the gap appears to be bridged.

In order to estimate the accuracy of Airy's approximation, let us consider the domain (4.39), where (4.35) is valid. The main contributions to the total scattering amplitude in this domain arise from the direct-reflection term I, (4.35), and from the rainbow term (4.35), which is dominant, due to the enhancement factor $\beta^{\frac{1}{3}}$. A numerical computation of the coefficients, taking $N = 1.33$, yields

$$\begin{aligned} f(\beta, \theta_R + \epsilon) \approx & -0.0786 \\ & \times \exp(-1.86i\beta) - 0.438e^{-i\pi/4}(2\beta)^{\frac{1}{3}} \\ & \times \exp[i\beta(3.038 + 0.862\epsilon - 0.230\epsilon^2)] \\ & \times \{\mathrm{Ai}[-0.369(2\beta)^{\frac{2}{3}}\epsilon(1 + 0.202\epsilon)] \\ & - 0.688i(2\beta)^{-\frac{1}{3}} \\ & \times \mathrm{Ai}'[-0.369(2\beta)^{\frac{2}{3}}\epsilon(1 + 0.202\epsilon)]\} \\ & (N = 1.33). \quad (4.43) \end{aligned}$$

If only the rainbow term is taken into account, the minima and maxima of the intensity still occur at the zeros of the Airy function and its derivative, respectively. Their angular positions are shifted with respect to Airy's theory by amounts proportional to $\mathcal{B}\epsilon$ [cf. (4.35)]. The corrections to the intensity also involve the term $\mathcal{C}$ in (4.35), which is again of order ϵ. Both corrections can attain several percent within the domain (4.39).

For β of the order of a few hundred, the correction term involving the derivative of the Airy function becomes of the same order of magnitude as the direct reflection term, so that interference with the first term in (4.43) must be taken into account. The correction term $\mathcal{A}$ to the phase of the rainbow term (4.35) will then also play a role.

In conclusion, within the domain (4.39), the corrections to Airy's theory can attain several percent; their value increases with the deviation from the rainbow angle.

5. THEORY OF THE GLORY

A. Introduction

The last region that remains to be treated is the neighborhood of the backward direction,

$$\theta = \pi - \epsilon, \quad 0 \leq \epsilon \ll \beta^{-\frac{1}{3}}. \quad (5.1)$$

This is the region where the glory is observed.

The glory is a strong enhancement in near-backward scattering by very small water droplets, with values of β ranging up to a few hundred. As a meteorological effect,[19a] it appears when an observer stands on a high point (mountain summit), looking at his own shadow prjoected on nearby thin clouds or mist (i.e., 180° away from the sun). Under favorable conditions, he sees the shadow of his head surrounded by a bright halo, sometimes accompanied by several colored rings. A color picture of the glory has recently been published.[19b] The glory is also frequently observed from airplanes (around the shadow of the plane). When several observers stand together, each one sees the glory only around the shadow of his own head, and not those of his companions, indicating that the effect is concentrated within a very small solid angle around 180°, corresponding to a narrow peak in the back-scattered intensity. [This remarkable effect was noticed already in the first recorded observations, made in 1735 by a Spanish captain, Antonio de Ulloa, from a mountain top in the Andes, in the course of a scientific expedition to Peru.[19]] The average value of β for which the observations have been made is of the order of 160, corresponding to water droplets with 0.028 mm average diameter (Ref. 7, p. 258).

A discussion of various attempts that have been made to explain the glory has been given by Van de Hulst (Refs. 6 and 7, p. 249). Although the first recorded observation was made more than two centuries ago, no satisfactory quantitative treatment has ever been given. The main facts that have to be explained may be classified as follows (cf. Ref. 7, p. 255):

(a) The anomalously large intensity near the backward direction for values of β ranging up to a few

[19] (a) J. M. Pernter and F. M. Exner, *Meteorologische Optik* (W. Braumüller, Vienna, 1910); (b) J. C. Brandt, Publ. Astron. Soc. Pacific **80**, 25 (1968).

hundred, as well as the fact that the phenomenon is no longer observed for larger water droplets (e.g., for $\beta \sim 10^3$).

(b) The angular distribution. With (5.1), if we denote by ϵ_j the angular radius of the jth dark ring (as it would be observed in yellow light), we have, roughly (Ref. 7, p. 257),

$$0.35 \leqslant \epsilon_1/\epsilon_2 \leqslant 0.45; \quad 1.6 \leqslant \epsilon_3/\epsilon_2 \leqslant 1.7. \quad (5.2)$$

The first dark ring is apparently rather hazy. We have

$$\epsilon_1 = \mathcal{O}(\beta^{-1}), \quad (5.3)$$

which is a measure of the narrowness of the backward peak.

The ratios (5.2) differ from those found in ordinary diffraction coronae, which correspond to the forward diffraction peak. The outer rings in the glory are also much more pronounced, i.e., the intensity decreases more slowly as we move away from the center. This disposes of an early theory according to which the glory would be a diffraction corona for light reflected from the clouds; it is undoubtedly contained in the back-scattered intensity from individual water droplets.

(c) The polarization: although few systematic data exist, there are indications that the glory is strongly polarized.

(d) Variability: the character of the rings (radius, brightness, etc.) frequently changes with time, even during a single observation.

Ultimately, the crucial test of a theory lies in how accurately it can reproduce the "exact" results, obtained by numerical summation of the partial-wave expansion. For the scalar problem, there do not seem to be many numerical results available. In the electromagnetic case, however, there exist several numerical calculations of the intensity at or near 180°. Most relevant to the present problem are those of Walter[20] and Bryant and Cox.[8]

The latter are particularly valuable, because the intensity at 180° was computed as a function of β, at intervals of 0.005, near $\beta = 200$ and $\beta = 500$. The results show a lot of fine structure that does not appear in other calculations. Specifically,

(e) Superimposed on a more slowly-varying background, the back-scattered intensity shows a rapidly-varying, quasiperiodic pattern. The period $\Delta\beta$ found for these fluctuations is given by

$$0.81 \leqslant \Delta\beta \leqslant 0.82. \quad (5.4)$$

[20] H. Walter, Optik **16**, 401 (1959)

(f) Within a single period, a few irregular peaks of varying heights and widths are found; the width ranges from $\sim$0.01 to $\sim$0.1 and the intensity can change by a factor of $\sim$100 (Ref. 8, Fig. 2), corresponding to enormous spikes.

Bryant and Cox also plotted on the same curve the intensity at 90° and the total cross section (Ref. 8, Fig. 2). They found that

(g) The total cross section also shows fluctuations with very similar character and the same period as the back-scattered intensity, but with greatly reduced magnitude, corresponding to changes of the order of one percent. At 90°, intermediate-size fluctuations are seen, but the period is *twice* that given by (5.4).

Except for the polarization, it is to be expected that most of the above features also appear in the scalar case. Thus, we shall investigate to what extent they are present here, although it must be stressed that an entirely adequate confrontation can only be made with the results obtained in the case of electromagnetic scattering.[11]

We shall see that, apart from the polarization effects, all the other features are indeed present and can be explained by the theory. However, for an explanation of the detailed structure of the intensity [(e) to (g)], higher-order terms in the Debye series have to be taken into account. Their effect is discussed in Sec. 6.

B. The Geometrical-Optic Contribution

The decomposition (3.10) made in the 2-ray region,

$$f_2(\beta, \theta) = f_{2,g}(\beta, \theta) + f_{2,\mathrm{res}}(\beta, \theta) + f'_{2,\mathrm{res}}(\beta, \theta), \quad (5.5)$$

is still valid in the domain (5.1), provided that we rewrite (3.11) in the form

$$f_{2,g}(\beta, \theta) = \frac{i}{\beta}\int_0^{\sigma_1\infty} \rho U P_{\lambda-\frac{1}{2}}(-\cos\theta) e^{i\pi\lambda} \tan(\pi\lambda)\lambda \, d\lambda. \quad (5.6)$$

This result is obtained by taking the path of integration in (3.11) to be symmetric about the origin, then splitting it at the origin, making $\lambda \to -\lambda$ in the lower half and employing the identity

$$Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta) - e^{2i\pi\lambda} Q^{(2)}_{-\lambda-\frac{1}{2}}(\cos\theta) = -e^{i\pi\lambda}\tan(\pi\lambda) P_{\lambda-\frac{1}{2}}(-\cos\theta), \quad (5.7)$$

which follows from N, Eq. (C6). The expressions (3.12), (3.13) for the residue-series contributions to (5.5) can be employed up to $\theta = \pi$, and so can (5.6).

Let us consider first the "geometrical-optic" term $f_{2,g}(\beta, \theta)$. Strictly speaking, this name is not entirely

appropriate, because geometrical optics would predict infinite intensity in the backward direction (which corresponds to a focal line). However, in view of the fact that in previous cases the saddle-point contributions were found to correspond to the geometrical-optic approximation, the same name will be applied here. As $\theta \to \pi$, the saddle point $\bar{\lambda}$ in (3.11) tends to the origin [cf. (3.2)]. This corresponds to the central ray, $\theta_1 = \theta_2 = 0$, which is transmitted through the sphere and then reflected backwards. Thus, we expect that the main contribution to (5.6) will arise from the neighborhood of $\lambda = 0$, or, more precisely, from the domain

$$|\lambda| \ll \beta^{\frac{1}{2}}, \tag{5.8}$$

which corresponds to the range of the saddle point.[13] [There is a misprint in the corresponding formula N, Eq. (9.48), which should read exactly like (5.8)].

We can therefore evaluate (5.6) by a method similar to that described in N, Sec. IX.C. We expand the integrand in powers of λ/β, keeping all correction terms up to $O(\beta^{-1})$, and making use of the asymptotic expansion N, Eq. (C9) for $P_{\lambda-\frac{1}{2}}(-\cos\theta)$.

With the change of variable

$$\lambda = e^{i\pi/4}\left(\frac{N\beta}{2-N}\right)^{\frac{1}{2}} x = \zeta x, \tag{5.9}$$

the result is

$$\begin{aligned} f_{2,g}(\beta, \pi - \epsilon) &= \frac{4iN^2(N-1)}{(2-N)(N+1)^3} \exp\left[2i(2N-1)\beta\right] \\ &\times \left\{\left[1 - \frac{i(2-N)}{4N\beta}\right] G_{0,1} - \frac{i(N^2-4N+1)}{2N(2-N)\beta} G_{0,3} \right. \\ &+ \frac{i(N^3-2)}{12N(2-N)^2\beta} G_{0,5} + \sin^2\frac{\epsilon}{2} \\ &\times \left.\left(\frac{\zeta}{3}\sin\frac{\epsilon}{2} G_{3,2} - G_{2,1} + \frac{G_{1,0}}{4\zeta\sin\frac{\epsilon}{2}}\right) + O(\beta^{-2})\right\}, \end{aligned} \tag{5.10}$$

where

$$\begin{aligned} G_{m,n}(\zeta, \epsilon) &= \int_0^\infty \exp(-x^2) \\ &\times J_m\left(2\zeta x \sin\frac{\epsilon}{2}\right) \tan(\pi\zeta x) x^n \, dx. \end{aligned} \tag{5.11}$$

Evaluating these integrals by the technique developed in N, Appendix F, we find the following final result:

$$\begin{aligned} f_{2,g}(\beta, \pi - \epsilon) &= -\frac{2N^2(N-1)}{(2-N)(N+1)^3} \\ &\times \exp\left[2i(2N-1)\beta\right] \exp\left[-\frac{iN\beta\epsilon^2}{4(2-N)}\right] \\ &\times \left\{1 + \frac{i(2N^3-10N^2+17N-8)}{2N(2-N)^2\beta} \right. \\ &- \left.\frac{(N^2+1)\epsilon^2}{8(2-N)^2} - \frac{iN(N^3-2)\beta\epsilon^4}{192(2-N)^4} + O(\beta^{-2})\right\} \end{aligned}$$

$$(0 \le \epsilon \ll \beta^{-\frac{1}{2}}). \tag{5.12}$$

It can be verified that (5.12) coincides with the expansion of (3.15)–(3.16) in powers of ϵ^2, within the domain under consideration. Thus, (3.15)–(3.16) are uniformly valid up to $\theta = \pi$.

No geometrical-optic rays other than the central one contribute to the second term of the Debye expansion in this region. As shown in Fig. 3(c), such rays can appear near the backward direction only for $N > \sqrt{2}$. (They are sometimes called "glory rays," but the corresponding effect should not be confused with the one under consideration.) Thus, the total scattering amplitude near the backward direction, in the geometrical-optic approximation, is given by

$$\begin{aligned} f_g(\beta, \pi - \epsilon) &= f_{0,g}(\beta, \pi - \epsilon) + f_{2,g}(\beta, \pi - \epsilon) \\ &+ f_{p>2,g}(\beta, \pi - \epsilon), \end{aligned} \tag{5.13}$$

where $f_{0,g}(\beta, \pi - \epsilon)$ is given by I, (4.52), $f_{2,g}(\beta, \pi - \epsilon)$ by (5.12), and $f_{p>2,g}(\beta, \pi - \epsilon)$ represents the total geometrical-optic contribution from higher-order terms in the Debye expansion. It corresponds essentially to the central-ray contributions after multiple internal reflections within the sphere, and may therefore be anticipated to be much smaller than the remaining two terms in (5.13). This is confirmed in Sec. 6B by explicit computation.

In particular, for $N = 1.33$, $\beta = 130$, which is close to the average value for which the glory is observed, the total contribution from the first two terms of (5.13) at $\theta = \pi$ is found to be

$$f_{0,g}(130, \pi) + f_{2,g}(130, \pi) \approx 0.101 + 0.176i \quad (N = 1.33). \tag{5.14}$$

The "exact" scattering amplitude corresponding to these values can be computed from its partial-wave expansion I, (2.1), with the help of partial-wave

tables[21] (the term $l = 0$ has to be separately added). The result is

$$f(130, \pi) \approx -0.0104 + 0.798i \quad (N = 1.33). \quad (5.15)$$

Comparing (5.14) with (5.15), we see that it not only has the wrong phase, but also accounts only for about 7% of the total intensity! As has already been mentioned (cf. Sec. 6B), higher-order geometrical-optic contributions are negligible. The angular distribution and β-dependence of (5.13) are also entirely different from those found in the glory.

We conclude that geometrical optics accounts only for a small fraction of the total intensity near the backward direction (in the relevant range of values of β) and is completely unable to explain the glory. The attempt by Ray[22] to explain the glory by means of diffraction of light rays reflected near the backward direction is thus seen to be incorrect. The same applies to a discussion by Bricard.[23]

C. Qualitative Discussion

Since the glory is not due to geometrical-optic contributions, it must arise from residue-series contributions. Thus, it must correspond to a case of strong "Regge-pole dominance" of the scattering amplitude. Heretofore, we have found such cases only in shadow regions (where the amplitude would vanish in the geometrical-optic approximation). This is the first example of such dominance in a lit region.

Physically, this implies that the glory is due to surface waves. This was first suggested by Van de Hulst (Refs. 6; 7, p. 373), who conjectured that diffracted rays taking two shortcuts across the sphere, i.e., of the type shown in Fig. 7, are responsible for the glory.

For $N = 1.33$, the total angle $\pi - \theta_L$ that must be described by the surface waves before emerging in the backward direction [cf. Fig. 7(a), (b)], is approximately 15°. The question then is whether the exponential damping of the surface waves along this arc would not prevent them from making an appreciable contribution. This quantitative problem was not treated by Van de Hulst.

There are two qualitative pieces of evidence that tend to support the general correctness of Van de Hulst's conjecture. One of them is Bryant and Cox's numerical study[8] of partial sums of the Mie series as a function of the number of partial waves retained. They found that, at $\theta = 180°$, by far the most important contribution to the sum arises from the edge domain I, (1.14), which, as we know, corresponds to nearly-grazing incident rays.

The other piece of evidence is experimental. It has been shown by Fahlen and Bryant[24] that the circumference of a water droplet, viewed at 180° with respect to the illuminating beam, appears like a thin luminous line. The explanation of this effect is that the surface of the droplet is a caustic of diffracted rays. Just as in the well-known phenomenon of the luminosity of a diffracting edge as seen from the shadow,[25] the eye (or the photographic plate) performs an inadmissible extrapolation. From the behavior at finite distances, it is inferred that the circumference of the droplet is an actual light source, whereas the true intensity there is, of course, finite. Thus, Fahlen and Bryant's observation provides direct experimental evidence for the existence of intense surface-wave contributions along the backward direction.

Both the above pieces of evidence strongly support the inference that surface waves are responsible for the dominant contribution to the glory. This is not necessarily equivalent to Van de Hulst's conjecture, which proposed a specific model for the surface-wave contributions, namely, diffracted rays of the type shown in Fig. 7. We shall see that, while these rays indeed give a significant contribution, surface-wave contributions from higher-order terms in the Debye expansion also play an important role.

The present treatment enables us to make a quantitative evaluation of the Van de Hulst-type surface-wave contribution. It corresponds to $f_{2,\mathrm{res}}(\beta, \pi - \epsilon)$ and is given by (3.18)–(3.21). Before performing a numerical evaluation, however, let us give a qualitative discussion of the behavior of the amplitude up to the third term in the Debye expansion. To this order, we have

$$f(\beta, \pi - \epsilon) \approx f_{0,g}(\beta, \pi - \epsilon) + f_{2,g}(\beta, \pi - \epsilon) + f_{2,\mathrm{res}}(\beta, \pi - \epsilon), \quad (5.16)$$

where the first two terms are the same as in (5.13) (the remaining contributions up to this order may be neglected).

For sufficiently large β and $\epsilon \gg \beta^{-1}$, the third term is approximately given by (3.22). In the domain under consideration, $\epsilon \lesssim \beta^{-\frac{1}{2}}$, the asymptotic expansion N,

[21] R. O. Gumprecht and C. M. Sliepcevich, *Tables of Light Scattering Functions for Spherical Particles* (University of Michigan Press, Ann Arbor, 1951).

[22] B. Ray, Proc. Ind. Assoc. Cultiv. Sci. **8**, 23 (1923); Nature **111**, 83 (1923).

[23] J. Bricard, in *Handbuch der Physik* (Springer-Verlag, Berlin, 1957), Bd. XLVIII, p. 351.

[24] T. S. Fahlen and H. C. Bryant, J. Opt. Soc. Am. **56**, 1635 (1966).

[25] A. Sommerfeld, *Optics* (Academic Press Inc., New York, 1954), p. 262.

(C11) for $P_{\lambda-\frac{1}{2}}(-\cos\theta)$, employed in the derivation of (3.22), is no longer valid and must be replaced by N, (C9). With this replacement and neglecting correction terms $\mathcal{O}(\beta^{-1})$ in I, (4.52) and (5.12), we find that (5.16) becomes

$$f(\beta, \pi-\epsilon) \approx -\frac{1}{2}\left(\frac{N-1}{N+1}\right) \times \exp(-2i\beta)\left[1+\frac{4N^2}{(2-N)(N+1)^2}\exp(4iN\beta)\right] + 2\frac{e^{i\pi/3}}{\gamma M^2}\exp(4iM\beta)(\pi-\theta_L)(\pi-\theta_L+M)J_0(\beta\epsilon) \times \sum_n (a_n')^{-2}\exp[i\lambda_n(\pi-\theta_L)] \quad (0 \leq \epsilon \ll \beta^{-1}). \tag{5.17}$$

In the residue series, we have neglected all terms beyond $m = 0$ [cf. (3.22)], which correspond to surface waves making more than one turn around the sphere, since such contributions are extremely small.

It must be emphasized that the expression for $f_{2,\mathrm{res}}(\beta, \pi-\epsilon)$ in (5.17), where only the lowest-order term in each asymptotic expansion has been kept, is certainly not a good approximation for $\beta \sim 10^2$. Many more terms would have to be included in the evaluation of the residues, as will be seen in Sec. 5D. However, our present purpose is to make a rough estimate of the order of magnitude of this term and of its qualitative behavior as a function of β and ϵ. For this purpose, the simple expression given in (5.17) is entirely adequate.

Taking $N = 1.33$ and employing the asymptotic expansions for the poles given in I, Appendix A, (5.17) becomes

$$\begin{aligned} f(\beta, \pi-\epsilon) &\approx -0.0708\exp(-2i\beta)[1+1.95\exp(5.32i\beta)] \\ &\quad + 1.69\exp\left(3.77i\beta + 0.243i\beta^{\frac{1}{3}} + i\frac{\pi}{3}\right) \\ &\quad \times J_0(\beta\epsilon)\beta^{\frac{1}{3}}\exp(-0.421\beta^{\frac{1}{3}}) \\ &\quad \times \{1+0.762\exp[(-0.315+0.182i)\beta^{\frac{1}{3}}] \\ &\quad + 0.657\exp[(-0.574+0.331i)\beta^{\frac{1}{3}}] + \cdots\}, \end{aligned} \tag{5.18}$$

where, within the curly brackets, we have taken into account only the contributions from the first three poles. Now let us compare the behavior of (5.18) as a function of β and ϵ with some of the features (a)–(g) of the glory, described in Sec. 5A.

(a) The ratio of the residue-series contribution to the geometrical-optic contribution to the amplitude is of the order of

$$|f_{2,\mathrm{res}}(\beta, \pi-\epsilon)/f_g(\beta, \pi-\epsilon)| \sim 15\beta^{\frac{1}{3}}\exp(-0.4\beta^{\frac{1}{3}}). \tag{5.19}$$

This is of order 10 for $\beta \sim 10^2$ and of order unity for $\beta \sim 10^3$.

Thus, in the domain where the glory is observed, the residue series is indeed the dominant term in the amplitude, and its order of magnitude is just right to account for the discrepancy between (5.14) and (5.15).

The physical factor that enhances the surface-wave contribution is their focusing along the axis, analogous to the Poisson spot: a whole cone of diffracted rays come together, rather than just two. This is responsible for the change from a factor $\beta^{-\frac{1}{6}}$ in (3.22) to a factor $\beta^{\frac{1}{3}}$ in (5.17); the amplification factor due to focusing is of order $\beta^{\frac{1}{2}}$ [cf. also N, (5.11)].

On the other hand, the damping coefficient in the attenuation factor of the surface waves also increases like $\beta^{\frac{1}{3}}$, so that, for large enough β (a few times 10^3), the geometrical-optic contribution becomes dominant. Together with the increasing smallness of the solid angle defined by (5.3), this explains why the glory is not observed for larger water droplets.

(b) Within the domain of values of β where the glory is observed, the angular distribution is determined by the dominant term in (5.18), namely,

$$i(\beta, \pi-\epsilon) \propto J_0^2(\beta\epsilon), \tag{5.20}$$

where i denotes the intensity.

The above angular distribution also follows directly from the fact that the dominant contribution to the glory arises from partial waves in the edge domain [cf. I, (1.14)]:

$$l_- \sim \beta - c\beta^{\frac{1}{3}} \ll l \ll l_+ \sim \beta + c\beta^{\frac{1}{3}}, \tag{5.21}$$

corresponding to nearly-grazing incident rays. In fact, for such values of l, N, (C9), yields

$$P_l[\cos(\pi-\epsilon)] \approx J_0(\beta\epsilon). \tag{5.22}$$

Similar considerations have been made by Van de Hulst (Refs. 6; 7, p. 253), who also observed that (5.20) would explain the slow intensity decrease at large angles, in contrast with ordinary diffraction coronae, for which

$$i(\theta) \propto J_1^2(\beta\theta)/(\beta\theta)^2. \tag{5.23}$$

In the former case, i decreases like $(\beta\epsilon)^{-1}$; in the latter, like $(\beta\theta)^{-3}$.

The ratios of dark-ring radii according to (5.20) are given by the ratios of zeros of $J_0(x)$:

$$\epsilon_1/\epsilon_2 \approx 0.44, \quad \epsilon_3/\epsilon_2 \approx 1.6. \tag{5.24}$$

These results are compatible with (5.2), and (5.3) is also verified, although the comparison is not too significant, because we are considering a scalar theory. For the same reason we cannot discuss feature (c).

(d) The observed variability of the glory pattern must be related to the variability of the average radius and the dispersion in the radii of water droplets in thin clouds or mist, and their evolution as a function of time. It is an indication that the back-scattered intensity is extremely sensitive to small variations in the parameter β. Thus, it is a consequence of feature (f), and it should be explained together with this feature.

In order to compare (5.18) with features (e)–(g), we have to consider its detailed behavior as a function of β, in the range $10^2 \leqslant \beta \leqslant 10^3$, and within a small interval of variation of β,

$$\beta = \beta_0 + \delta\beta, \quad |\delta\beta| \leqslant 1, \quad |\delta\beta|/\beta_0 \ll 1. \tag{5.25}$$

It follows that

$$\beta^{\frac{1}{3}} \approx \beta_0^{\frac{1}{3}} + \frac{1}{3}\frac{\delta\beta}{\beta_0^{\frac{2}{3}}} \tag{5.26}$$

may actually be replaced by $\beta_0^{\frac{1}{3}}$ in (5.18).

Thus, (5.18) may be rewritten as

$$f(\beta_0 + \delta\beta, \pi - \epsilon) \approx A[1 + B\exp(-0.45i\delta\beta) + C\exp(-5.77i\delta\beta)], \quad |B| \leqslant \tfrac{1}{2}, \quad |C| \leqslant \tfrac{1}{4} \quad (10^2 \leqslant \beta_0 \leqslant 10^3, |\delta\beta| \leqslant 1), \tag{5.27}$$

where A, B, and C are complex parameters depending on β_0, which remain approximately constant within the above interval $\delta\beta$. The first term within the square brackets arises from the dominant term $f_{2,\mathrm{res}}$ in (5.16), the second one from $f_{2,g}$ and the third one from $f_{0,g}$.

It is clear that (5.27) cannot explain features (e)–(g). Instead of a quasiperiodic pattern, with period given by (5.4), and rapid intensity variations, by factors of up to 100, (5.27) describes two much less prominent modulations, resulting from the interference between geometrical-optic and surface-wave contributions. The largest modulation corresponds to a much greater period ($\sim$14) and a much smaller intensity variation (by less than a factor of 4).

While (5.17) is only a rough approximation for $\beta \sim 10^2$, the more exact evaluation of the residue series that will now be undertaken cannot account for the discrepancy between (5.27) and features (e)–(g). Thus, these features must arise from the interference with surface-wave contributions to higher-order terms in the Debye expansion. It will be shown in Sec. 6D that this is indeed the correct explanation.

D. The Residue-Series Contribution

For a more accurate evaluation of the residue-series contribution $f_{2,\mathrm{res}}$, we start from the exact expressions (3.18)–(3.20). We have to compute the terms appearing in (3.21).

The partial derivatives $\dot{d}$, $\ddot{d}$, and $\dddot{d}$ in (3.21) can be computed with the help of I, (A25)–(A27), (for the terms involving $[1\ \beta]$) and I, (A23) (for the terms involving $[2\ \alpha]$). The Hankel functions and their derivatives can be computed by means of I, (A11)–(A20).

By taking the logarithmic derivative of (3.20) with respect to λ, we find

$$\frac{\dot{c}_m}{c_m} = \frac{1}{\lambda} + i(2m+1)\pi + \frac{\dot{H}_\lambda^{(1)}(\alpha)}{H_\lambda^{(1)}(\alpha)} - 3\frac{\dot{H}_\lambda^{(2)}(\alpha)}{H_\lambda^{(2)}(\alpha)} - 2\frac{\dot{H}_\lambda^{(1)}(\beta)}{H_\lambda^{(1)}(\beta)} + \frac{[1\dot{\ }\beta] - N[1\dot{\ }\alpha]}{[1\ \beta] - N[1\ \alpha]} + \frac{\dot{P}_{\lambda-\frac{1}{2}}(-\cos\theta)}{P_{\lambda-\frac{1}{2}}(-\cos\theta)}, \tag{5.28}$$

and, differentiating once more with respect to λ,

$$\frac{\ddot{c}_m}{c_m} = \left(\frac{\dot{c}_m}{c_m}\right)^2 - \frac{1}{\lambda^2} + \psi\{H_\lambda^{(1)}(\alpha)\} - 3\psi\{H_\lambda^{(2)}(\alpha)\} - 2\psi\{H_\lambda^{(1)}(\beta)\} + \psi\{[1\ \beta] - N[1\ \alpha]\} + \psi\{P_{\lambda-\frac{1}{2}}(-\cos\theta)\}, \tag{5.29}$$

where we have introduced the notation

$$\psi\{f(\lambda)\} = \frac{\dot{\dot{f}}}{f} - \left(\frac{\dot{f}}{f}\right)^2. \tag{5.30}$$

In order to evaluate (3.20) and (5.28)–(5.29), we again employ the expansions given in I, Appendix A for $H_\lambda^{(1)}(\beta)$, $[1\ \beta]$ and their derivatives, the expansion N, (A16) for $H_\lambda^{(1,2)}(\alpha)$ and their derivatives (thus, $[1\ \alpha]$ is given by I, (A23) with $i \to -i$) and the expansion N, (C11) for $P_{\lambda-\frac{1}{2}}(-\cos\theta)$.

The numerical evaluation of $f_{2,\mathrm{res}}(\beta, \theta)$ has been carried out at the point $\beta = 130$, $\theta = \pi$, for $N = 1.33$. The first neglected term in all asymptotic expansions employed was $\mathcal{O}(\beta^{-2})$, and contributions from the first five poles λ_n were taken into account. The result is given by

$$f_{2,\mathrm{res}}(130, \pi) \approx -0.165 + 0.483i \quad (N = 1.33). \tag{5.31}$$

Comparing this with (5.14), we see that $f_{2,\mathrm{res}}$ is indeed dominant over the geometrical-optic contribution. The order of magnitude of (5.31) (but not the numerical value!) also agrees with the estimates made with the help of (5.18).

Adding (5.31) to (5.14), we find

$$f_{0,g}(130, \pi) + f_{2,g}(130, \pi) + f_{2,\mathrm{res}}(130, \pi) \approx -0.064 + 0.659i \quad (N = 1.33). \tag{5.32}$$

Comparing this with the exact result (5.15), we see that $f_{2,\mathrm{res}}$ corrects the phase in the right direction and leads to a value for $|f|$ of about 85% of the exact value (70% for the intensity). The remainder of the discrepancy must be accounted for by contributions from higher-order terms in the Debye expansion. The discussion given in Sec. 6 leads us to expect that, for other values of β, higher-order terms in the Debye expansion may account for a larger fraction of the intensity, and the relatively good agreement between (5.32) and (5.15) may be somewhat fortuitous. This should be checked by extending the computation to other values of β.

In conclusion, we see that Van de Hulst-type surface waves indeed give rise to an important contribution to the glory, but we must still investigate the effect of higher-order terms.

6. HIGHER-ORDER TERMS

A. Introduction

So far we have discussed only the first three terms in the Debye expansion I, (3.21). With regard to the remaining terms, the following questions may be asked: (i) Can they be evaluated by similar procedures? (ii) Do they give a significant contribution? (iii) Do they give rise to any new physical effects?

The answer to (i) is clearly affirmative. The higher the order of a term in the Debye expansion, the larger will be the number of associated saddle points and the number of regions to be treated. However, the techniques for the evaluation of higher-order terms are essentially the same as those developed for the first three terms, with only slight extensions required.

For $N = 1.33$, as has already been mentioned (I, Sec. 3C), more than 98.5% of the total intensity is contained in the first three terms. For higher values of N, geometrical-optic contributions decrease less rapidly with the order, because the internal reflection coefficient increases. However, the amplitude of the direct-reflection term also increases and the transmitted contribution becomes relatively less important. Thus, the first three terms probably suffice for most applications.

In the neighborhood of some special directions, higher-order terms can give appreciable contributions. Thus, for $N = 1.33$, the secondary rainbow (around $\theta = 128.7°$), though much fainter than the primary one, still has noticeable intensity. It can be treated by exactly the same method as the primary rainbow (Sec. 4A). We have also found indications that higher-order residue-series contributions may be important in the glory (Sec. 5C). We shall see that they give rise to the rapid fluctuations in intensity mentioned in Sec. 5A, and that this effect occurs in all directions, although the amplitude of the fluctuations is largest near the backward direction.

We shall confine our attention almost entirely to the backward and forward directions. The results are not limited to the range $1 < N < \sqrt{2}$. However, the cases $N > 1$ and $N < 1$ still require separate treatments.

B. Higher-Order Geometrical-Optic Contributions to $f(\beta, 0)$ and $f(\beta, \pi)$

The $(p + 1)$th term of the Debye expansion is given by I, (3.23) and I, (3.26). With the help of the reflection properties (2.2), as well as the identity I, (2.12), these representations may be rewritten in different ways, depending on whether p is even or odd:

$$\begin{aligned} f_{2j}(\beta, \theta) &= (-1)^{j+1} \frac{i}{\beta} \sum_{m=0}^{\infty} (-1)^m \\ &\quad \times \int_{-\infty}^{\infty} U \rho^{2j-1} P_{\lambda-\frac{1}{2}}(\cos\theta) e^{2i(m+j)\pi\lambda} \lambda \, d\lambda \\ &= (-1)^{j+1} \frac{i}{2\beta} \int_{-\infty+i\epsilon}^{\infty+i\epsilon} U(e^{i\pi\lambda}\rho)^{2j-1} P_{\lambda-\frac{1}{2}}(\cos\theta) \frac{\lambda \, d\lambda}{\cos(\pi\lambda)} \\ &= (-1)^{j} \frac{i}{2\beta} \int_{-\infty-i\epsilon}^{\infty-i\epsilon} U(e^{i\pi\lambda}\rho)^{2j-1} P_{\lambda-\frac{1}{2}}(\cos\theta) \frac{\lambda \, d\lambda}{\cos(\pi\lambda)} ; \end{aligned} \tag{6.1}$$

$$\begin{aligned} f_{2j+1}(\beta, \theta) &= \frac{(-1)^{j+1}}{\beta} \sum_{m=0}^{\infty} (-1)^m \\ &\quad \times \int_{-\infty}^{\infty} U(e^{i\pi\lambda}\rho)^{2j} P_{\lambda-\frac{1}{2}}(-\cos\theta) e^{i(2m+1)\pi\lambda} \lambda \, d\lambda \\ &= \frac{(-1)^{j+1}}{2\beta} \int_{-\infty+i\epsilon}^{\infty+i\epsilon} U(e^{i\pi\lambda}\rho)^{2j} P_{\lambda-\frac{1}{2}}(-\cos\theta) \frac{\lambda \, d\lambda}{\cos(\pi\lambda)} \\ &= \frac{(-1)^{j}}{2\beta} \int_{-\infty-i\epsilon}^{\infty-i\epsilon} U(e^{i\pi\lambda}\rho)^{2j} P_{\lambda-\frac{1}{2}}(-\cos\theta) \frac{\lambda \, d\lambda}{\cos(\pi\lambda)} . \end{aligned} \tag{6.2}$$

By procedures similar to those employed in (2.4)–(2.12), these results can also be written in the form

$$f_{2j}(\beta, \theta) = f_{2j,0}(\beta, \theta) + f_{2j,r}(\beta, \theta), \tag{6.3}$$

$$f_{2j+1}(\beta, \theta) = f_{2j+1,0}(\beta, \theta) + f_{2j+1,r}(\beta, \theta), \tag{6.4}$$

where

$$f_{2j,r}(\beta, \theta) = \frac{(-1)^j}{2\beta} \int_{-\infty - i\epsilon}^{\infty - i\epsilon} U(e^{i\pi\lambda}\rho)^{2j-1} \times e^{-i\pi\lambda} P_{\lambda-\frac{1}{2}}(-\cos\theta) \frac{\lambda\, d\lambda}{\cos(\pi\lambda)}, \tag{6.5}$$

$$f_{2j+1,r}(\beta, \theta) = \frac{(-1)^{j+1} i}{2\beta} \int_{-\infty - i\epsilon}^{\infty - i\epsilon} U(e^{i\pi\lambda}\rho)^{2j} \times e^{i\pi\lambda} P_{\lambda-\frac{1}{2}}(\cos\theta) \frac{\lambda\, d\lambda}{\cos(\pi\lambda)}, \tag{6.6}$$

$$\begin{aligned} f_{2j,0}(\beta, \theta) &= (-1)^j \frac{i}{\beta} \int_{-\infty - i\epsilon}^{\infty + i\epsilon} U(e^{i\pi\lambda}\rho)^{2j-1} \times e^{-i\pi\lambda} Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\, \lambda\, d\lambda \\ &= (-1)^{j+1} \frac{i}{\beta} \int_0^{\infty + i\epsilon} U(e^{i\pi\lambda}\rho)^{2j-1} \times P_{\lambda-\frac{1}{2}}(-\cos\theta) \tan(\pi\lambda)\, \lambda\, d\lambda, \end{aligned} \tag{6.7}$$

$$\begin{aligned} f_{2j+1,0}(\beta, \theta) &= (-1)^j \frac{i}{\beta} \int_{-\infty - i\epsilon}^{\infty + i\epsilon} U(e^{i\pi\lambda}\rho)^{2j} Q^{(2)}_{\lambda-\frac{1}{2}}(\cos\theta)\, \lambda\, d\lambda \\ &= (-1)^{j+1} \frac{i}{\beta} \int_0^{\infty + i\epsilon} U(e^{i\pi\lambda}\rho)^{2j} \times P_{\lambda-\frac{1}{2}}(\cos\theta) \tan(\pi\lambda)\, \lambda\, d\lambda. \end{aligned} \tag{6.8}$$

Note that (2.6)–(2.12) are particular cases of these results.

If we take $f_{2j,0}$ at $\theta = \pi$ and $f_{2j+1,0}$ at $\theta = 0$, the corresponding integrals (6.7), (6.8) have a saddle point at $\lambda = 0$. For $N < 2j$ and $N < 2j + 1$, respectively, the corresponding steepest-descent path makes an angle of $\pi/4$ with the positive λ-axis. The integrand differs from that of (2.12) only by powers of $e^{i\pi\lambda}\rho$, so that, according to Fig. 1 and I, Fig. 21, the path of integration can be deformed into the steepest-descent path.

Neglecting corrections of order β^{-1}, we can employ the approximations

$$\tan(\pi\lambda) \approx i, \tag{6.9}$$

$$U(\lambda, \beta) \approx \frac{4N}{(N+1)^2} \exp\left[2i(N-1)\beta - \frac{i\lambda^2}{N\beta}(N-1)\right], \tag{6.10}$$

$$e^{i\pi\lambda}\rho(\lambda, \beta) \approx -i \frac{(N-1)}{(N+1)} \exp\left(2iN\beta + \frac{i\lambda^2}{N\beta}\right), \tag{6.11}$$

valid near the saddle point.

The evaluation of the saddle-point contribution finally yields

$$f^{(c)}_{2j,0}(\beta, \pi) = -\frac{N^2}{N^2-1} \exp(-2i\beta) \times \frac{z^j}{\left(j - \frac{N}{2}\right)} [1 + \mathcal{O}(\beta^{-1})], \tag{6.12}$$

$$f^{(c)}_{2j+1,0}(\beta, 0) = \frac{N^2}{(N+1)^2} \exp[2i(N-1)\beta] \times \frac{z^j}{\left[j - \left(\frac{N-1}{2}\right)\right]} [1 + \mathcal{O}(\beta^{-1})], \tag{6.13}$$

where

$$z = \left(\frac{N-1}{N+1}\right)^2 \exp(4iN\beta). \tag{6.14}$$

Note that (5.12) and I, (5.48) are particular cases of these results.

The superscript (c) in (6.12) and (6.13) is to indicate that they represent contributions corresponding to the centrally incident ray in geometrical optics. The parameter z is identical to that which appears in the theory of the Fabry–Perot interferometer (Ref. 25, p. 47), representing the amplitude and phase change for double traversal of the sphere diameter. In general there may be other geometrical-optic contributions to the amplitude at $\theta = 0$ or π, arising from incident rays with nonzero impact parameters.

The total geometrical-optic contribution from central rays to the scattering amplitude at $\theta = \pi$ and $\theta = 0$ from higher-order terms in the Debye expansion is given by

$$\begin{aligned} f^{(c)}_{p>2,g}(\beta, \pi) &= \sum_{j=2}^{\infty} f^{(c)}_{2j,0}(\beta, \pi) \\ &= -\frac{N^2}{N^2-1} \exp(-2i\beta) \times \left[\varphi\left(z, \frac{N}{2}\right) - \frac{2z}{2-N}\right][1 + \mathcal{O}(\beta^{-1})], \end{aligned} \tag{6.15}$$

$$\begin{aligned} f^{(c)}_{p>2,g}(\beta, 0) &= \sum_{j=1}^{\infty} f^{(c)}_{2j+1,0}(\beta, 0) \\ &= \frac{N^2}{(N+1)^2} \exp[2i(N-1)\beta] \times \varphi\left(z, \frac{N-1}{2}\right)[1 + \mathcal{O}(\beta^{-1})], \end{aligned} \tag{6.16}$$

where

$$\varphi(z, \lambda) = \sum_{j=1}^{\infty} \frac{z^j}{(j - \lambda)} \quad (|z| < 1, \lambda \neq 1, 2, 3, \cdots). \tag{6.17}$$

This function is related to Lerch's transcendent[26]

$$\Phi(z, s, \alpha) = \sum_{n=0}^{\infty} \frac{z^n}{(n + \alpha)^s} \quad (|z| < 1, \alpha \neq 0, -1, -2, \cdots) \tag{6.18}$$

by

$$\varphi(z, \lambda) = \Phi(z, 1, -\lambda) + \lambda^{-1}. \tag{6.19}$$

For $N = 1.33$, we have $|z| \approx 0.02$, so that (6.15) is a very small correction. For instance,

$$f^{(c)}_{p>2,g}(130, \pi) \approx -0.0007 + 0.0001i, \tag{6.20}$$

is to be compared with (5.14). As mentioned in Sec. 5B, the correction is negligible.

C. Higher-Order Residue-Series Contributions to $f(\beta, \pi)$ for $N > 1$

The residue-series contribution at the poles λ_n to $f_p(\beta, \pi)$ is of the form

$$f_{p,\mathrm{res}}(\beta, \pi) = -\frac{2\pi i^r}{\beta} \sum_{m=0}^{\infty} (-1)^m \times \sum_n \text{residue } [\lambda U \rho^{p-1} e^{i(2m+s)\pi\lambda}]_{\lambda_n}, \tag{6.21}$$

where r and s are integers related to p, that have to be determined by detailed study of the deformation of the path of integration in (6.2), (6.5) near $\theta = \pi$. According to (3.12) and I, (5.7), we have

$$r = s = 1 \quad \text{for} \quad p = 1, \quad p = 2. \tag{6.22}$$

We shall evaluate only the dominant high-frequency contribution to (6.21). Thus, we restrict ourselves to the term $m = 0$ and we keep only the lowest-order term in each asymptotic expansion. The result, like (5.17), is certainly not a good approximation for $\beta \sim 10^2$, although it does yield the right order of magnitude. However, it is adequate for a qualitative discussion of the effects due to higher-order terms. For an accurate numerical computation, techniques similar to those employed in Sec. 5D would be required.

[26] W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, Berlin, 1966), 3rd ed., p. 32.

Substituting $U(\lambda, \beta)$ and $\rho(\lambda, \beta)$ by their explicit expressions, we find [cf. (3.18)–(3.20)]

$$f_{p,\mathrm{res}}(\beta, \pi) \approx (-1)^{p+1} i^r \frac{32}{\pi\beta^3} \sum_n r_{n,p}, \tag{6.23}$$

where

$$r_{n,p} = \text{residue} \left\{ \frac{c_p(\lambda, \beta)}{[d(\lambda, \beta)]^{p+1}} \right\}_{\lambda_n}, \tag{6.24}$$

$$c_p(\lambda, \beta) = \frac{\lambda e^{is\pi\lambda} [H^{(1)}_\lambda(\alpha)]^{p-1}}{[H^{(1)}_\lambda(\beta)]^2 [H^{(2)}_\lambda(\alpha)]^{p+1}} ([1\ \beta] - N[1\ \alpha])^{p-1}, \tag{6.25}$$

and $d(\lambda, \beta)$ is given by (3.19).

The evaluation of the dominant term in $r_{n,p}$ is carried out in Appendix C. Substituting the result, given by (C26), in (6.23), we get

$$f_{p,\mathrm{res}}(\beta, \pi) \approx i^{r+1} \frac{e^{i\pi/3}}{\gamma} \exp\left[ip\left(2M\beta - \frac{\pi}{2}\right)\right] L_p^{(-1)}\left(\frac{-2\zeta_p}{M}\right) \times \sum_n (a'_n)^{-2} \exp(i\lambda_n\zeta_p)[1 + \mathcal{O}(\gamma^2)], \tag{6.26}$$

where $L_p^{(-1)}$ is a generalized Laguerre polynomial, defined by (C24), and M and ζ_p are defined by (2.38) and (C19), respectively. The value of the integers in (6.21) and (C19) is determined by the requirement that ζ_p corresponds to an angle between 0 and 2π,

$$\zeta_p \equiv \pi - p\theta_t \,(\mathrm{mod}\, 2\pi), \quad 0 \leq \zeta_p < 2\pi. \tag{6.27}$$

In particular, for $p = 1$ and $p = 2$, it follows from (6.22) that (6.26) is in agreement with I, (5.20), and with the extension of (3.46) to $\theta = \pi$. Similarly to I, (5.24), and to (3.24), the above result can also be rewritten as follows [cf. (C24)]:

$$f_{p,\mathrm{res}}(\beta, \pi) \approx i^{r+1} e^{i\pi/4} (2\pi\beta)^{\frac{1}{2}} \exp\left[ip\left(2M\beta - \frac{\pi}{2}\right)\right] \times \sum_n D_n^2 D_{21} D_{12} \Big[(\tilde{R}_{11})^{p-1} \zeta_p + (p-1)(\tilde{R}_{11})^{p-2} D_{12} D_{21} \frac{\zeta_p^2}{2!} + \frac{(p-1)(p-2)}{2!} (\tilde{R}_{11})^{p-3} (D_{12}D_{21})^2 \frac{\zeta_p^3}{3!} + \cdots + (D_{12}D_{21})^p \frac{\zeta_p^p}{p!} \Big] \times \exp(i\lambda_n\zeta_p)[1 + \mathcal{O}(\gamma^2)], \tag{6.28}$$

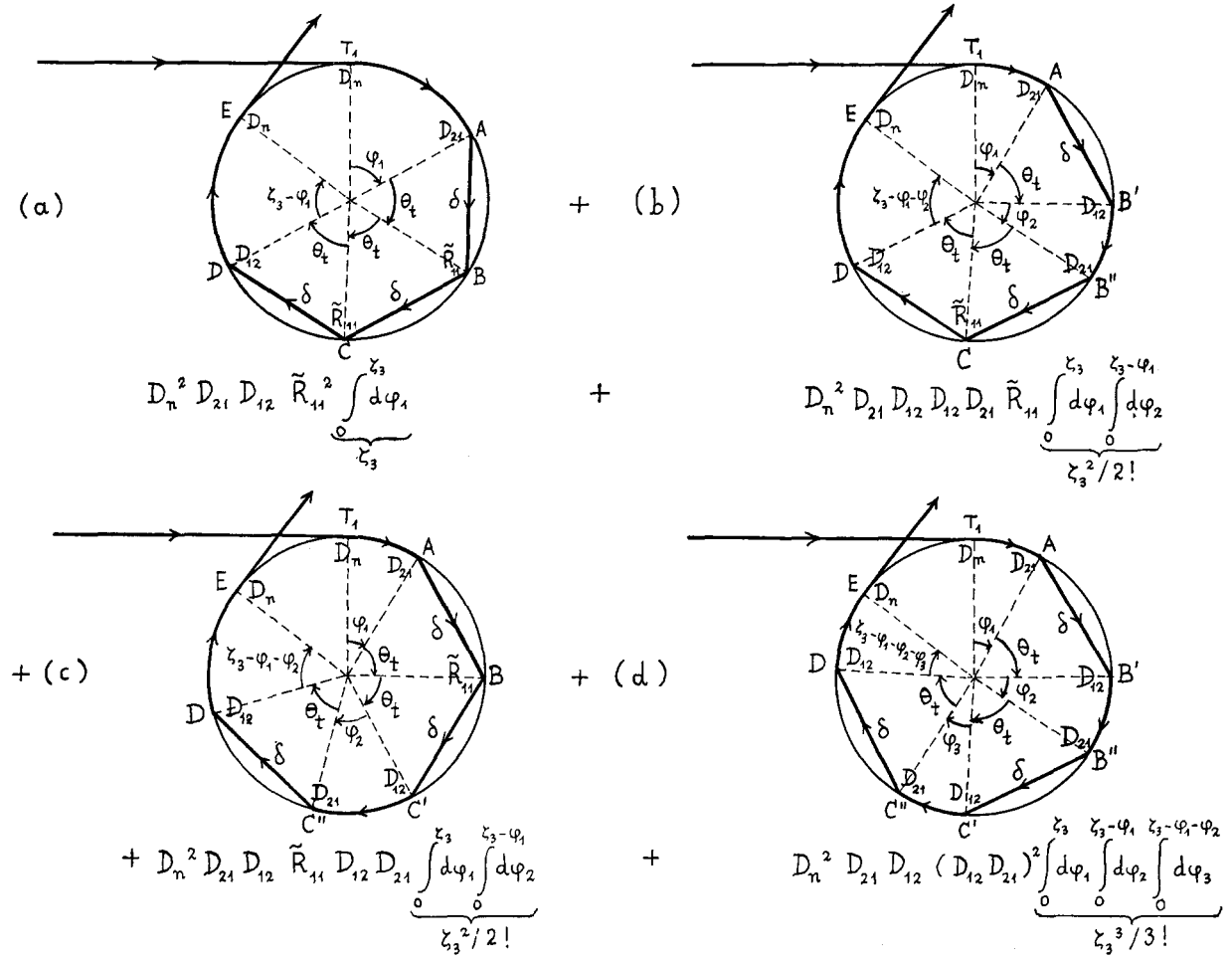


FIG. 10. Physical interpretation of (6.28) for $p = 3$. The four types of diagram that contribute in this case are shown, together with the contribution from each type. The diffraction, transmission, or reflection coefficients at each vertex are indicated. The total angle described along the surface is ζ_3. There is a phase factor exp $(3i\delta)$, where $\delta = 2M\beta$ is the optical phase difference associated with each "shortcut."

where D_n^2 is given by (3.25), $D_{21}D_{12}$ by (3.26) and $\tilde{R}_{11} = 1$, as in (3.27). An equivalent result for a cylinder was obtained by Chen [Ref. 9, Eq. (1.33)], by applying the geometrical theory of diffraction.

The physical interpretation of (6.28) is a generalization of that given in Fig. 7 for $p = 2$. The terms which arise for $p = 3$ are shown in Fig. 10. For simplicity, this figure is drawn for a scattering angle $\theta \neq \pi$. Referring to this figure as an illustration, we can describe the physical interpretation of each term in (6.28).

As has been emphasized in I, Sec. 3A, the Debye expansion corresponds to a description in terms of surface interactions, and its pth term represents the effect of $(p + 1)$ interactions at the surface. For a surface wave, one of them is its excitation at the point T_1 (with diffraction coefficient D_n) and final reconversion into a tangentially emerging ray at E (again with coefficient D_n). Another one is the initial critical refraction into the sphere at A (coefficient D_{21}) and final reemergence at D (factor D_{12}). These two interactions account for the common factor $D_n^2 D_{21} D_{12}$ in (6.28).

Once inside the sphere, there remain $(p - 1)$ interactions at the surface. Each of them can belong to either one of two types [cf. Figs. 7(c), 7(d)]: (I), internal reflection, with coefficient $\tilde{R}_{11}$; (II), critical refraction to the outside (coefficient D_{12}), followed by traveling along an arc as a surface wave, and by a new critical refraction into the sphere (coefficient D_{21}). These two types of elementary interactions are illustrated in Fig. 11. Each of them can be regarded as a "vertex," provided that the path V′V″ traveled along the surface for a type-II vertex is separately taken into account. The "coupling constant" associated with a type-I vertex is $\tilde{R}_{11}$, and for a type-II vertex it is $D_{12}D_{21}$. With this interpretation, the terms of (6.28) correspond to diagrams with $(p - 1)$ "internal"

FIG. 11. The two possible types of elementary interactions of a diffracted ray at the surface ("vertices") and the corresponding "coupling constants."

vertices, besides the two "external" ones already described above. An equivalent way to classify them is that they are all associated with p shortcuts across the sphere.

The simplest diagram with $(p-1)$ internal vertices is one with $(p-1)$ type-I vertices [Fig. 10(a)]. Diagrams of this kind can have any value for the angle φ_1 between 0 and ζ_p, so that they contribute

$$(\tilde{R}_{11})^{p-1}\int_0^{\zeta_p} d\varphi_1 = (\tilde{R}_{11})^{p-1}\zeta_p,$$

which is the first term within square brackets in (6.28).

If we now substitute one type-I vertex in each diagram of the above class by a type-II vertex, there are $(p-1)$ different ways to do this [Figs. 10(b), (c)], so that we get a contribution [cf. (3.29)]

$$(p-1)(\tilde{R}_{11})^{p-2}D_{12}D_{21}\int_0^{\zeta_p} d\varphi_1\int_0^{\zeta_p-\varphi_1} d\varphi_2 = (p-1)(\tilde{R}_{11})^{p-2}D_{12}D_{21}\frac{\zeta_p^2}{2!},$$

which is the second term in (6.28).

Similarly, if we substitute two type-I vertices by type-II vertices, this can be done in $(p-1)(p-2)$ ways, but an interchange between the two type-II vertices leaves the result unchanged, so that this class of diagrams [Fig. 10(d)] contributes

$$\frac{(p-1)(p-2)}{2!}(\tilde{R}_{11})^{p-3}(D_{12}D_{21})^2 \times\int_0^{\zeta_p} d\varphi_1\int_0^{\zeta_p-\varphi_1} d\varphi_2\int_0^{\zeta_p-\varphi_1-\varphi_2} d\varphi_3,$$

which is the third term in (6.28)—and so on.

The "propagator" between two vertices is either $\exp(2iM\beta)$, the phase factor associated with a shortcut, or $\exp(i\lambda_n\phi_j)$, the damping factor for a surface wave along the angle ϕ_j. Since there are p shortcuts and the total angle described along the surface is ζ_p, this leads to the factor $\exp(2ipM\beta)\exp(i\lambda_n\zeta_p)$ in (6.28). The factors $\exp(-i\pi/2)$ represent the phase delay associated with passage through the focal points for diffracted rays at the poles.

It also follows from the above argument that, for an angle θ such that $\pi-\theta \gg \beta^{-\frac{1}{2}}$, the dominant terms of the residue-series contribution at high frequencies must be of the form

$$f_{p,\mathrm{res}}(\beta,\theta) = f^{+}_{p,\mathrm{res}}(\beta,\theta) + f^{-}_{p,\mathrm{res}}(\beta,\theta), \quad (6.29)$$

where

$$f^{\pm}_{p,\mathrm{res}}(\beta,\theta) = \frac{i^{n_\pm}}{(\sin\theta)^{\frac{1}{2}}}\exp(2ipM\beta) \times\sum_{m=0}^{\infty}(-1)^m\sum_n D_n^2 D_{21}D_{12}\Big[(\tilde{R}_{11})^{p-1}\zeta^{\pm}_{m,p} + (p-1)(\tilde{R}_{11})^{p-1}D_{12}D_{21}\frac{(\zeta^{\pm}_{m,p})^2}{2!} + \cdots + (D_{12}D_{21})^{p-1}\frac{(\zeta^{\pm}_{m,p})^p}{p!}\Big]\exp(i\lambda_n\zeta^{\pm}_{m,p}) \quad (\pi-\theta \gg \beta^{-\frac{1}{2}}), \quad (6.30)$$

where $n_\pm$ is an integer and

$$\zeta^{\pm}_{m,p} = \zeta^{\pm}_p + 2m\pi, \quad (6.31)$$

the angles $\zeta^{\pm}_p$ being the minimum angles described by surface waves excited at T_1 or T_2 (Fig. 7) before emerging in the direction θ. In (6.30), waves making any number of turns around the sphere have been added, but usually only $m=0$ needs to be taken into account. The difference between the factors appearing in (6.28) and (6.30) corresponds to the replacement [cf. N, (C8)]

$$P_{\lambda-\frac{1}{2}}(1) = 1 \to P_{\lambda-\frac{1}{2}}(-\cos\theta) \approx (2\pi\beta\sin\theta)^{-\frac{1}{2}} \times\left\{\exp\left[i\lambda(\pi-\theta)-i\frac{\pi}{4}\right] + \exp\left[-i\lambda(\pi-\theta)+i\frac{\pi}{4}\right]\right\}. \quad (6.32)$$

The extra factor $\beta^{\frac{1}{2}}$ in (6.28) is a measure of the focusing effect along the axis. Note that (3.24) is a particular case of (6.29).

D. Higher-Order Effects in the Glory

In order to discuss the effect of the higher-order contributions (6.26), the first question that must be answered is: How many such contributions need to be taken into account? The slow convergence of the Debye expansion for residue-series contributions, arising from the high internal reflection coefficient (3.27), is apparent from (6.28).

Let us investigate the asymptotic behavior of (6.26) for large p. The asymptotic behavior of $L_p^{(-1)}(-x)$ for large p and fixed x is given by[27]

$$L_p^{(-1)}(-x) = \sqrt{\frac{x}{p}}\, e^{-x/2}\Big\{I_1[2(px)^{\frac{1}{2}}] + \frac{x}{4p} I_3[2(px)^{\frac{1}{2}}] + \cdots\Big\}, \quad (6.33)$$

where $I_n(z)$ is the modified Bessel function of order n. In particular, if $\sqrt{px} \gg 1$, (6.33) becomes

$$L_p^{(-1)}(-x) = \frac{x^{\frac{1}{4}} e^{-x/2}}{2(\pi)^{\frac{1}{2}} p^{\frac{3}{4}}} \exp\,[2(px)^{\frac{1}{2}}]\left[1 + \mathcal{O}\left(\frac{1}{(px)^{\frac{1}{2}}}\right)\right] \quad [(px)^{\frac{1}{2}} \gg 1]. \quad (6.34)$$

Under these conditions, (6.26) becomes

$$f_{p,\mathrm{res}}(\beta, \pi) \approx \frac{i^{r+1} e^{i\pi/3}}{2(\pi)^{\frac{1}{2}}\gamma}\left(\frac{2\zeta_p}{M}\right)^{\frac{1}{4}} p^{-\frac{3}{4}} \times \exp\left[2^{\frac{3}{2}}\left(\frac{p\zeta_p}{M}\right)^{\frac{1}{2}} + ip\left(2M\beta - \frac{\pi}{2}\right)\right] \times \sum_n (a_n')^{-2} \exp\left[i\left(\lambda_n + \frac{i}{M}\right)\zeta_p\right] \times [1 + \mathcal{O}(\gamma^2)] \quad [(p\zeta_p/M)^{\frac{1}{2}} \gg 1]. \quad (6.35)$$

It would appear from this result that $|f_{p,\mathrm{res}}|$ is unbounded as $p \to \infty$. However, it must be remembered that (6.26) is the dominant term in an asymptotic expansion for *fixed* p and sufficiently large β, whereas we are now interested in the asymptotic behavior for *fixed* β and increasingly large p. Since the number of correction terms [indicated in (6.26) as $\mathcal{O}(\gamma^2)$] also increases with p, (6.26) eventually no longer represents the dominant term for sufficiently large p: It is modified by the accumulated effect of a large number of correction terms (e.g., γ^{-2} terms, each of order γ^2).

We shall now give a heuristic argument to show that the resultant effect due to correction terms must be to bring about an exponential damping factor for large p. To see this, let us go back to the discussion of the rate of convergence of the Debye expansion in I, Sec. 3A. In terms of the partial-wave series, the Debye expansion I, (3.21) can be rewritten as follows:

$$f(\beta, \pi) - f_0(\beta, \pi) = -\frac{i}{\beta}\sum_{l=0}^{\infty}(-1)^l(l + \tfrac{1}{2})U_l\sum_{p=1}^{\infty}(\rho_l)^{p-1}, \quad (6.36)$$

where

$$U_l(\beta) = U(l + \tfrac{1}{2}, \beta), \quad \rho_l(\beta) = \rho(l + \tfrac{1}{2}, \beta). \quad (6.37)$$

According to the discussion given in Sec. 5C, the residue-series contributions are associated with partial waves in the edge domain [cf. I, (1.14)], so that, at least in order of magnitude, we can identify

$$f_{p,\mathrm{res}}(\beta, \pi) \sim -\frac{i}{\beta}\sum_{l=l_-}^{l_+}(-1)^l(l + \tfrac{1}{2})U_l(\rho_l)^{p-1}, \quad (6.38)$$

where l_- and l_+ are given by (5.21). Thus, the rate of convergence of the Debye expansion for the residue-series contributions is determined by the magnitude of the spherical reflection coefficient $|\rho_l|$ in the edge domain (5.21).

It follows from I, (3.15) and I, (3.8)–(3.11), that

$$|\rho_l|^2 = 1 - \frac{16}{\pi^2\beta^2} \times |H_{l+\frac{1}{2}}^{(1)}(\beta)H_{l+\frac{1}{2}}^{(2)}(\alpha)([1\,\beta] - N[2\,\alpha])|^{-2}. \quad (6.39)$$

Substituting the Hankel functions and their logarithmic derivatives by the corresponding asymptotic expansions in the edge domain (I, Appendix A), we finally get [cf. I, (4.58)]

$$|\rho_l|^2 \approx 1 - \frac{\gamma}{M}|\mathrm{Ai}\,(-z_l)|^{-2} = 1 - 2\epsilon_l \quad (l_- \lesssim l \lesssim l_+), \quad (6.40)$$

where

$$z_l = e^{-i\pi/3}\gamma(l + \tfrac{1}{2} - \beta), \quad (6.41)$$

so that $|z_l| = \mathcal{O}(1)$ in the edge domain.

On the other hand, it follows from I, (3.24), I, (3.5)–(3.8), and I, Appendix A, that

$$|U_l(\beta)| = |T_{21}T_{12}| \approx \frac{\gamma}{\pi M}|\mathrm{Ai}\,(-z_l)|^{-2} \quad (l_- \lesssim l \lesssim l_+). \quad (6.42)$$

[27] *The Bateman Manuscript Project: Higher Transcendental Functions, Vol. II*, A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, Eds. (McGraw-Hill Book Co., Inc., New York, 1953), p. 199.

Substituting these results in the remainder after P terms of (6.38), we find

$$\left|\sum_{p=P+1}^{\infty} f_{p,\mathrm{res}}(\beta,\pi)\right| \leqslant \frac{\gamma}{\pi M}\sum_{l=l_-}^{l_+}|\mathrm{Ai}\,(-z_l)|^{-2}\frac{|\rho_l|^P}{|1-\rho_l|}$$

$$\approx \frac{2}{\pi}\sum_{l=l_-}^{l_+}|\rho_l|^P \approx 2c\beta^{\frac{1}{3}}\bar{\rho}^P, \quad (6.43)$$

where

$$\bar{\rho} = 1-\epsilon, \quad \epsilon \sim \gamma, \quad (6.44)$$

is an average value of ρ_l in the edge domain, and c is defined by (5.21).

Finally, (6.43) becomes, for large enough P,

$$\left|\sum_{p=P+1}^{\infty} f_{p,\mathrm{res}}(\beta,\pi)\right| \leqslant 2c\beta^{\frac{1}{3}}(1-\epsilon)^P \sim 2c\beta^{\frac{1}{3}}e^{-\epsilon P}$$

$$\sim 2c\beta^{\frac{1}{3}}e^{-\gamma P}. \quad (6.45)$$

Comparing this with (5.18), we see that the remainder after P terms of the Debye expansion for the residue-series contributions is negligible, as compared with the second term $f_{2,\mathrm{res}}(\beta,\pi)$, if

$$P \sim \beta^{\frac{2}{3}}. \quad (6.46)$$

This gives the maximum number of terms that would have to be kept in the Debye expansion.

Actually, (6.46) is probably an overestimate. We can interpret (6.43) as implying that, due to the correction factors indicated in (6.26), the internal reflection coefficient for diffracted rays is brought down from its "geometrical-optic" value $\tilde{R}_{11} = 1$ to

$$\tilde{R}_{11} \sim \bar{\rho} = 1-\epsilon. \quad (6.47)$$

From (6.28), this is seen to imply that, in (6.26), we should make the replacement

$$L_p^{(-1)}\left(-\frac{2\zeta_p}{M}\right) \to \bar{\rho}^P L_p^{(-1)}\left(-\frac{2\zeta_p}{M\bar{\rho}}\right). \quad (6.48)$$

According to (6.45), the damping factor $\bar{\rho}^p$ becomes effective for $p \gtrsim \gamma^{-1}$, leading to the estimate

$$\beta^{\frac{1}{3}} \leqslant P \leqslant \beta^{\frac{2}{3}}. \quad (6.49)$$

Since the number of terms in (6.38) is $\sim\beta^{\frac{1}{3}}$, it might seem more expedient, in practice, to evaluate the residue-series contribution directly, by numerical summation of the edge-domain terms in the partial-wave expansion. This is related to a proposal made by Ljunggrén.[28] However, the objections to this procedure would be: (i) the identification (6.38) should be regarded merely as an order-of-magnitude estimate; (ii) it is difficult to determine the precise values of l_- and l_+ in (6.38), and the value of the sum undergoes considerable fluctuations as extra terms are added (cf. Ref. 8, Fig. 3); (iii) the physical interpretation in terms of surface waves enables us to understand the qualitative behavior of the results, as will now be seen.

In order to determine the resultant effect of higher-order surface-wave contributions, we have to sum the contributions (6.26) for all values of p, up to a maximum value P verifying (6.49). One of the main difficulties in this summation is the dependence of ζ_p on p, corresponding to the different position of the shadow boundary for each term of the Debye expansion.

We want to discuss the qualitative behavior of the resultant surface-wave contribution. For this purpose, an accurate evaluation is not required. We shall carry out the summation by making several simplifying assumptions:

(A) Only the contribution from the first pole λ_1 is taken into account.

This is certainly adequate for an order-of-magnitude evaluation. According to (6.26), the total residue-series contribution to the backward scattering amplitude is then given by

$$f_{\mathrm{res}}(\beta,\pi) \approx -\frac{e^{i\pi/3}}{a_1'^2\gamma}\Psi(N,\beta), \quad (6.50)$$

where

$$\Psi(N,\beta) = \sum_p \exp\left[ip\left(2M\beta-\frac{\pi}{2}\right)+i\lambda_1\zeta_p\right]$$

$$\times L_p^{(-1)}\left(-\frac{2\zeta_p}{M}\right). \quad (6.51)$$

The next problem is: Over what values of p does the sum range? In principle, we have to sum over all p, up to P. However, we can clearly restrict ourselves to the diffracted rays that emerge closest to the backward direction, because other contributions contain an extra damping factor of at least $\exp(i\lambda_n\theta_t)$, corresponding to an additional shortcut (cf. Fig. 10). Thus, in (6.27), we impose the extra condition

$$0 \leq \zeta_p < \theta_t. \quad (6.52)$$

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[28] T. Ljunggrén, Arkiv Fysik 1, 1 (1949).

TABLE I. Values of ζ_p for the lowest values of p.

$N = 1.33, \quad \theta_t = 1.43978$

p	2	6	10	15	19	24	28
ζ_p	0.26204	0.78612	1.31021	0.39452	0.91860	0.00029	0.52699

$N = 1.40, \quad \theta_t = 1.55039$

p	2	6	10	14	18	22	26
ζ_p	0.040819	0.12246	0.20410	0.28574	0.36738	0.44901	0.53065

The values of ζ_p satisfying the conditions (6.27), (6.52) for the lowest values of p are listed in Table I for $N = 1.33$ and for $N = 1.40$. The latter value is close to the critical refractive index $N = \sqrt{2}$, for which the diffracted rays are "at resonance." In fact, for $N = \sqrt{2}$, as shown in Fig. 12, a diffracted ray comes back to the starting point after each four additional shortcuts taken through the sphere. Moreover, in this limiting case, there are diffracted rays emerging exactly in the backward direction, i.e., with $\zeta_p = 0$, for

$$p = 4n + 2 \quad (n = 0, 1, 2, \cdots). \tag{6.53}$$

For $N = 1.40$, the angle ζ_2 corresponds to only 2.3°, as compared with 15° for $N = 1.33$. For $N = \sqrt{2}$, there are additional complications, as we see from Figs. 3(b), 3(c), for $p = 2$, because this is the borderline between having one ray or three rays near the backward direction; thus, a special treatment would be required.

There is another resonance, corresponding to a period of five shortcuts (inscribed regular pentagon instead of square), for

$$N = [\cos(\pi/5)]^{-1} \approx 1.236. \tag{6.54}$$

The value $N = 1.33$ is about halfway between this value and $N = \sqrt{2}$ (but still closer to $\sqrt{2}$), so that the corresponding values of p given by Table I:

$$p = 2, 6, 10, 15, 19, 24, 28, \cdots \quad (N = 1.33) \tag{6.55}$$

show a mixture of periodicities 4 and 5, with predominance of the period 4.

On the other hand, for $N = 1.40$, the values of p are of the form (6.53) up to $p = 74$. According to (6.49), larger values of p would not give any appreciable contribution within the range of values of β for which the glory is observed. Thus, we can make a further simplifying assumption:

(B) The summation in (6.51) is restricted to the values of p given by (6.53).

This is certainly a much better approximation for $N = 1.40$ than for $N = 1.33$, and it becomes better the closer N is to $\sqrt{2}$. The effect of deviations from assumption (B), like those found in (6.55), will be discussed later.

For $N = 1.40$, it follows from (6.30) and Table I that

$$\zeta_{4n+2} = (2n + 1)\zeta_2, \tag{6.56}$$

up to the same value of p for which (B) holds. Thus, it is consistent with (B) to assume also that

(C) The angles ζ_{4n+2} are given by (6.56) for all n.

For large enough n, (6.56) will violate condition (6.52). In particular, the damping factor $\exp(i\lambda_1\zeta_p)$ in (6.51), which would be bounded by $|\exp(i\lambda_1\theta_t)|$, will decrease exponentially as $n \to \infty$, according to (6.56). However, for large values of n, where the exponential decrease becomes significant, there would be such a decrease anyway, arising from the multiple internal reflection factor $\tilde{p}^p$ [cf. (6.45)]. Thus, for N sufficiently close to $\sqrt{2}$, (C) is a reasonable assumption.

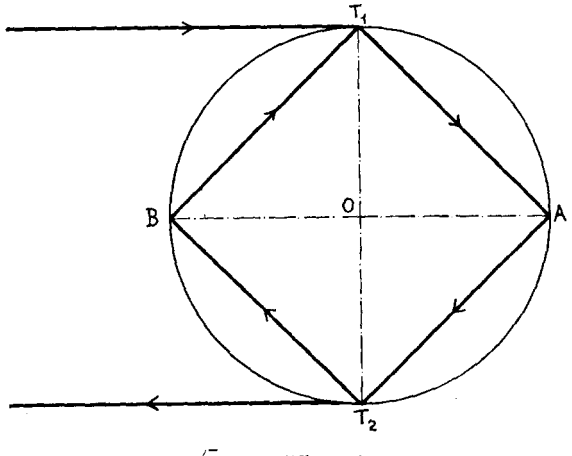


FIG. 12. For $N = \sqrt{2}$, the diffracted rays are at resonance: they come back to the starting point after four shortcuts, forming a square.

The last simplifying assumption we shall make is

(D) The angle ζ_p may be replaced by an average value $\bar{\zeta}$ in the argument of the Laguerre polynomial in (6.51):

$$L_p^{(-1)}(-2\zeta_p/M) \to L_p^{(-1)}(-x), \tag{6.57}$$

where

$$x = 2\bar{\zeta}/M \quad (0 \leq \bar{\zeta} < \theta_t). \tag{6.58}$$

Since the Laguerre polynomial is a slowly varying function of ζ_p as compared with $\exp(i\lambda_1\zeta_p)$ [cf. (6.34)], assumption (D) is also reasonable for an order-of-magnitude evaluation.

The effect of the simplifying assumptions (A) to (D) is to replace (6.51) by

$$\Psi(N, \beta) \approx \Psi(x, \delta) = \sum_{n=0}^{\infty} e^{i(4n+2)\delta} L_{4n+2}^{(-1)}(-x), \tag{6.59}$$

where δ is a complex number given by

$$\delta = 2M\beta - \frac{\pi}{2} + \tfrac{1}{2}\lambda_1\zeta_2 + i\epsilon \quad (\operatorname{Im}\delta > 0). \tag{6.60}$$

The term $i\epsilon$ ($\epsilon > 0$) has been added to represent the effective damping due to other contributions. It corresponds mainly to the effect of the internal reflection coefficient $\tilde{\rho}$ [cf. (6.48)]. This source of damping would still be present even for $\zeta_2 = 0$ ($N = \sqrt{2}$), and it is, in fact, responsible for the convergence of the Debye expansion for the residue-series contributions, as we have seen above.

The main virtue of the approximation (6.59) is that $\Psi(x, \delta)$ can be evaluated exactly, with the help of the generating function for generalized Laguerre polynomials (Ref. 27, p. 242):

$$\sum_{p=0}^{\infty} L_p^{(\alpha)}(x) z^p = (1 - z)^{-\alpha-1} \exp\left(\frac{xz}{z-1}\right) \quad (|z| < 1). \tag{6.61}$$

Setting $\alpha = -1$ and $z = e^{i\delta}$ ($\operatorname{Im}\delta > 0$), we get [cf. (C24)–(C25)]

$$\Phi(x, \delta) = \sum_{p=0}^{\infty} e^{ip\delta} L_p^{(-1)}(-x) = \exp\left(\frac{xe^{i\delta}}{1 - e^{i\delta}}\right)$$
$$= \exp\left(-\frac{x}{2}\right) \exp\left(\frac{ix}{2}\cot\frac{\delta}{2}\right) \quad (\operatorname{Im}\delta > 0). \tag{6.62}$$

To get $\Psi(x, \delta)$, it suffices to take

$$\Psi(x, \delta) = \frac{1}{4}\left[\Phi(x, \delta) - \Phi\left(x, \delta + \frac{\pi}{2}\right) + \Phi(x, \delta + \pi) - \Phi\left(x, \delta + \frac{3\pi}{2}\right)\right], \tag{6.63}$$

so that

$$\Psi(x, \delta) = \tfrac{1}{4}\exp\left(-\frac{x}{2}\right) \times \left\{\exp\left(\frac{ix}{2}\cot\frac{\delta}{2}\right) + \exp\left(-\frac{ix}{2}\tan\frac{\delta}{2}\right) - \exp\left[\frac{ix}{2}\cot\left(\frac{\delta}{2} + \frac{\pi}{4}\right)\right] - \exp\left[-\frac{ix}{2}\tan\left(\frac{\delta}{2} + \frac{\pi}{4}\right)\right]\right\}. \tag{6.64}$$

In particular, if $\operatorname{Im}\delta$ is large, i.e.,

$$\exp(-\operatorname{Im}\delta) \ll 1, \tag{6.65}$$

we can employ the approximation

$$\tan\frac{\delta}{2} \approx i + 2\exp(-\operatorname{Im}\delta)\sin(\operatorname{Re}\delta), \tag{6.66}$$

so that (6.64) becomes

$$\Psi(x, \delta) \approx \tfrac{1}{2}\{\cos[xe^{-\operatorname{Im}\delta}\sin(\operatorname{Re}\delta)] - \cos[xe^{-\operatorname{Im}\delta}\cos(\operatorname{Re}\delta)]\}$$
$$\approx \frac{x^2}{4}\exp(-2\operatorname{Im}\delta)\cos(2\operatorname{Re}\delta)$$
$$= \frac{x^2}{4}\operatorname{Re}(e^{2i\delta}) \quad (e^{-\operatorname{Im}\delta} \ll 1,\ x \lesssim 1). \tag{6.67}$$

Let us study the behavior of $\Psi(x, \delta)$ as a function of δ. We have [cf. (6.59)]:

$$\Psi\left(x, \delta + \frac{\pi}{2}\right) = -\Psi(x, \delta), \tag{6.68}$$

so that it suffices to consider the interval

$$0 \leq \operatorname{Re}\delta < \pi/2. \tag{6.69}$$

The behavior of Ψ within this interval depends very sensitively on the magnitude of the damping, i.e., on $\operatorname{Im}\delta$.

For strong damping, $e^{-\operatorname{Im}\delta} \ll 1$, we have, by (6.67), $|\Psi| \ll 1$, and Ψ oscillates like $\cos(2\operatorname{Re}\delta)$. In the opposite extreme of weak damping, $\operatorname{Im}\delta \ll 1$, it follows from (6.64) that $|\Psi|$ has oscillations with rapidly-varying period within the interval (6.69), but it is still bounded by

$$|\Psi(x, \delta)| \lesssim 1. \tag{6.70}$$

We shall now discuss the implications of these results for the theory of the glory. It follows from (6.50) and (6.59) that

$$|f_{\text{res}}(\beta, \pi)| \approx 2.034(\beta/2)^{\frac{1}{3}}|\Psi(x, \delta)|. \tag{6.71}$$

On the other hand, according to Sec. 5, the intensity

in the glory is dominated by the residue-series contribution:

$$i(\beta, \pi) \approx |f_{\text{res}}(\beta, \pi)|^2. \tag{6.72}$$

Let us consider the behavior of $i(\beta, \pi)$ as a function of β. It follows from (6.68) and (6.71)–(6.72) that the intensity is a periodic function of Re δ, with period $\pi/2$. According to (6.60), the corresponding period $\Delta\beta$ in β, near $\beta = \beta_0$, is given by

$$\Delta\beta = \frac{\pi}{4M + \zeta_2\left(\dfrac{d \operatorname{Re} \lambda_1}{d\beta}\right)_{\beta_0}}. \tag{6.73}$$

Within the domain of validity of the approximation I, (3.29), for λ_1, this becomes

$$\Delta\beta \approx \frac{\pi}{4M + \zeta_2\left[1 + \dfrac{x_1}{12}\left(\dfrac{2}{\beta_0}\right)^{\frac{2}{3}}\right]} \quad (\beta_0^{\frac{1}{3}} \gg 1). \tag{6.74}$$

Notice that, actually, (6.71) is not strictly periodic in β, both because $\Delta\beta$ depends (not very strongly) on β and because Im δ also changes with β. Furthermore, the strict periodicity in Re δ follows from assumptions (B) and (C), which are not very good approximations for $N = 1.33$. However, we should still find a quasi-periodic pattern, with period given approximately by (6.73), superimposed on a more slowly varying background.

For $\beta_0 = 200$, $N = 1.333$, (6.74) gives

$$\Delta\beta \approx 0.83, \tag{6.75}$$

in excellent agreement with the corresponding value (5.4) found by Bryant and Cox.[8] This provides the explanation of feature (e) in the glory (Sec. 5A). We see that the quasiperiodicity arises from the proximity to the resonance situation shown in Fig. 12, with a return to nearly the original position after each four additional shortcuts.

Let us now turn to feature (f), the behavior of $i(\beta, \pi)$ within a single period. For $\beta_0 \approx 200$, $N = 1.33$, it follows from (6.60), I, (3.29) and Table I, that $e^{-\operatorname{Im}\delta} \sim 10^{-2} \ll 1$, so that (6.67) holds. According to (6.67), the total residue-series contribution has the same order of magnitude as the second term in the Debye expansion. As we have seen in Sec. 5C, this term accounts correctly for the order of magnitude of the intensity in the glory.

On the other hand, the relatively slow oscillations of $|\Psi|$ given by (6.67) do not agree with the behavior described in feature (f) (Sec. 5A). However, the assumptions made in the derivation of this result are violated for $N = 1.33$. In particular, assumptions (B) and (C), which led to strong damping of high-p contributions, are already violated for $p = 15$ and $p = 24$ (cf. Table I). The latter, in particular, corresponds to a very small ζ_p. According to (6.49), these terms are still significant for $\beta_0 \sim 200$. In view of (6.33)–(6.35), their contributions can be quite large, and they probably account for the large spikes in the backward intensity; e.g., the interference between $p = 2$ and $p = 15$ may give rise to narrow peaks. The irregular behavior of the intensity within a period is thus related to the mixture of periodicities 4 and 5 in (6.55).

As N approaches closer to the resonance at $\sqrt{2}$, the assumptions leading to (6.71) become increasingly better justified. The damping also decreases with ζ_2 [cf. (6.60)], so that (6.64) should be applied. Thus we should find a number of oscillations with rapidly varying period within a single interval $\Delta\beta$. The character of these oscillations is strongly dependent on the damping, i.e., on the deviation of the refractive index from resonance. This extremely sensitive dependence of the intensity on β and N explains feature (d) (Sec. 5A), the variability of the glory.

The ratio of the surface-wave contribution to $f(\beta, \pi)$ to the geometrical-optic contribution is roughly given by [cf. (5.19)]:

$$|f_{\text{res}}(\beta, \pi)/f_g(\beta, \pi)| \sim \beta^{\frac{1}{3}} \exp(-\bar{\zeta} \operatorname{Re} \lambda_1), \tag{6.76}$$

but it can become much larger at resonance. However, by (6.70) and (6.71), the magnitude of the resonance peaks is bounded by

$$|f_{\text{res}}(\beta, \pi)| \leqslant \beta^{\frac{1}{3}}, \tag{6.77}$$

and this is also the upper bound for the ratio (6.76).

The origin of this upper bound can be understood by going back to the partial-wave series. By I, (2.1) and (6.38), we have

$$f_{\text{res}}(\beta, \pi) \approx \frac{1}{i\beta} \sum_{l=l_-}^{l_+} (-1)^l (l + \tfrac{1}{2})[S_l(k) - 1]. \tag{6.78}$$

The unitarity condition for the S matrix gives

$$|S_l(k) - 1| \leq 2, \tag{6.79}$$

where the extreme value 2 is attained when the lth partial wave is resonant. Substituting (6.79) in (6.78), and taking into account (5.21), we are led to an upper bound of the form (6.77).

Thus, the upper bound (6.77) corresponds to *saturation of the unitarity limit*. It would arise from having most partial waves within the edge domain

(5.21) close to resonance. This provides a link between the geometrical picture of diffracted-ray resonances illustrated in Fig. 12 and the more familiar concept of resonances in individual partial waves. The former are due to poles of the Debye expansion; the latter correspond to Regge poles close to the real axis [cf. I, Fig. 3 and the discussion about the physical interpretation of I, (2.34)–(2.35)]. The relationship between the two sets of poles and the two pictures is similar to that between the Debye expansion and the partial-wave description: surface-wave resonances can be regarded as a collective effect of many nearly-resonant partial waves, and conversely.

In conclusion, we see that higher-order surface-wave contributions are responsible for the main features of the glory that were left unexplained in Sec. 5 (quasiperiodicity, behavior within a period, and variability). All these effects are related to the existence of resonances like that shown in Fig. 12.

E. The Total Cross Section and the Ripple

Let us now go over to the forward scattering amplitude. According to I, (4.67), I, (5.48), and (6.16), it can be written in the following form:

$$f(\beta, 0) = f_d(\beta, 0) + f_F(\beta, 0) + f_g(\beta, 0) + \tilde{f}_{\text{res}}(\beta, 0), \tag{6.80}$$

where

$$f_d(\beta, 0) = i\beta/2 \tag{6.81}$$

is the contribution from the forward diffraction peak,

$$f_F(\beta, 0) = i\left[\frac{M_0}{\gamma} - \frac{i}{M} + \frac{8}{15}M_1\gamma - \frac{iM_0}{6}\frac{(4N^2-3)}{M^3}\gamma^2 + \mathcal{O}(\gamma^3)\right] \tag{6.82}$$

is the contribution from the Fock correction terms,

$$f_g(\beta, 0) = -\frac{2N^2}{(N-1)(N+1)^2}\exp[2i(N-1)\beta] \times \left\{1 + \frac{i}{\beta}\left[1 - \frac{1}{N} + \frac{1}{2(N-1)}\right] + \mathcal{O}(\beta^{-2})\right\} + \frac{N^2}{(N+1)^2}\exp[2i(N-1)\beta]\varphi\left(z, \frac{N-1}{2}\right) \tag{6.83}$$

is the geometrical-optic contribution (neglecting noncentral rays) and, finally, $\tilde{f}_{\text{res}}(\beta, 0)$ is the residue-series contribution.

In particular, taking $N = 1.33$, $\beta = 130$, we find

$$f_d(130, 0) + f_F(130, 0) + f_g(130, 0) \approx 65i + (-3.223 + 2.449i) + (1.081 + 1.644i) = -2.142 + 69.093i \quad (N = 1.33), \tag{6.84}$$

whereas the corresponding "exact" result, computed in the same way as (5.15), is

$$f(130, 0) = -2.529 + 68.988i \quad (N = 1.33). \tag{6.85}$$

Thus, the residue-series contribution must be given by

$$\tilde{f}_{\text{res}}(130, 0) \approx -0.387 - 0.105i \quad (N = 1.33). \tag{6.86}$$

Though smaller than the Fock and geometrical-optic contributions in (6.84), this still has comparable order of magnitude.

The total cross section is related to $f(\beta, 0)$ by the optical theorem:

$$\sigma_{\text{tot}} = \frac{4\pi a^2}{\beta}\,\text{Im}\, f(\beta, 0). \tag{6.87}$$

Taking into account (6.80)–(6.83), we find

$$\frac{\sigma_{\text{tot}}}{2\pi a^2} = 1 + \left\{\text{Re}\, M_0\gamma^2 + \tfrac{8}{15}\text{Re}\, M_1\gamma^4 + \frac{\text{Im}\, M_0}{6}\frac{(4N^2-3)}{M^3}\gamma^5\right\} + \frac{2N^2}{(N+1)^2\beta}\left\{-\frac{2}{N-1}\sin[2(N-1)\beta] + \text{Im}\left[e^{2i(N-1)\beta}\varphi\left(z, \frac{N-1}{2}\right)\right]\right\} + \frac{\sigma_{\text{res}}}{2\pi a^2} + \mathcal{O}(\beta^{-2}), \tag{6.88}$$

where the first term arises from the diffraction peak, the second and third ones (expressions within curly brackets) from the Fock and (central-ray) geometrical-optic contributions, and σ_{res} denotes the residue-series contribution.

The diffraction and Fock terms in (6.88) give rise to a slowly varying background which is monotonically decreasing, approaching the asymptotic value unity as $\beta \to \infty$. This leads to the well-known result that the asymptotic cross section is twice the geometrical cross section ($\sigma_{\text{tot}} \to 2\pi a^2$).

The geometrical-optic contribution gives rise to relatively slow oscillations with period

$$\Delta_1\beta = \frac{\pi}{N-1} \tag{6.89}$$

and amplitude decreasing like β^{-1}, superimposed on the background. These oscillations arise from interference between waves diffracted around the sphere and those geometrically transmitted through it. An analogous effect has been observed in neutron

scattering at energies of several million electron volts ("giant resonances"), and a similar explanation has been proposed.[29]

Very accurate numerical calculations of the total cross section, based on the partial-wave series and done at very small intervals, have shown, superimposed on these broad oscillations, a quasiperiodic structure, corresponding to rather irregular fluctuations with short period and variable amplitude. These secondary fluctuations are generally known as the "ripple" (Ref. 7, p. 177, Fig. 32[30]). Most calculations have been performed for $\beta \leqslant 20$, but the ripple also appears in Bryant and Cox's curves for σ_{tot} near $\beta = 200$ (Ref. 8, Fig. 2). Moreover, as has already been mentioned in Sec. 5A [feature (g)], these curves show a striking parallelism with the scattered intensity at 180°, with similar peaks, located at nearly the same values of β, but with greatly reduced amplitude. This parallelism strongly suggests that the ripple must correspond to the contribution from σ_{res} in (6.88).

Let us compute the contribution. According to I, (5.30), (3.38), and (6.21), the residue-series contribution to $f_p(\beta, 0)$ must be of the form

$$\tilde{f}_{p,\text{res}}(\beta, 0) = -\frac{2\pi}{\beta} i^{r-1} \sum_{m=0}^{\infty} (-1)^m \sum_n \text{residue}\, \{\lambda U \rho^{p-1} \times \exp[i(2m + s + 1)\pi\lambda]\}_{\lambda_n}, \quad (6.90)$$

where r and s are integers related to p, and (6.22) remains valid.

By comparison with (6.21), we see that the only difference in (6.90) is an additional factor $-ie^{i\pi\lambda}$. Thus, according to (6.26),

$$\tilde{f}_{p,\text{res}}(\beta, 0) \approx i^r \frac{e^{i\pi/3}}{\gamma} \times \exp\left[ip\left(2M\beta - \frac{\pi}{2}\right)\right] L_p^{(-1)}(-2\tilde{\zeta}_p/M) \times \sum_n (a_n')^{-2} \exp(i\lambda_n \tilde{\zeta}_p)[1 + \mathcal{O}(\gamma^2)], \quad (6.91)$$

where [cf. (6.30)]

$$\tilde{\zeta}_p \equiv 2\pi - p\theta_t \,(\text{mod } 2\pi), \quad 0 \leq \tilde{\zeta}_p < 2\pi. \quad (6.92)$$

In particular, for $p = 1$ and $p = 2$, (6.91) agrees with I, (5.32), and with the extension of (3.46) to $\theta = 0$ [cf. (6.32)].

[29] J. M. Peterson, Phys. Rev. **125**, 955 (1962); K. W. McVoy, L. Heller, and M. Bolsterli, Rev. Mod. Phys. **39**, 245 (1967); K. W. McVoy, Ann. Phys. (N.Y.) **43**, 91 (1967).

[30] P. Walstra, Proc. Koninkl. Nederl. Akad. Wetensch. **B67**, 491 (1964).

The dominant contributions arise from values of p such that [cf. (6.52)]

$$0 \leq \tilde{\zeta}_p < \theta_t. \quad (6.93)$$

For $N = 1.33$, this implies that the lowest value of p to contribute is $p = 4$. Employing (6.91) to estimate the order of magnitude of this contribution for $\beta = 130$, we find that it is of order unity, in agreement with (6.86).

For $N = 1.40$, up to large values of p, the dominant contributions arise from [cf. (6.53)]

$$p = 4n \quad (n = 1, 2, 3, \cdots), \quad (6.94)$$

whereas, for $N = 1.33$, we find deviations from (6.94) already for rather low values of p, as in Table I.

By employing assumptions similar to those made for the derivation of (6.50), we find

$$\tilde{f}_{\text{res}}(\beta, 0) = \sum_p \tilde{f}_{p,\text{res}}(\beta, 0) \approx -\frac{(-i)^r e^{i\pi/3}}{\gamma a_1'^2} \tilde{\Psi}(N, \beta), \quad (6.95)$$

where

$$\tilde{\Psi}(N, \beta) \approx \tilde{\Psi}(\tilde{x}, \delta) = \sum_{n=1}^{\infty} \exp(4in\delta) L_{4n}^{(-1)}(-\tilde{x}), \quad (6.96)$$

with

$$\tilde{x} = 2\tilde{\zeta}/M \quad (0 \leq \tilde{\zeta} < \theta_t), \quad (6.97)$$

where $\tilde{\zeta}$ is an average value of $\tilde{\zeta}_p$, and δ is given by the *same* expression (6.60). In fact, (6.56) is replaced by

$$\tilde{\zeta}_{4n} = n\tilde{\zeta}_4 = 2n\zeta_2, \quad (6.98)$$

with ζ_2 still given by (6.30).

It is readily seen, with the help of (C25), that (6.63)–(6.64) are replaced by

$$\begin{aligned}\tilde{\Psi}(\tilde{x}, \delta) &= \frac{1}{4}\left[\Phi(\tilde{x}, \delta) + \Phi\left(\tilde{x}, \delta + \frac{\pi}{2}\right) + \Phi(\tilde{x}, \delta + \pi) + \Phi\left(\tilde{x}, \delta + \frac{3\pi}{2}\right)\right] - 1 \\ &= \frac{1}{4}\exp\left(-\frac{\tilde{x}}{2}\right)\left\{\exp\left(\frac{i\tilde{x}}{2}\cot\frac{\delta}{2}\right) + \exp\left(-\frac{i\tilde{x}}{2}\tan\frac{\delta}{2}\right) + \exp\left[\frac{i\tilde{x}}{2}\cot\left(\frac{\delta}{2} + \frac{\pi}{4}\right)\right] + \exp\left[-\frac{i\tilde{x}}{2}\tan\left(\frac{\delta}{2} + \frac{\pi}{4}\right)\right]\right\} - 1. \quad (6.99)\end{aligned}$$

Instead of (6.68), we now have

$$\tilde{\Psi}\left(\tilde{x}, \delta + \frac{\pi}{2}\right) = \tilde{\Psi}(\tilde{x}, \delta). \quad (6.100)$$

Thus, $f_{\rm res}(\beta, 0)$, and consequently also the ripple, given by

$$\sigma_{\rm res} = \frac{4\pi a^2}{\beta} \operatorname{Im} f_{\rm res}(\beta, 0), \tag{6.101}$$

have the same quasiperiodicity in β as the intensity in the glory, with period given by (6.73)–(6.74).

For $N = 1.33$, the behavior of the cross section within one period is again determined by deviations from (6.94) at relatively low p. The type of deviation and the conditions for constructive interference are similar to those found for the back-scattered intensity. This explains the parallelism found by Bryant and Cox [feature (g), Sec. 5A].

Strictly speaking, the above results cannot be applied to the range $1 \leqslant \beta \leqslant 20$ for which most data on the ripple are available, since they are based upon asymptotic approximations that break down for such low β. However, we can try to employ them for a qualitative understanding of the behavior of the ripple within this range.

According to (6.49) and (6.94), the dominant contribution to the ripple for low β and $N = 1.33$ should arise from $p = 4$ (diffracted rays taking four shortcuts). It then follows from (6.91) and (6.101), again restricting ourselves to the contribution from the pole λ_1, that

$$\sigma_{\rm res} \sim A(\beta)\beta^{-\frac{2}{3}} \exp(-\tilde{\zeta}_4 \operatorname{Im} \lambda_1) \sin(4 \operatorname{Re} \delta + \chi), \tag{6.102}$$

where A is an amplitude factor, δ is given by (6.60), and χ is a constant phase.

As a function of β, (6.102) shows a sinusoidal behavior with variable amplitude. This agrees with the calculated curves up to $\beta \sim 10$.[30] As β increases, higher values of p start to contribute [cf. (6.49)] and deviations from the sinusoidal pattern should appear. Since the damping of the surface waves is not very strong for low β, interference with the contributions from values of p other than (6.94) and from poles other than λ_1 should also give rise to such deviations. This again agrees with the results of numerical calculations.[30]

The period of the oscillations, according to (6.102), is the same as that at 180°, given by (6.73). If we apply the approximation (6.74), neglecting the correction $\beta_0^{-\frac{2}{3}}$ in the denominator, we find

$$\Delta\beta \sim \frac{\pi}{4M + \zeta_2}, \tag{6.103}$$

if the dominant contribution arises from $p = 4$, as for $N = 1.33$. In general, for other values of N, (6.103) must be replaced by

$$\Delta\beta \sim \frac{2\pi}{2Mp + \tilde{\zeta}_p}, \tag{6.104}$$

where p is the lowest term that contributes. These results should not be very accurate at low β, since they are based upon the high-frequency approximation (6.74).

The expression (6.104) for the period was derived by Van de Hulst (Ref. 7, p. 377) on the basis of a model in which only the lowest p verifying (6.93) contributes. It was compared with the period observed in numerical calculations for $\beta \leqslant 20$ and several values of N, by Walstra.[30] It was found that (6.104) is in very good agreement with the data, although it predicts values systematically in excess of the observed ones.

This is exactly what should be expected. In fact, (6.104) should be replaced by a more accurate expression, corresponding to (6.73), and we have

$$d \operatorname{Re} \lambda_1 / d\beta > 1. \tag{6.105}$$

Physically, this corresponds to the fact that the phase velocity of the surface waves is slightly smaller than that in free space (they are delayed due to the curvature of the surface). This was not taken into account by Van de Hulst in his computation of the optical path difference.

No ripple is observed in the total cross section for $N < 1$,[30] and, indeed, none should be expected, as the diffracted rays cannot take any shortcuts through the sphere in this case (cf. Sec. 6F).

The present theory also leads us to predict that the ripple must be damped for an absorbing sphere (complex refractive index), and that the attenuation must increase with the absorption. This follows from the fact that each shortcut is then accompanied by absorption, i.e., $\operatorname{Im} \delta$ in (6.60) has an additional component due to absorption. This attenuation of the ripple has indeed been observed in numerical computations for complex N.[31]

For sufficiently small β ($\beta \leqslant 4$), the peaks in the ripple may be attributed to resonances in successively higher partial waves.[30] However, as β increases, more than one partial wave may be near resonance, and we finally come to the surface-wave model of the ripple. As we have seen in connection with the glory (Sec. 6D), the two pictures actually merge together, each effect in one description corresponding to a collective effect produced by several terms in the other one.

[31] D. Deirmendjian, R. Clasen, and W. Viezee, J. Opt. Soc. Am. **51**, 620 (1961).

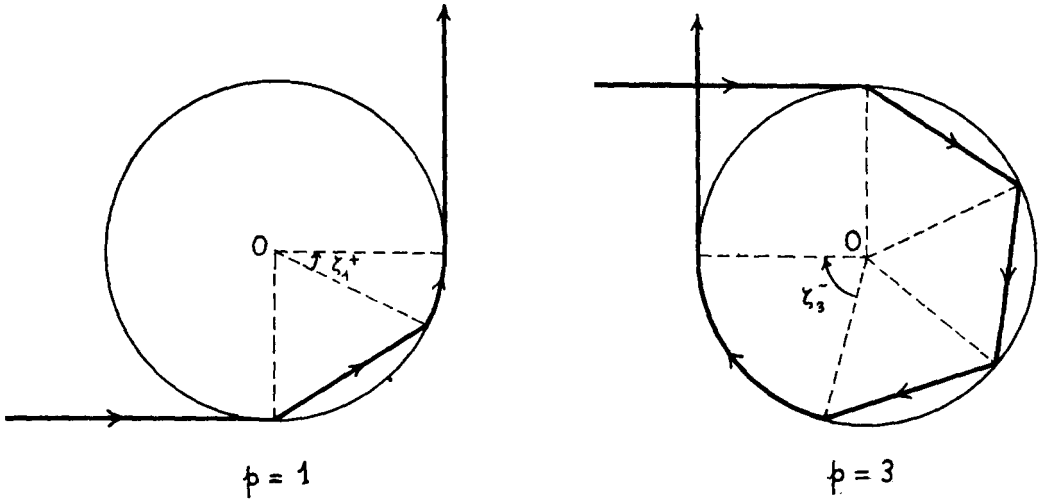


FIG. 13. The lowest-order residue-series contributions to the intensity at $\theta = 90°$.

Heretofore, we have restricted our discussion of higher-order surface-wave effects to the forward and backward directions. However, it is clear from (6.30) that similar ripple effects should also be observed in any other direction. For $\theta = 90°$, they have actually been found in Bryant and Cox's calculations, and the corresponding period is *twice* that found for $\theta = 0°$ and 180° (Ref. 8, Fig. 2).

The reason for this is indicated in Fig. 13, which shows the lowest-order contributions at 90° for $N = 1.33$: They correspond to $f^{+}_{1,\mathrm{res}}$ and $f^{-}_{3,\mathrm{res}}$ in (6.30). Instead of (6.53) and (6.94), the dominant contributions at 90° arise from $p = 2n + 1$ $(n = 0, 1, 2, \cdots)$, and the relative phase shift between successive contributions is $\frac{1}{2}$ Re δ, where δ is still given by (6.60). Thus, the period is $2\Delta\beta$, with $\Delta\beta$ given by (6.73). This completes the explanation of feature (g) for the glory (Sec. 5A).

We have seen that the amplitude of the ripple component relative to the remaining contributions to the scattering amplitude is at most of order $\beta^{-\frac{2}{3}}$ at $\theta = 0°$ [cf. (6.102)] and at most of order $\beta^{\frac{1}{3}}$ at $\theta = 180°$ [cf. (6.77)], where the ripple is the dominant term (glory). In other directions, far away from forward and backward, it follows from (6.30) [cf. also I, (5.32) and I (5.45)] that the relative amplitude of the ripple is of order $\beta^{-\frac{1}{6}}$. [This is related to the focusing factor $\beta^{\frac{1}{2}}$ in (6.32).]

Thus, *the relative amplitude of the ripple far away from the forward and backward directions is the geometric mean of the values found in these directions.* This is in good agreement with the estimates made by Penndorf.[10] From numerical calculations ranging up to $\beta \sim 400$, he found that the ripple is present in all directions (curves for $\theta = 10°$, 20°, and 40° are given), with increasing relative amplitude as θ increases from 0° to 180°, and he estimated the average amplitude as roughly 0.1 at 0°, 5 at 90°, and 500 at 180°.

We conclude, therefore, that the ripple is a very general phenomenon, that affects the intensity in any direction, but only becomes dominant near the backward direction, where it gives rise to the glory. It is a general manifestation of the resonance phenomena for diffracted rays discussed in Sec. 6D. A practical implication of this result for numerical calculations is that very closely spaced points in β are required for an accurate interpolation for the intensity in any direction.

F. Higher-Order Residue-Series Contributions to $f(\beta, \pi)$ for $N < 1$

Finally, let us consider the residue-series contributions to $f(\beta, \theta)$ for $N < 1$, e.g., at $\theta = \pi$. According to I, (5.8) and to (3.13), the contribution to $f_p(\beta, \pi)$ from the residue series at the poles $-\lambda'_n$ is of the form

$$f'_{p,\mathrm{res}}(\beta, \pi) = -\frac{2\pi i}{\beta}\sum_{m=0}^{\infty}(-1)^m \times \sum_n \text{residue}\,\{\lambda U(\rho e^{2i\pi\lambda})^{p-1} \times \exp[i(2m+1)\pi\lambda]\}_{-\lambda_n'}. \quad (6.106)$$

Taking into account (2.2) and restricting ourselves to $m = 0$, this becomes

$$f'_{p,\mathrm{res}}(\beta, \pi) \approx -\frac{2\pi i}{\beta}\sum_n \text{residue}\,(\lambda e^{-i\pi\lambda} U \rho^{p-1})_{\lambda_n'}. \quad (6.107)$$

Substituting U and ρ by their explicit expressions [cf. (3.20)], we find

$$f'_{p,\mathrm{res}}(\beta, \pi) \approx (-1)^{p+1} i\,\frac{32}{\pi\beta^3}\sum_n r'_{n,p}, \quad (6.108)$$

where

$$r'_{n,p} = \text{residue}\left\{\frac{c'_p(\lambda,\beta)}{[d(\lambda,\beta)]^{p+1}}\right\}_{\lambda_n'}, \tag{6.109}$$

$$c'_p(\lambda,\beta) = \frac{\lambda e^{-i\pi\lambda}[H_\lambda^{(1)}(\alpha)]^{p-1}}{[H_\lambda^{(1)}(\beta)]^2[H_\lambda^{(2)}(\alpha)]^{p+1}}([1\ \beta] - N[1\ \alpha])^{p-1}, \tag{6.110}$$

and $d(\lambda, \beta)$ is given by (3.19).

The evaluation of the dominant term in $r'_{n,p}$ is performed in Appendix D. Substituting the result, given by (D18), in (6.108), we finally get

$$f'_{p,\text{res}}(\beta,\pi) \approx 4i\pi\frac{N^2}{M'} \times \exp(-2iM'\beta)\sum_n \frac{1}{p!}[\mathfrak{D}_n(\pi-\theta)]^p \times \exp[-i\lambda'_n(\pi-\theta_t)][1+\mathcal{O}(\gamma^2)], \tag{6.111}$$

where, as in I, (4.76) and I, (5.67),

$$\theta_t = 2\cos^{-1}N, \tag{6.112}$$

$$\mathfrak{D}_n = \frac{e^{-i\pi/3}}{2\pi a_n'^2\gamma'}, \quad \gamma' = (2/\alpha)^{\frac{1}{3}}. \tag{6.113}$$

In particular, for $p = 1$, the result agrees with I, (5.64), and for $p = 2$ it agrees with the analytic continuation of (3.33) (extended to $\theta = \pi$) to $N < 1$. Actually, as is readily verified, (6.111) reduces to the residue series in I, (4.85), for $p = 0$, so that it can be employed even in that case.

The physical interpretation of (6.111) is a generalization of that given in I, Sec. 5E for $p = 1$. It is illustrated in Fig. 14 for $p = 3$. Since no shortcuts through the sphere are possible for $N < 1$, the only possible "elementary interaction" of the surface waves at any point of the surface, as they travel along on the inner side, is a kind of "internal diffraction," described by the internal diffraction coefficient $\mathfrak{D}_n$, each time they shed a ray to the outside region.

Since the shadow boundary S_1S_1' is the same for all terms in the Debye expansion, all surface waves describe the same total angle $\pi - \theta_t$ before emerging in the backward direction; in between, however, they can undergo any number of internal diffractions, and $f'_{p,\text{res}}$ corresponds to a term with p internal diffractions.

For instance, for $p = 3$ (Fig. 14), the corresponding contribution is proportional to

$$\mathfrak{D}_n^3\int_0^{\pi-\theta_t}d\varphi_1\int_0^{\pi-\theta_t-\varphi_1}d\varphi_2 \times\int_0^{\pi-\theta_t-\varphi_1-\varphi_2}d\varphi_3 = \mathfrak{D}_n^3\frac{(\pi-\theta_t)^3}{3!},$$

and for the general case this gives rise to the factor $[\mathfrak{D}_n(\pi - \theta_t)]^p/p!$ in (6.111). The physical interpretation of the remaining factors has already been given in I, Sec. 4E.

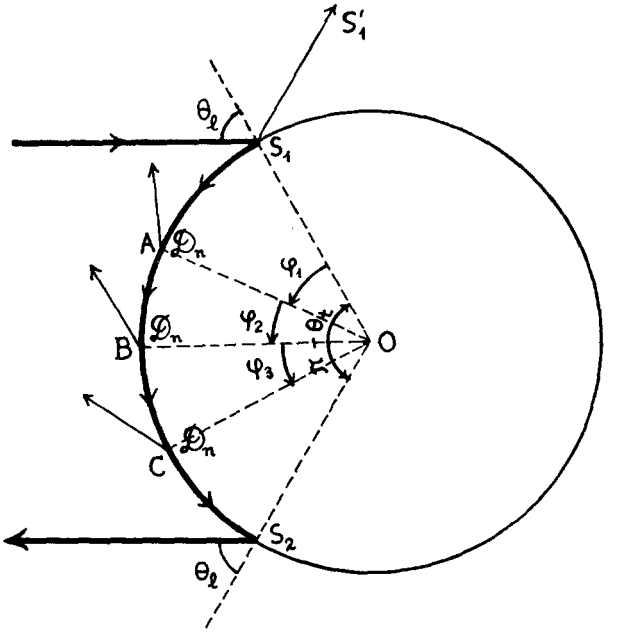


FIG. 14. Physical interpretation of (6.111) for $p = 3$. The only possible surface interaction of the diffracted rays as they travel along the surface on the inner side is "internal diffraction," described by the coefficient $\mathfrak{D}_n$, that can occur any number of times.

Since (6.111) is valid also for $p = 0$, the total (dominant) contribution to $f(\beta, \pi)$ from the residue series at the poles λ'_n is

$$f'_{\text{res}}(\beta,\pi) = \sum_{p=0}^{\infty} f'_{p,\text{res}}(\beta,\pi) \approx 4\pi i\frac{N^2}{M'}\exp(-2iM'\beta) \times\sum_n \exp[-i\lambda'_n(\pi-\theta_t)] \times\sum_{p=0}^{\infty}\frac{[\mathfrak{D}_n(\pi-\theta_t)]^p}{p!}[1+\mathcal{O}(\gamma^2)], \tag{6.114}$$

which can be rewritten as

$$f'_{\text{res}}(\beta,\pi) \approx 4\pi i\frac{N^2}{M'}\exp(-2iM'\beta) \times\sum_n \exp[-i\lambda''_n(\pi-\theta_t)][1+\mathcal{O}(\gamma^2)], \tag{6.115}$$

where

$$\lambda''_n = \lambda'_n + i\mathfrak{D}_n. \tag{6.116}$$

Thus, the total (dominant) effect of all residue-series contributions is equivalent to that from $p = 0$ [cf. I, (4.85)], but now evaluated with poles at shifted positions, given by (6.116). We can also say that the effect of higher-order contributions is to "renormalize" the phase velocities and damping constants of the surface waves.

In the approximation I, (3.35), for the poles,

$$\lambda_n' \approx \alpha + e^{-i\pi/3}\frac{x_n}{\gamma'} + i\frac{N}{M'}, \qquad (6.117)$$

the pole shift (6.116) corresponds to the replacement [cf. (6.113)]

$$x_n \to x_n + (i/2\pi a_n'^2). \qquad (6.118)$$

For large n, the correction term in (6.118) is $\mathcal{O}(n^{-\frac{1}{3}})$ [N, (D8)], but it has an appreciable effect for the lowest values of n, which are responsible for the dominant contribution.

In conclusion, we see that the behavior of the scattering amplitude for $N < 1$ is simpler in several respects than that for $N > 1$. The surface waves excited by the critically incident ray have the same shadow boundary for all terms in the Debye expansion, and they cannot make any shortcuts through the sphere. Their resultant effect, at least for the dominant term, can easily be summed (without the simplifying assumptions employed for $N > 1$), and leads simply to a renormalization of the propagation constants. There are no resonance effects, and, consequently, no ripple: the intensity in any direction, as well as the total cross section, have a much smoother behavior than for $N > 1$. In the quantum-mechanical interpretation we can say that a repulsive interaction leads to a simpler structure than an attractive one.

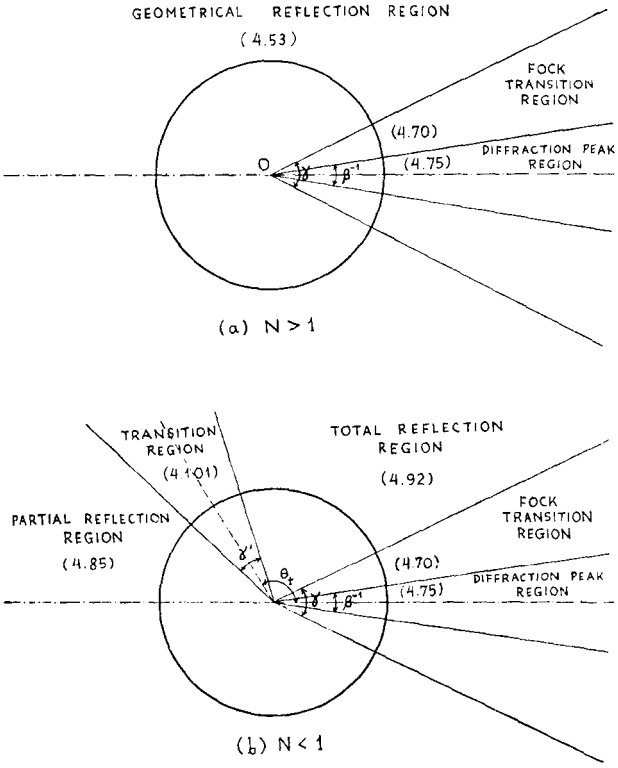


FIG. 15. Basic formulas applicable in each region for the first term $f_0(\beta, \theta)$ of the Debye expansion: (a) for $N > 1$; (b) for $N < 1$. All equation numbers refer to Paper I.

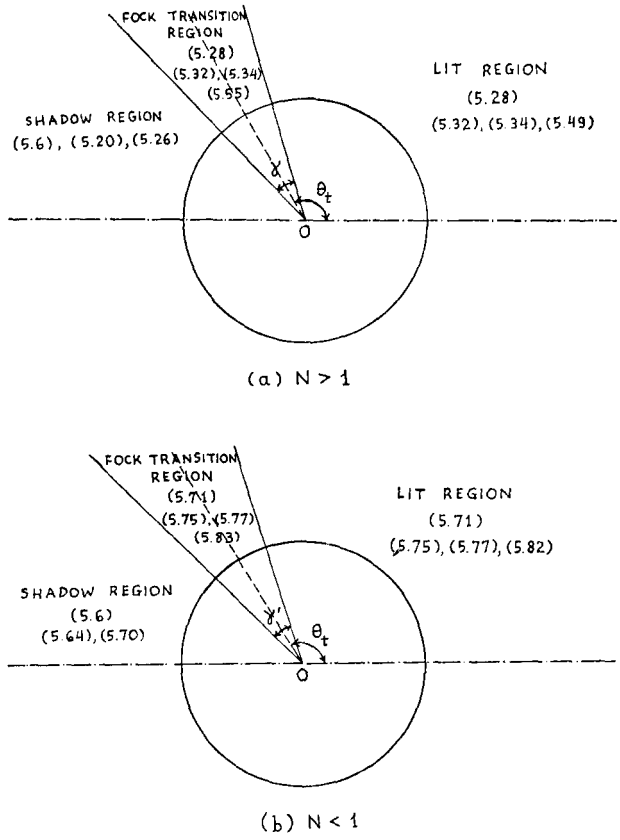


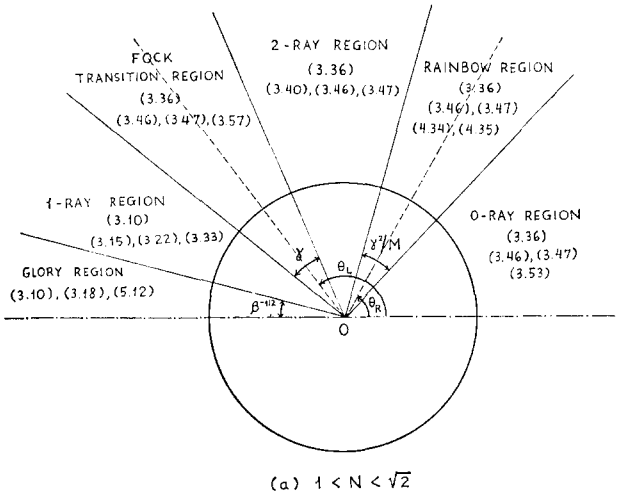
FIG. 16. Basic formulas applicable in each region for the second term $f_1(\beta, \theta)$ of the Debye expansion: (a) for $N > 1$; (b) for $N < 1$ All equation numbers refer to Paper I.

On the other hand, as remarked at the end of I, Sec. 5E, the structure of the transition region around the shadow boundary $\theta = \theta_t$ is quite complicated, because contributions from all terms in the Debye expansion must be taken into account.

7. CONCLUSION

The main conclusion that may be drawn from the present work is that the modified Watson transformation enables us to extract from the partial-wave expansion the complete asymptotic behavior of the scattering amplitude in any direction in the high-frequency domain I, (1.1). This is the purpose for which the Watson transformation was originally introduced.

To facilitate practical application of the results, it is convenient to list the basic formulas that should be applied within each angular region, for each term of the Debye expansion treated in Papers I and II. This is done in Figs. 15 to 17, which provide a graphical summary of the main results. The equations listed in Figs. 15 and 16 refer to Paper I; those in Fig. 17 to



(a) $1 < N < \sqrt{2}$

(b) HIGHER-ORDER RESIDUE-SERIES CONTRIBUTIONS

$N > 1$: $\theta = \pi -$ (6.50), (6.59), (6.64); $\theta = 0 -$ (6.95), (6.96), (6.99)

$N < 1$: $\theta = \pi -$ (6.115)

FIG. 17. Basic formulas applicable in each region: (a) for the third term $f_2(\beta, \theta)$ of the Debye expansion, for $1 < N < \sqrt{2}$; (b) for the effect of higher-order residue-series contributions. All equation numbers refer to Paper II.

Paper II. The angular width of the transition regions is greatly exaggerated in these figures. Only the main formulas are listed, without including the simplified versions given in the text for special ranges of values of the parameters within each region. The total scattering amplitude in any direction is obtained by summing the corresponding contributions from the first three terms of the Debye expansion and taking into account higher-order correction terms.

The subdivision into angular regions for each term of the Debye expansion corresponds to that predicted by geometrical optics for the associated class of rays, together with transition regions.

In lit regions, the dominant term is usually (not always!) given by the geometrical-optic contribution. Although these contributions were known, their precise domain of validity had not been established. The first correction term, representing the second-order WKB approximation, has been evaluated in each case; the first neglected term is $O(\beta^{-2})$.

In shadow regions, the behavior is usually dominated by surface-wave contributions. The most convenient language for the description and physical interpretation of the results is provided by the geometrical theory of diffraction, although it must be used with due care.

For $N > 1$, the surface waves are excited by tangentially incident rays, just like those found for an impenetrable sphere. However, penetration into the sphere leads to several new effects. The diffracted rays can have two types of elementary interactions at the surface, as illustrated in Fig. 11. The combination of these two types leads to a series of diagrams characterized by the number of interactions or, equivalently, by the number of shortcuts taken through the sphere.

For $N < 1$, we have found a new class of surface waves excited by critically incident rays. They are related to Schmidt head waves, but their sense of propagation disagrees with that predicted by the geometrical theory of diffraction. The physical requirement is that surface waves always propagate from the shadow boundary into the shadow. The formulation of the geometrical theory of diffraction should be modified to take this requirement into account. It implies that the local behavior of a ray at the surface is determined not only by the tangent plane, but also by the distinction between shadow and lit sides.

Some of the most interesting phenomena appear in the transition regions. We have found essentially four different types of transition regions: (a) normal (Fock-type) transitions; (b) the region around the shadow boundary for $N < 1$; (c) the rainbow; (d) the glory.

Transition regions of type (a) are similar to those found for an impenetrable sphere. Their angular width is usually of order γ. The amplitude within these regions can be described in terms of generalized Fock functions. They include the region around the forward diffraction peak (I, Sec. 4D).

The transition region (b) has a more complicated structure, because it is a common transition region for all terms in the Debye expansion, and the transition is of a different nature for different terms (I, Secs. 4E and 5E).

The rainbow (c) is associated with the transformation of a pair of real rays into complex rays. The Chester–Friedman–Ursell method allows us to treat this situation. It leads to a uniform asymptotic expansion, which contains the Airy theory as a particular case, but represents a considerable extension beyond the domain of validity of this theory.

The glory (d) represents an impressive example of "Regge-pole dominance" of the scattering amplitude in near-backward directions. Van de Hulst's conjecture that the glory is due to surface waves is confirmed, although his model, corresponding to two shortcuts, must be supplemented by taking into account higher-order surface-wave contributions.

The present theory enables us to explain all the features of the glory listed in Sec. 5A, except, of course, the polarization. These features arise from a competition between four different effects: (1) the exponential damping of the surface waves as they travel along the surface of the sphere; (2) the focusing of diffracted rays along the axis, which enhances the back-scattered contribution; (3) the high internal reflectivity of diffracted rays at the surface, implying that a large number of internal reflections must be taken into account (At the same time, the deviation of the reflection coefficient from unity eventually leads to exponential damping of the surface-wave contributions.); (4) The resonance effects associated with nearly-closed circuits after four successive shortcuts (Fig. 12).

Although an accurate evaluation of the higher-order residue-series contributions would require techniques similar to those discussed in Sec. 5D, we have been able to estimate their resultant effect and to discuss its qualitative behavior, with the help of several simplifying assumptions. The technique is essentially equivalent to finding a generating function for an infinite class of diagrams and then employing it for their summation.

The resonance effects found for the diffracted rays lead to rapid quasiperiodic intensity fluctuations, which are present in all directions, but only become dominant near the backward direction, where they lead to the large intensity variations that appear in the glory. The ripple in the total cross section is a manifestation of the same effect, with greatly reduced amplitude. The relative amplitude of the surface-wave contributions also decreases as β increases (due to the exponential damping), and eventually, for large enough β, geometrical-optic terms again become dominant.

We have also established a link between diffracted-ray resonances and collective effects due to resonances in individual partial waves contained in the edge domain. This corresponds to the relation between the Debye expansion and the physical interpretation of Regge poles given in I, Sec. 2. In both descriptions, a large number of terms have to be taken into account. In fact, interference between many contributions is clearly required to explain the complicated structure of the curves for the back-scattered intensity obtained by Bryant and Cox.[8] However, the surface-wave picture is physically more appealing and it leads naturally to an explanation of all observed effects.

From the mathematical point of view, several problems have received only cursory treatment (if any) in the present work: (a) We have given only a heuristic discussion of the convergence of the Debye expansion for the residue-series contributions (Sec. 6D). It would be desirable to show that a more accurate evaluation of the residues leads to the same result. (b) The detailed shape of steepest-descent contours far away from the saddle points has not been discussed. (c) A more careful derivation of the residue-series contributions, by taking a sequence of contours passing between the poles, is required.[32]

From the point of view of numerical computation, an extensive program should be carried out for a detailed comparison between the present results and those obtained by numerical summation of the partial-wave expansion. The ripple effects require close spacing between calculated points for accurate interpolation. The knowledge of the behavior of the solution provided by the present results should be of considerable help for performing the interpolation. The irregular fluctuations due to the ripple may also be washed out by suitable averaging. If only average results are required, as is the case in many applications, the present approximations may already be adequate. A more ambitious program would be to substitute tables of partial waves or scattered intensities by tables of coefficients of WKB-expansion and residue-series contributions.

Finally, from the physical point of view, several applications and extensions of the present work can be envisaged:

(i) For the third term of the Debye expansion, only the range $1 < N < \sqrt{2}$ has been treated. Several interesting effects appear in other ranges, particularly in the neighborhood of transition points between different ranges (Fig. 3). For instance, one can have a confluence of saddle points near $\theta = \pi$, leading to a mixture of rainbow and glory effects. The neighborhood of these transition points should be investigated both theoretically and experimentally.

In the range $\sqrt{2} < N < 2$, where the neighborhood of the backward direction is a 3-ray region (Fig. 3), anomalously large back-scattering (e.g., from ice spheres) has already been found[33] and discussed by means of surface waves.[34] In this context, back-scattered rays corresponding to noncentral incident rays are sometimes called "glory rays," but this phenomenon is clearly quite different from that discussed in the present work, although the one discussed here can be regarded as a virtual continuation of the other one.

[32] R. F. Goodrich and N. D. Kazarinoff, Proc. Cambridge Phil. Soc. 59, 167 (1963).

[33] D. Atlas and K. M. Glover, in *Electromagnetic Scattering*, M. Kerker, Ed. (The Macmillan Co., New York, 1963), p 213.

[34] J. R. Probert-Jones, in *Electromagnetic Scattering*, M. Kerker, Ed. (The Macmillan Co., New York, 1963), p. 237.

(ii) In Van de Hulst's chart of the $N - \beta$ domain (Ref. 7, Fig. 20, p. 132), we have treated the right-hand side of the square, excluding a neighborhood of the corners. It would be of interest to discuss also the transition to neighboring regions, such as the anomalous-diffraction and Rayleigh–Gans regions (where N is so close to 1 that the positions of the poles are strongly affected), and the region $N \gg 1$ (where the Debye expansion converges more slowly, but direct reflection is dominant). The relation with the resonance region has already appeared in the discussion of surface-wave resonances and the transition to low values of β (Sec. 6E).

(iii) Only the scattering amplitude has been treated. The behavior of the wavefunction in the near region should also be discussed, along similar lines to the discussion given in N for an impenetrable sphere. In particular, this would allow us to determine the behavior within the sphere, which is of interest near resonance. Instead of plane-wave scattering, one can also investigate Green's function. This may provide a useful model for focusing effects in the presence of a point source.

(iv) The extension to a complex refractive index, to represent an absorptive sphere, should not be difficult. Actually, the convergence of the Debye expansion would be improved in this case, in view of the increased damping due to absorption. The propagation of radio waves around the earth is an example.[35]

(v) The extension to complex N would be of particular interest for applications to nuclear physics, in connection with the optical model. Applications to atomic physics, including rainbow effects, have already been discussed.[36] The application to giant resonances in neutron scattering[29] has already been mentioned (Sec. 6E).

Although the nuclear surface does not seem to be very sharp, some evidence for nuclear glory scattering has been given by Bryant and Jarmie.[37] They have obtained a good fit to near-backward alpha-scattering from spinless nuclei at energies between 18 and 50 MeV with an angular distribution of the type (5.20), where a is the nuclear radius. As discussed in Sec. 5C, this indicates that high partial waves, with impact parameters close to the nuclear surface, play an important role. However, a model for the excitations near the nuclear surface that might be involved has not been given.

(vi) The treatment should be extended to bodies of different shapes, and the effect of the geometry on the propagation of surface waves should be discussed. Extension to inhomogeneous bodies should also be considered. In quantum mechanics, this corresponds to a discussion of the classical limit of quantum scattering for more general potentials.

(vii) Finally, in order to account for polarization effects, the scattering of an electromagnetic field should be considered. As will be shown in a forthcoming paper,[11] the present treatment can readily be extended to the electromagnetic case, allowing us to discuss the scattering of light by a transparent sphere.

ACKNOWLEDGMENTS

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APPENDIX A: DETERMINATION OF THE SADDLE POINTS FOR $1 < N < \sqrt{2}$

According to (2.47) and (2.20), the saddle points of (2.43) are given by (2.48), where

$$2\theta_2 - \theta_1 = (\pi - \theta)/2, \quad \sin\theta_1 = N \sin\theta_2. \quad \text{(A1)}$$

It follows from (A1) that

$$\cos\frac{\theta}{2} = \frac{2\sin\theta_1}{N^2}\left\{[(1 - \sin^2\theta_1)(N^2 - \sin^2\theta_1)]^{\frac{1}{2}} - \frac{N^2}{2} + \sin^2\theta_1\right\}, \quad \text{(A2)}$$

where the positive square root is taken, because, for the real saddle points, we must have $0 \leq \theta_1 \leq \pi/2$, $0 \leq \theta_2 \leq \pi/2$.

Introducing

$$z = \sin\theta_1 = \bar{\lambda}/\beta, \quad d = 2\cos(\theta/2), \quad m = N^2/4, \quad \text{(A3)}$$

we find that (A2) becomes

$$z\{[(1 - z^2)(4m - z^2)]^{\frac{1}{2}} + z^2 - 2m\} - md = 0. \quad \text{(A4)}$$

Transposing the square root to the other side and squaring, we find

$$z^4 - 2m\,d\,z^3 - 4m(1 - m)z^2 + 4m^2\,d\,z + m^2 d^2 = 0. \quad \text{(A5)}$$

[35] H. Bremmer, *Terrestrial Radio Waves* (Elsevier Publ. Co., Amsterdam, 1949).

[36] K. W. Ford and J. A. Wheeler, Ann. Phys. (N.Y.) 7, 259, 287 (1959).

[37] H. C. Bryant and N. Jarmie, Ann. Phys. (N.Y.) (to be published).

The roots of this fourth-degree equation include, in addition to those of (A4), spurious roots, which verify (A4) with opposite sign for the square root.

The standard procedure for solving an algebraic equation of the fourth degree[38] is to reduce it to a pair of quadratic equations, the coefficients of which are obtained by solving an auxiliary third-degree equation, the resolvent equation. One must first choose the appropriate root of the resolvent; in the present range of values for N, where at least two of the roots are spurious [cf. Fig. 3(b)], one must also choose the appropriate quadratic equation, such that its roots verify (A4).

This can be done by identifying first a particular solution, corresponding to specific value of d (i.e., θ), and then following it by continuity as d changes. A suitable choice for θ is the rainbow angle θ_R; according to (2.35)–(2.36), we must then have

$$d = d_R = \frac{4}{m}\left(\frac{1-m}{3}\right)^{\frac{3}{2}} \Rightarrow z = z_R = 2\left(\frac{1-m}{3}\right)^{\frac{1}{2}}, \tag{A6}$$

and this must be a double root [cf. Fig. 3(b)].

Applying the procedure indicated above, we find that the correct roots are given by

$$z' = b + (b^2 - c)^{\frac{1}{2}}, \quad z'' = b - (b^2 - c)^{\frac{1}{2}}, \tag{A7}$$

where

$$b = \tfrac{1}{2}(md + e), \tag{A8}$$

$$c = \frac{1}{2}\left[u + \frac{md}{e}(u + 4m)\right], \tag{A9}$$

$$e = [u + 4m(1-m) + m^2d^2]^{\frac{1}{2}} \quad \text{(positive square root)}, \tag{A10}$$

and u, the solution of the cubic resolvent equation, is given by

$$u = s_1 + s_2 - \tfrac{4}{3}m(1-m), \tag{A11}$$

$$s_{1,2} = [r \pm (\Delta)^{\frac{1}{2}}]^{\frac{1}{3}}, \tag{A12}$$

where

$$r = \tfrac{4}{3}m^3\{-\tfrac{16}{9}(1-m)^3 + 4[(1-m)^2 + \tfrac{3}{2}m]d^2 + \tfrac{3}{2}md^4\}, \tag{A13}$$

and Δ is the discriminant, given by

$$\Delta = \tfrac{64}{27}m^6d^2\{-16(1-m)^3 + [8(1-m)^3 + 27m^2]d^2 - \tfrac{1}{2}[2(1-m)^3 + 27m^2]d^4 + \tfrac{27}{16}m^2d^6\}. \tag{A14}$$

The condition for a double root is $\Delta = 0$. This indeed happens for $d = d_R$, leading to the solution (A6). For $d < d_R$, i.e., $\theta < \theta_R$, corresponding to the 0-ray region in Fig. 3(b), we have $\Delta > 0$, and the positive cube root is to be taken in (A12). In this region, (A7) gives a pair of complex-conjugate solutions which leave the real axis at right angles (cf. Fig. 4).

For $d < d_R$, i.e., $\theta > \theta_R$, we have $\Delta < 0$ and (A12) becomes

$$s_{1,2} = [r \pm i(|\Delta|)^{\frac{1}{2}}]^{\frac{1}{3}} = \rho^{\frac{1}{3}} \exp(\pm i\phi/3), \tag{A15}$$

where the phase ϕ must be so chosen that

$$0 < \phi < \pi \tag{A16}$$

and ϕ increases as d decreases. The roots z', z'' are now real and they move away from the point z_R, in opposite directions, as d decreases. The smaller root z'' tends to the origin as $d \to 0$ ($\theta \to \pi$). The larger root z' tends first to the point $z = 1$ ($\theta_1 = \pi/2$), which is reached for $\theta = \theta_L$, the 1-ray/2-ray shadow boundary given by (2.30), corresponding to

$$d = d_L = m^{-1} - 2. \tag{A17}$$

Thus, in the domain $d_L < d < d_R$, we have two real roots, corresponding to the 2-ray region in Fig. 3(b).

As d decreases from d_L to 0, the larger root z' decreases from 1 to $2[m(1-m)]^{\frac{1}{2}}$. However, it is now a spurious root, verifying (A4) with opposite sign for the square root. Thus, only the smaller root z'' is acceptable. This corresponds to the 1-ray region in Fig. 3(b).

To determine the behavior of the roots in the neighborhood of $\theta = \theta_R$, it is simpler to go back to (A1) and to expand θ in a Taylor series around $\theta_1 = \theta_{1R}$, making use of (2.34)–(2.36), as well as of the relation

$$d\theta_2/d\theta_1 = \cos\theta_1/(N\cos\theta_2). \tag{A18}$$

This leads to

$$\epsilon = \frac{3s}{4c}\delta^2 + \frac{(3+c^2)}{16c^2}\delta^3 + \frac{s(17c^2+3)}{256c^3}\delta^4 + \frac{(25c^4+6c^2-15)}{1024c^4}\delta^5 + \frac{s(721c^4-1770c^2-855)}{122\,880}\delta^6 + \mathcal{O}(\delta^7), \tag{A19}$$

where

$$\epsilon = \theta - \theta_R, \quad \delta = \theta_1 - \theta_{1R}, \tag{A20}$$

and s and c are given by (2.35).

Inverting (A19), we find the two solutions

$$\begin{Bmatrix}\delta' \\ \delta''\end{Bmatrix} = \pm p\epsilon^{\frac{1}{2}} - q\epsilon \pm \frac{1}{2p}\left[5q^2 - \frac{(17c^2+3)}{108s^2}\right]\epsilon^{\frac{3}{2}} - \left[8\frac{q^3}{p^2} + \frac{(c^4-6c^2+3)}{108s^3c}\right]\epsilon^2 + \mathcal{O}(\epsilon^{\frac{5}{2}}), \tag{A21}$$

[38] J. V. Uspensky, *Theory of Equations* (McGraw-Hill Book Co., Inc., New York, 1948), p. 94.

where

$$p = \left(\frac{4c}{3s}\right)^{\frac{1}{2}}, \quad q = \frac{3 + c^2}{18s^2}. \tag{A22}$$

The corresponding roots z', z'', according to (A3) and (A20), are

$$\begin{Bmatrix} z' \\ z'' \end{Bmatrix} = s \pm cp\epsilon^{\frac{1}{2}} - \left(cq + \frac{s}{2}p^2\right)\epsilon \pm \left[\frac{5}{2}c\frac{q^2}{p} - \frac{c(17c^2+3)}{216s^2p} + spq - \frac{c}{6}p^3\right]\epsilon^{\frac{3}{2}} + \mathcal{O}(\epsilon^2), \tag{A23}$$

where upper signs correspond to z' and lower ones to z''.

For $\epsilon > 0$, (A23) gives the two real saddle points around the rainbow angle. For $\epsilon < 0$, we must substitute

$$\epsilon^{\frac{1}{2}} \to -i\,|\epsilon|^{\frac{1}{2}} = -i(\theta_R - \theta)^{\frac{1}{2}} \quad (\theta < \theta_R), \tag{A24}$$

and (A23) then gives the two complex-conjugate saddle points shown in Fig. 4, where we have arbitrarily associated the root z' with the lower saddle point and z'' with the upper one.

The corresponding values of $\cos\theta_1$ and $N\cos\theta_2$ are

$$\begin{Bmatrix} \cos\theta_1' \\ \cos\theta_1'' \end{Bmatrix} = c \mp sp\epsilon^{\frac{1}{2}} + \left(sq - \frac{c}{2}p^2\right)\epsilon \mp \left\{\frac{s}{2p}\left[5q^2 - \frac{(17c^2+3)}{108s^2}\right] - cpq - \frac{s}{6}p^3\right\}\epsilon^{\frac{3}{2}} + \mathcal{O}(\epsilon^2), \tag{A25}$$

$$\begin{Bmatrix} N\cos\theta_2' \\ N\cos\theta_2'' \end{Bmatrix} = 2c \mp \frac{sp}{2}\epsilon^{\frac{1}{2}} + \left[\frac{sq}{2} + \frac{p^2}{16c}(3 - 7c^2)\right]\epsilon \mp \left\{\frac{s}{4p}\left[5q^2 - \frac{(17c^2+3)}{108s^2}\right] + \frac{pq}{8c}(3 - 7c^2) - \frac{sp^3}{192c^3}(43c^2 + 9)\right\}\epsilon^{\frac{3}{2}} + \mathcal{O}(\epsilon^2). \tag{A26}$$

The expansion of $N\cos\theta_2 - \frac{1}{2}\cos\theta_1$ will also be required. It is given by

$$\begin{Bmatrix} N\cos\theta_2' - \frac{1}{2}\cos\theta_1' \\ N\cos\theta_2'' - \frac{1}{2}\cos\theta_1'' \end{Bmatrix} = \frac{3c}{2} + \frac{s}{4}\epsilon \pm \frac{cp}{6}\epsilon^{\frac{3}{2}} + \frac{c(11c^2 - 15)}{144s^2}\epsilon^2 \pm \frac{p}{34\,560c^2s^3} \times (875c^6 - 1257c^4 + 657c^2 + 45)\epsilon^{\frac{5}{2}} + \mathcal{O}(\epsilon^3). \tag{A27}$$

APPENDIX B: THE METHOD OF CHESTER, FRIEDMAN, AND URSELL

Let us consider the integral

$$F(\kappa, \epsilon) = \int g(w)\exp\left[\kappa f(w, \epsilon)\right] dw, \tag{B1}$$

where κ is a large positive parameter and g and f are sufficiently regular functions of their arguments (cf. Refs. 3, 4).

We assume that, for some range of values of the parameter ϵ, the integrand has two saddle points, $w'(\epsilon)$ and $w''(\epsilon)$, and that, for some value of ϵ, e.g., $\epsilon = 0$, the two saddle points coincide. For fixed $\epsilon \neq 0$, the ordinary method of steepest descents may be applied, provided that κ is sufficiently large, $\kappa > \kappa_0(\epsilon)$. However, $\kappa_0(\epsilon) \to \infty$ as $\epsilon \to 0$, so that the corresponding asymptotic expansions are not uniform. In order to obtain a uniform asymptotic expansion in a region containing $\epsilon = 0$, the following procedure is applied.

A new variable μ is introduced by

$$f(w, \epsilon) = \tfrac{1}{3}\mu^3 - \zeta(\epsilon)\mu + A(\epsilon). \tag{B2}$$

The two saddle points w', w'' must correspond, respectively, to $\pm\zeta^{\frac{1}{2}}$, i.e.,

$$w = w' \to \mu = -\zeta^{\frac{1}{2}}(\epsilon); \quad w = w'' \to \mu = \zeta^{\frac{1}{2}}(\epsilon). \tag{B3}$$

This allows us to determine $\zeta(\epsilon)$ and $A(\epsilon)$, by solving the equations

$$\begin{aligned} f(w', \epsilon) &= \tfrac{2}{3}\zeta^{\frac{3}{2}}(\epsilon) + A(\epsilon); \\ f(w'', \epsilon) &= -\tfrac{2}{3}\zeta^{\frac{3}{2}}(\epsilon) + A(\epsilon). \end{aligned} \tag{B4}$$

The transformation $w \leftrightarrow \mu$ has one branch that is uniformly regular and one-to-one near $\mu = 0$. This branch is characterized by the fact that (B3) holds on it. On this branch, for small μ and ϵ, we can expand

$$G(w, \epsilon) = g(w)\frac{dw}{d\mu} = \sum_m p_m(\epsilon)(\mu^2 - \zeta)^m + \sum_m q_m(\epsilon)\mu(\mu^2 - \zeta)^m, \tag{B5}$$

where the coefficients $p_m(\epsilon)$, $q_m(\epsilon)$ can be determined by repeatedly differentiating (B5) and setting $w = w'$, $\mu = -\zeta^{\frac{1}{2}}$ and $w = w''$, $\mu = \zeta^{\frac{1}{2}}$.

It follows that

$$F(\kappa, \epsilon) \approx 2\pi i \exp\left[\kappa A(\epsilon)\right]\left\{\sum_m p_m(\epsilon)F_m(\zeta, \kappa, C) + \sum_m q_m(\epsilon)G_m(\zeta, \kappa, C)\right\}, \tag{B6}$$

where

$$F_m(\zeta, \kappa, C) = \frac{1}{2\pi i}\int_C (\mu^2 - \zeta)^m \exp\left[\kappa(\tfrac{1}{3}\mu^3 - \zeta\mu)\right] d\mu, \tag{B7}$$

$$G_m(\zeta, \kappa, C) = \frac{1}{2\pi i}\int_C \mu(\mu^2 - \zeta)^m \exp\left[\kappa(\tfrac{1}{3}\mu^3 - \zeta\mu)\right] d\mu, \tag{B8}$$

and C is the transformed contour of integration, where the limits of integration are formally extended to infinity.

The functions F_m and G_m can be expressed in terms of the Airy function and its derivative. In particular, if C is the contour C_1 defined by

$$\int_{C_1} = \int_{e^{-i\pi/3}\infty}^{e^{i\pi/3}\infty}, \tag{B9}$$

we have

$$\begin{aligned} F_0(\zeta, \kappa, C_1) &= \kappa^{-\frac{1}{3}} \operatorname{Ai}(\kappa^{\frac{2}{3}}\zeta), \\ G_0(\zeta, \kappa, C_1) &= -\kappa^{-\frac{2}{3}} \operatorname{Ai}'(\kappa^{\frac{2}{3}}\zeta), \\ F_1(\zeta, \kappa, C_1) &= 0, \\ G_1(\zeta, \kappa, C_1) &= -\kappa^{-\frac{4}{3}} \operatorname{Ai}(\kappa^{\frac{2}{3}}\zeta), \end{aligned} \tag{B10}$$

and higher-order functions are determined by the recurrence relations

$$\begin{aligned} F_m(\zeta, \kappa, C_1) &= -\frac{2}{\kappa}(m-1)G_{m-2}(\zeta, \kappa, C_1), \\ G_m(\zeta, \kappa, C_1) &= -\frac{1}{\kappa}[(2m-1)F_{m-1}(\zeta, \kappa, C_1) \\ &\quad + 2(m-1)\zeta F_{m-2}(\zeta, \kappa, C_1)]. \end{aligned} \tag{B11}$$

Substituting these results in (B6), we are led to an asymptotic expansion of the type

$$\begin{aligned} F(\kappa, \epsilon) = \exp[\kappa A(\epsilon)] &\times \left\{ \frac{\operatorname{Ai}(\kappa^{\frac{2}{3}}\zeta)}{\kappa^{\frac{1}{3}}} \left[\sum_{s=0}^{M} \frac{a_s(\epsilon)}{\kappa^s} + \mathcal{O}\left(\frac{1}{\kappa^{M+1}}\right) \right] \right. \\ &\left. + \frac{\operatorname{Ai}'(\kappa^{\frac{2}{3}}\zeta)}{\kappa^{\frac{2}{3}}} \left[\sum_{s=0}^{M} \frac{b_s(\epsilon)}{\kappa^s} + \mathcal{O}\left(\frac{1}{\kappa^{M+1}}\right) \right] \right\}, \end{aligned} \tag{B12}$$

where the coefficient functions $a_s(\epsilon)$ and $b_s(\epsilon)$ are regular for small ϵ and the error terms are uniform in ϵ for small ϵ. Thus, (B12) is valid in a region $|\epsilon| \leq R_\epsilon$, independently of κ.

If appropriate regularity conditions are satisfied,[4] the domain of validity of the uniform asymptotic expansion (B12) can be extended to a larger region by matching it with the steepest-descent expansion, with which it has a common domain of validity.

For this purpose, one makes use of the asymptotic expansions of the Airy function and its derivative[39]:

$$\operatorname{Ai}(z) \approx \frac{z^{-\frac{1}{4}}}{2(\pi)^{\frac{1}{2}}} \exp(-\eta)\left[1 - \frac{5}{72\eta} + \mathcal{O}(\eta^{-2})\right] \quad (|\arg z| < \pi), \tag{B13}$$

$$\operatorname{Ai}'(z) \approx -\frac{z^{\frac{1}{4}}}{2(\pi)^{\frac{1}{2}}} \exp(-\eta)\left[1 - \frac{7}{72\eta} + \mathcal{O}(\eta^{-2})\right] \quad (|\arg z| < \pi), \tag{B14}$$

[39] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (National Bureau of Standards, Washington, 1964), p. 448.

$$\operatorname{Ai}(-z) \approx \frac{z^{-\frac{1}{4}}}{(\pi)^{\frac{1}{2}}}\left\{[1 + \mathcal{O}(\eta^{-2})]\sin\left(\eta + \frac{\pi}{4}\right) - \frac{5}{72\eta}[1 + \mathcal{O}(\eta^{-2})]\cos\left(\eta + \frac{\pi}{4}\right)\right\} \quad (|\arg z| < \tfrac{2}{3}\pi), \tag{B15}$$

$$\operatorname{Ai}'(-z) \approx -\frac{z^{\frac{1}{4}}}{(\pi)^{\frac{1}{2}}}\left\{[1 + \mathcal{O}(\eta^{-2})]\cos\left(\eta + \frac{\pi}{4}\right) - \frac{7}{72\eta}[1 + \mathcal{O}(\eta^{-2})]\sin\left(\eta + \frac{\pi}{4}\right)\right\} \quad (|\arg z| < \tfrac{2}{3}\pi), \tag{B16}$$

where

$$\eta = \tfrac{2}{3}z^{\frac{3}{2}}. \tag{B17}$$

APPENDIX C: EVALUATION OF $r_{n,p}$

According to (6.24), we have

$$r_{n,p} = \frac{1}{p!}\frac{d^p}{d\epsilon^p}\left\{\epsilon^{p+1}\frac{c_p(\lambda, \beta)}{[d(\lambda, \beta)]^{p+1}}\right\}_{\epsilon=0}, \tag{C1}$$

where

$$\epsilon = \lambda - \lambda_n. \tag{C2}$$

Only the behavior of $d(\lambda, \beta)$ near $\epsilon = 0$ is relevant for the evaluation of the residue. Thus, we can employ the Taylor series expansion

$$d(\lambda, \beta) = d(\lambda_n, \beta)\sum_{k=1}^{\infty}\frac{d^{(k)}(\lambda_n, \beta)}{d(\lambda_n, \beta)}\frac{\epsilon^k}{k!}, \tag{C3}$$

where $d^{(k)}$ denotes the kth derivative with respect to λ and $d^{(1)} = \dot{d}$.

It follows from I, (A11)–(A18), that

$$\dot{H}^{(1)}_{\lambda_n}(\beta)/H^{(1)}_{\lambda_n}(\beta) = iM + \mathcal{O}(\gamma^2), \tag{C4}$$

where $M = (N^2 - 1)^{\frac{1}{2}}$, as in (2.38), whereas all other ratios that appear in I, (A25)–(A27), such as $\dot{H}'^{(1)}_{\lambda_n}(\beta)/H^{(1)}_{\lambda_n}(\beta)$, $\ddot{H}^{(1)}_{\lambda_n}(\beta)/H^{(1)}_{\lambda_n}(\beta), \cdots$ are at least $\mathcal{O}(\gamma^2)$. Similarly, by I, (A23), the derivatives of $[1\ \alpha]$ are at least $\mathcal{O}(\gamma^3)$. Therefore, it follows from I, (A22) and I, (A25) that

$$\begin{aligned} d(\lambda_n, \beta) &= -[1\ \beta]\dot{H}^{(1)}_{\lambda_n}(\beta)/H^{(1)}_{\lambda_n}(\beta) + \mathcal{O}(\gamma^2) \\ &= -M^2 + \mathcal{O}(\gamma^2). \end{aligned} \tag{C5}$$

Similarly, by complete induction, one can show that

$$d^{(k+1)}(\lambda_n, \beta) = -(k+1)\,d^{(k)}(\lambda_n, \beta) \times \dot{H}^{(1)}_{\lambda_n}(\beta)/H^{(1)}_{\lambda_n}(\beta) + \mathcal{O}(\gamma^2), \tag{C6}$$

so that, by (C4) and (C5),

$$d^{(k)}(\lambda_n, \beta)/d(\lambda_n, \beta) = k!\,(-iM)^{k-1} + \mathcal{O}(\gamma^2). \tag{C7}$$

Substituting this result in (C3), we find

$$d(\lambda, \beta) = d(\lambda_n, \beta) \epsilon \sum_{k=0}^{\infty} (-iM\epsilon)^k + \mathcal{O}(\gamma^2)$$
$$= -\frac{M^2\epsilon}{1 + iM\epsilon} + \mathcal{O}(\gamma^2). \quad \text{(C8)}$$

On the other hand, according to I, (3.6),

$$[2\,\alpha] - [1\,\alpha] = -\frac{4i}{\pi\alpha H_\lambda^{(1)}(\alpha) H_\lambda^{(2)}(\alpha)}, \quad \text{(C9)}$$

so that

$$[1\,\beta] - N[1\,\alpha] = d(\lambda, \beta) - \frac{4i}{\pi\beta H_\lambda^{(1)}(\alpha) H_\lambda^{(2)}(\alpha)}. \quad \text{(C10)}$$

Near $\lambda = \lambda_n$, N, (A16) and I, (A6) give

$$H_\lambda^{(1,2)}(\alpha) = \left(\frac{2}{\pi M\beta}\right)^{\frac{1}{2}} \times \exp\left[\pm i\left(\beta M - \lambda \cos^{-1}\frac{1}{N} - \frac{\pi}{4}\right)\right] \times [1 + \mathcal{O}(\gamma^2)], \quad \text{(C11)}$$

so that (C10) becomes, with the help of (C8),

$$[1\,\beta] - N[1\,\alpha] \approx d(\lambda, \beta) - 2iM = \frac{M^2\epsilon - 2iM}{1 + iM\epsilon} + \mathcal{O}(\gamma^2). \quad \text{(C12)}$$

Similarly, let

$$u(\lambda, \beta) = [H_\lambda^{(1)}(\beta)]^{-2}. \quad \text{(C13)}$$

Then, just as for (C6), one can prove by complete induction that

$$u^{(k)}(\lambda_n, \beta) = (-1)^k (k+1)!\, u(\lambda_n, \beta) \times \left[\frac{\dot{H}_{\lambda_n}^{(1)}(\beta)}{H_{\lambda_n}^{(1)}(\beta)}\right]^k [1 + \mathcal{O}(\gamma^2)], \quad \text{(C14)}$$

i.e., with the help of (C4),

$$u^{(k)}(\lambda_n, \beta)/u(\lambda_n, \beta) = (k+1)!\,(-iM)^k[1 + \mathcal{O}(\gamma^2)]. \quad \text{(C15)}$$

Thus, near $\lambda = \lambda_n$, neglecting $\mathcal{O}(\gamma^2)$,

$$u(\lambda, \beta) = u(\lambda_n, \beta) \sum_{k=0}^{\infty} \frac{u^{(k)}(\lambda_n, \beta)}{u(\lambda_n, \beta)} \frac{\epsilon^k}{k!}$$
$$= \sum_{k=0}^{\infty} (k+1)(-iM\epsilon)^k = \frac{1}{(1 + iM\epsilon)^2}. \quad \text{(C16)}$$

Taking into account I, (A11), I, (A19), I, (A8), this becomes

$$\frac{1}{[H_\lambda^{(1)}(\beta)]^2} = \frac{M^2 e^{i\pi/3}}{4a_n'^2\gamma^4} \cdot \frac{[1 + \mathcal{O}(\gamma^2)]}{(1 + iM\epsilon)^2}. \quad \text{(C17)}$$

Substituting (C11), (C12), and (C17) in (6.25), we finally get, near $\lambda = \lambda_n$,

$$c_p(\lambda, \beta) = (-i)^p e^{i\pi/3} \frac{\pi\beta^3}{16} \frac{M^3}{a_n'^2\gamma} \times \exp(2ipM\beta + i\lambda_n\zeta_p) \frac{(-2iM + M^2\epsilon)^{p-1}}{(1 + iM\epsilon)^{p+1}} \times \exp(i\epsilon\zeta_p)[1 + \mathcal{O}(\gamma^2)], \quad \text{(C18)}$$

where [cf. I, (5.21)]:

$$\zeta_p = s\pi - 2p\cos^{-1}\frac{1}{N} = s\pi - p\theta_t. \quad \text{(C19)}$$

Taking into account (C8) and (C18), we find that (C1) becomes

$$r_{n,p} = -i^p \frac{e^{i\pi/3}}{\gamma} \frac{\pi\beta^3}{16} \frac{e^{2ipM\beta}}{M^{2p-1}} \times \frac{\exp(i\lambda_n\zeta_p)}{a_n'^2} \mathcal{F}_p(M, \zeta_p)[1 + \mathcal{O}(\gamma^2)], \quad \text{(C20)}$$

where

$$\mathcal{F}_p(M, \zeta_p) = \frac{1}{p!}\frac{d^p}{d\epsilon^p}[(-2iM + M^2\epsilon)^{p-1} \exp(i\epsilon\zeta_p)]_{\epsilon=0}. \quad \text{(C21)}$$

With the change of variable

$$-2iM + M^2\epsilon = \frac{M^2}{i\zeta_p} x, \quad \text{(C22)}$$

we finally get

$$\mathcal{F}_p(M, \zeta_p) = \frac{i}{2} M^{2p-1} L_p^{(-1)}(-2\zeta_p/M), \quad \text{(C23)}$$

where

$$L_p^{(-1)}(-x) = \frac{xe^{-x}}{p!}\frac{d^p}{dx^p}(x^{p-1}e^x) = \sum_{m=1}^{p}\binom{p-1}{m-1}\frac{x^m}{m!} = \frac{x}{p} L_{p-1}^{(1)}(-x) = L_p(-x) - L_{p-1}(-x) \quad (p \geq 1) \quad \text{(C24)}$$

is a generalized Laguerre polynomial (Ref. 26, p. 239). We define

$$L_0^{(-1)}(-x) = 1. \quad \text{(C25)}$$

From (C20) and (C23) we obtain the final result

$$r_{n,p} = -i^{p+1} \frac{e^{i\pi/3}}{\gamma} \frac{\pi\beta^3}{32} \exp(2ipM\beta) L_p^{(-1)}(-2\zeta_p/M)(a_n')^{-2} \times \exp(i\lambda_n\zeta_p)[1 + \mathcal{O}(\gamma^2)]. \quad \text{(C26)}$$

APPENDIX D: EVALUATION OF $r'_{n,p}$

From (6.109), we get

$$r'_{n,p} = \frac{1}{p!}\frac{d^p}{d\epsilon^p}\left\{\epsilon^{p+1}\frac{c_p'(\lambda, \beta)}{[d(\lambda, \beta)]^{p+1}}\right\}_{\epsilon=0}, \quad \text{(D1)}$$

where

$$\epsilon = \lambda - \lambda_n'. \quad \text{(D2)}$$

Again, only the behavior of $d(\lambda, \beta)$ near $\epsilon = 0$ is relevant, so that, as in (C3), we expand

$$d(\lambda, \beta) = d(\lambda'_n, \beta) \sum_{k=1}^{\infty} \frac{d^{(k)}(\lambda'_n, \beta)}{d(\lambda'_n, \beta)} \frac{\epsilon^k}{k!}. \tag{D3}$$

From I, (A11)–(A18), we find that,

$$\dot{H}^{(2)}_{\lambda'_n}(\alpha)/H^{(2)}_{\lambda'_n}(\alpha) = -iM'/N + \mathcal{O}(\gamma^2), \tag{D4}$$

where $M' = (1 - N^2)^{\frac{1}{2}}$, as in I, (3.31), whereas all other ratios that appear in the analogs of I, (A25)–(A27) for $[2\ \alpha]$ are at least $\mathcal{O}(\gamma^2)$. Similarly, by I, (2.39), the derivatives of $[1\ \beta]$ are at least $\mathcal{O}(\gamma^3)$. Thus, we find

$$d(\lambda'_n, \beta) = [1\dot{\beta}] - N[2\dot{\alpha}] = N \frac{\dot{H}^{(2)}_{\lambda'_n}(\alpha)}{H^{(2)}_{\lambda'_n}(\alpha)} [2\ \alpha] + \mathcal{O}(\gamma^2)$$

$$= \frac{M^2}{N'} + \mathcal{O}(\gamma^2). \tag{D5}$$

One can show by complete induction that

$$d^{(k+1)}(\lambda'_n, \beta) = -(k+1) \frac{\dot{H}^{(2)}_{\lambda'_n}(\alpha)}{H^{(2)}_{\lambda'_n}(\alpha)} d^{(k)}(\lambda'_n, \beta) + \mathcal{O}(\gamma^2), \tag{D6}$$

so that

$$\frac{d^{(k)}(\lambda'_n, \beta)}{d(\lambda'_n, \beta)} = k! \left(i \frac{M'}{N}\right)^{k-1} + \mathcal{O}(\gamma^2). \tag{D7}$$

Substituting this result in (D3) and (D5), we find

$$d(\lambda, \beta) = \epsilon d(\lambda'_n, \beta) \sum_{k=0}^{\infty} (iM'\epsilon/N)^k + \mathcal{O}(\gamma^2)$$

$$= \frac{M'^2 \epsilon}{N - iM'\epsilon} + \mathcal{O}(\gamma^2). \tag{D8}$$

On the other hand, we have [cf. (3.31)]

$$H^{(1)}_{\lambda}(\alpha) \approx 2 \frac{e^{-i\pi/3}}{\gamma'} \operatorname{Ai}(e^{i\pi/3} x), \tag{D9}$$

where

$$x = e^{i\pi/3}(\lambda - \alpha)/\gamma', \quad \gamma' = (2/\alpha)^{\frac{1}{3}}, \tag{D10}$$

and, by (3.32),

$$H^{(1)}_{\lambda}(\alpha) \approx H^{(1)}_{\lambda'_n}(\alpha) \approx -\frac{e^{-i\pi/6}}{\pi a'_n \gamma'}. \tag{D11}$$

Similarly, from (D9),

$$[1\ \alpha] = \mathcal{O}(\gamma'), \quad [1\dot{\alpha}] = \mathcal{O}(\gamma'^2), \tag{D12}$$

so that, near λ'_n,

$$[1\ \beta] - N[1\ \alpha] \approx [1\ \beta]_{\lambda_n'} = iM', \tag{D13}$$

with the help of I, (2.39). To the present order of accuracy, (D11) and (D13) may be directly substituted in (6.110). Similarly, we may replace $H^{(1)}_{\lambda}(\beta)$ by [cf. (C11)]

$$H^{(1)}_{\lambda}(\beta) \approx \left(\frac{2}{\pi M'\beta}\right)^{\frac{1}{2}} \exp\left(iM'\beta - i\lambda \frac{\theta_t}{2} - i\frac{\pi}{4}\right), \tag{D14}$$

where θ_t is given by I, (4.76).

On the other hand, by I, (A1), and by (D10),

$$H^{(2)}_{\lambda}(\alpha) \approx 2e^{i\pi/3} \operatorname{Ai}(-x)/\gamma', \tag{D15}$$

and, with the help of (D4), we find

$$H^{(2)}_{\lambda}(\alpha) \approx H^{(2)}_{\lambda'_n}(\alpha) + \epsilon \dot{H}^{(2)}_{\lambda'_n}(\alpha) \approx H^{(2)}_{\lambda'_n}(\alpha)\left(1 - i\frac{M'}{N}\epsilon\right)$$

$$= 2e^{i\pi/6} \frac{N}{M'} \gamma'^2 a'_n \left(1 - i\frac{M'}{N}\epsilon\right), \tag{D16}$$

with all higher derivatives yielding higher-order contributions.

Substituting (D11)–(D16) in (6.110), we finally get, near $\lambda = \lambda'_n$,

$$c'_p(\lambda, \beta)$$

$$= -\frac{\pi^2 M' N \beta^3}{8} \exp\left[-2iM'\beta - i\lambda'_n(\pi - \theta_t)\right]$$

$$\times \left(-\frac{e^{i\pi/6} M'^2}{2\pi N a'^2_n \gamma'}\right)^p \frac{\exp\left[-i\epsilon(\pi - \theta_t)\right]}{\left(1 - i\frac{M'}{N}\epsilon\right)^{p+1}} [1 + \mathcal{O}(\gamma^2)]. \tag{D17}$$

Replacing (D8) and (D17) in (D1), we find

$$r'_{n,p} = -\frac{\pi^2 N^2 \beta^3}{8M'}$$

$$\times \exp\left[-2iM'\beta - i\lambda'_n(\pi - \theta_t)\right]\left(-\frac{e^{i\pi/6}}{2\pi a'^2_n \gamma'}\right)^p$$

$$\times \frac{1}{p!}\left\{\frac{d^p}{d\epsilon^p}\left[e^{-i\epsilon(\pi - \theta_t)}\right]\right\}_{\epsilon=0} [1 + \mathcal{O}(\gamma^2)],$$

so that, finally,

$$r'_{n,p} = -\frac{\pi^2 N^2 \beta^3}{8M'} \exp\left[-2iM'\beta - i\lambda'_n(\pi - \theta_t)\right]$$

$$\times \frac{1}{p!}\left[-\frac{e^{-i\pi/3}(\pi - \theta_t)}{2\pi a'^2_n \gamma'}\right]^p [1 + \mathcal{O}(\gamma^2)]. \tag{D18}$$

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Problem of Two Spin Deviations in a Linear Chain with Next-Nearest-Neighbor Interactions

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The problem of two spin deviations from the fully aligned state is studied in a linear chain for the Hamiltonian $[J(i,j) > 0]$:

$$H = -\tfrac{1}{2}\sum_{(\mathrm{nn})} J(i,j)\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{2}\alpha \sum_{(\mathrm{nnn})} J(i,j)\mathbf{S}_i \cdot \mathbf{S}_j,$$

where (nn) and (nnn) mean nearest- and next-nearest-neighbor interactions, respectively. The behavior of the bound state, which is found to exist for $\alpha \geq 0$ only, is discussed.

INTRODUCTION

Recently we studied the ground state properties of the Hamiltonian

$$H = -\tfrac{1}{2}J\sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} - \tfrac{1}{2}J\alpha \sum_{i=1}^{N} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+2} \qquad (1)$$

$(N+1 \equiv 1,\ N+2 \equiv 2)$.[1] Short chains of up to eight particles were exactly studied, and upper and lower bounds for the ground-state energy per particle for arbitrarily large N were found. In this paper we present some results on the study of a few excited states of the Hamiltonian (1). Specifically, we shall study the one and two spin deviations from the completely aligned state. The fully aligned state is the exact ground state for the case $J > 0$, $\alpha > 0$ (i.e., all interactions ferromagnetic). So our considerations have relevance to the low-lying excited states for this case. For J negative (antiferromagnetic case), the completely aligned state is a highly excited state, such that our considerations are not particularly useful. In this paper we consider only the ferromagnetic case, $J > 0$. For α negative with $J > 0$, the ferromagnetic state may no longer be the ground state. In fact, it was conjectured that the ground state for $J > 0$ and $\alpha < 0$ is of spin zero and that $\alpha = 0$ is itself a singular point. Although no proof has as yet been found, we shall offer here some illustrations of the singular nature of the point $\alpha = 0$.

With $\alpha = 0$ in (1) (that is, the linear chain having only nearest-neighbor interactions), the problem has been the subject of several well-known investigations.[2] Bethe[3] considered two and more spin deviations, and was able to solve the resulting difference equations. His method depends crucially on his famous ansatz that, for example, the two-spin-deviation states have the form

$$\Psi = \sum_{m,n} a(m,n)\psi(m,n),$$

$$a(m,n) = \exp(ik_1 m + ik_2 n + \tfrac{1}{2}i\varphi) + \exp(ik_2 m + ik_1 n - \tfrac{1}{2}i\varphi). \qquad (2)$$

Here $\psi(m,n)$ denotes a spin function having up spins at the mth and the nth sites. k_1 and k_2 are wavevectors and φ may be called the phase shift. With appropriate boundary conditions, Bethe found that the states with two spin deviations formed a continuum (k_1, k_2 real) and that there was a bound state (k_1, k_2 complex, with imaginary parts equal but of opposite signs), produced by interaction of the spin waves. One can define a wavenumber $K = k_1 + k_2$, which is a constant of the motion and can be thought of as the wavevector corresponding to the center-of-mass motion of the two excitations of up spins. The bound-state energy varies with K—a characteristic feature of this problem—and for each value of K there exists only one bound state below the continuum. Bethe's method was extended by Dyson to two and three dimensions in his work on the Heisenberg model.[4]

The one-spin-deviation problem—the simple spin waves—for the Hamiltonian (1) can be handled by Bethe's method. The two spin deviations lead, however, to a set of difference equations difficult to solve. No simple guess corresponding to Bethe's ansatz has so far been found. Fortunately, alternative methods are now available, which are sufficient to reveal the nature of the spectrum and give some idea of the bound state. Some picture of the wavefunction can also be obtained. The method of Green's functions was used by Wortis[5] in the examination of the problem of the bound states of the Heisenberg model. Wortis's equations can be directly extended to our Hamiltonian.

[1] C. K. Majumdar and D. K. Ghosh (to be published).
[2] The literature may be traced from C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321 (1966).
[3] H. Bethe, Z. Physik **71**, 205 (1930); L. Hulthén, Arkiv Astron, Fysik **24**, No. 12 (1938).
[4] F. J. Dyson, Phys. Rev. **102**, 1217 (1956).
[5] M. Wortis, Phys. Rev. **132**, 85 (1963).

However, we find another method used by Fukuda and Wortis,[6] one that is simpler and more convenient. This method employs nothing more than the Schrödinger equation. The derivation of the equations by the Green's function method (along the line followed by Wortis) is completely straightforward and is left to the interested reader.

The first section gives the solution of the trivial one spin deviation problem. Then we take up the two spin deviations and discuss the continuum and bound states for $\alpha \geq 0$. For $\alpha < 0$, the continuum is easily discussed, but we have not been able to find any bound states.

I. SPIN WAVES

In the simple case of one spin deviation, we can allow α to be positive as well as negative: $-1 \leq \alpha \leq 1$. It is convenient to write the Hamiltonian (1) as

$$H = -\tfrac{1}{2}\sum_{i,j} J(i,j)\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{2}\sum_{i,j} Y(i,j)\mathbf{S}_i \cdot \mathbf{S}_j. \quad (3)$$

Here,

$$J(i,j) = \begin{cases} J, & \text{if } i \text{ and } j \text{ are nearest neighbors,} \\ 0, & \text{otherwise.} \end{cases}$$

Similarly,

$$Y(i,j) = \begin{cases} J\alpha, & \text{if } i \text{ and } j \text{ are next nearest neighbors,} \\ 0, & \text{otherwise.} \end{cases}$$

Notice the unimportant change in the magnitude of J from Eq. (1) by a factor 2. The commutation relations of the spin operators are the usual ones:

$$\begin{aligned} S^{\pm} &= S^x \pm iS^y, \\ [S^z, S^{\pm}] &= \pm S^{\pm}, \\ [S^+, S^-] &= 2S^z. \end{aligned} \quad (4)$$

The spin-deviation-number operator is

$$n = NS + \sum_i S_i^z. \quad (5)$$

n commutes with H and, for the fully aligned state $|0\rangle$, $n = 0$. The spin waves correspond to the state with one spin flipped up, $n = 2S$, and the wavefunction can be written as

$$\Psi = \sum_i u(i) S_i^+ |0\rangle. \quad (6)$$

The Schrödinger equation is

$$E\Psi = H\Psi. \quad (7)$$

If E_0 is the energy of the state $|0\rangle$ of all down spins,

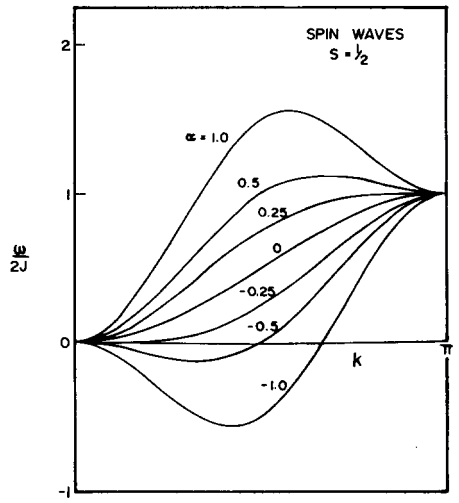

FIG. 1. The spin-wave spectrum ($S = \frac{1}{2}$) with the next-nearest-neighbor interaction present. For $\alpha < -0.25$, the fully aligned state is unstable with respect to the spin waves for small k.

we get

$$(E - E_0)\Psi = \sum_i u(i)[H, S_i^+] |0\rangle. \quad (8)$$

Define the spin-wave energy $\omega = E - E_0$. Then, using (4), we get

$$\begin{aligned} &[\omega - 2SJ(1 + \alpha)]u(l) \\ &\qquad = -S\sum_m [J(l,m) + Y(l,m)]u(m). \end{aligned} \quad (9)$$

Define the Fourier transform as

$$u(l) = \frac{1}{N}\sum_k e^{ikl}\tilde{u}(k), \quad (10)$$

where the wavevectors k fill up the Brillouin zone $-\pi < k \leq \pi$. Then we get the spin-wave spectrum as

$$\omega = 2SJ(1 + \alpha) - 2SJ\cos k - 2SJ\alpha\cos 2k. \quad (11)$$

In Fig. 1 we represent the spectrum for $-1 \leq \alpha \leq 1$. While, for α positive, the fully aligned state remains always stable with respect to the spin-wave excitation, this is not true for α negative. For $\alpha < -0.25$ the spin waves lie lower in energy for small k; in other words, there, a state of total spin $S(N - 2)$ lies lower in energy than the state of total spin SN.

II. TWO SPIN DEVIATIONS

Following Fukuda and Wortis,[6] the eigenstate Ψ of two spin deviations can be written as

$$\Psi = \sum_{i,j} U(i,j) S_i^+ S_j^+ |0\rangle, \quad (12)$$

$$U(i,j) = U(j,i). \quad (13)$$

For $S = \frac{1}{2}$, $U(i,i)$ is not defined. The normalized two-spin-deviation wavefunction with spins up at the

[6] N. Fukuda and M. Wortis, J. Phys. Chem. Solids **24**, 1675 (1963).

sites i and j is

$$\psi(i,j) = 4S\left(1 - \frac{\delta(ij)}{2S}\right)^{\frac{1}{2}} U(i,j). \tag{14}$$

Writing the energy with respect to the aligned state of energy E_0 as ω (not to be confused with that of Sec. I), i.e.,

$$H|0\rangle = E_0|0\rangle, \quad H\Psi = E\Psi,$$
$$\omega = E - E_0, \tag{15}$$

we get

$$\omega\Psi = \sum_{i,j} U(i,j)[H, S_i^+ S_j^+]|0\rangle. \tag{16}$$

Utilizing (4), we can write down the equations determining $U(i,j)$:

$$\begin{aligned}[\omega - 4JS(1+\alpha)]U(i,j) &= -S\sum_l \{[J(j,l) + Y(j,l)]U(i,l) \\ &\quad + [J(i,l) + Y(i,l)]U(j,l)\} \\ &\quad + [J(i,j) + Y(i,j)]\{\tfrac{1}{2}[U(i,i) + U(j,j)] - U(i,j)\}.\end{aligned} \tag{17}$$

As Fukuda and Wortis remarked, for $S = \frac{1}{2}$, the $i = j$ component of (17) does not follow from (16). It is clear that for $S = \frac{1}{2}$ the components $U(l,l)$ entirely cancel out of (17) for $i \neq j$. Thus the Schrödinger equation leaves $U(i,i)$ totally undetermined. The set of equations (17) for $i \neq j$ is complete for the determination of the $S = \frac{1}{2}$ problem. In order to take Fourier transforms, it is convenient not to have a special situation at $i = j$. So for $S = \frac{1}{2}$, we choose to let the $i = j$ component of (17) define the unphysical $U(i,i)$ in terms of the physical $U(i,j)$, $i \neq j$. This definition can have no effect on the physical $U(i,j)$'s and, by (14), is not reflected in the wavefunction. All the components of (17) now hold for arbitrary S.

Define now the center of mass and the relative coordinates

$$2R = R_i + R_j, \quad r = R_i - R_j \tag{18}$$

and introduce the Fourier transform

$$U(i,j) = \frac{1}{N}\sum_K e^{iKR} U_K(r), \quad U_K(r) = U_K(-r). \tag{19}$$

The sum over K runs over the first Brillouin zone. Then the periodicity condition on U is $U_K(r) = \exp(iKL/2)U_K(r+L)$, where L is the size of our chain. Since each unit distance of the chain is of length one, $L = N$. So Eq. (17) becomes

$$\begin{aligned}[\omega - 4JS(1+\alpha)]U_K(r) &+ 2SJ\{\cos\tfrac{1}{2}K[U_K(r+1) + U_K(r-1)] \\ &+ \alpha\cos K[U_K(r+2) + U_K(r-2)]\} \\ &= J(r)[\cos\tfrac{1}{2}KrU_K(0) - U_K(r)] \\ &+ Y(r)[\cos\tfrac{1}{2}KrU_K(0) - U_K(r)].\end{aligned} \tag{20}$$

The right-hand side represents the interaction between the spin waves. We now introduce a further Fourier transform

$$U_K(r) = \frac{1}{N}\sum_{k\in F} e^{ikr} U_K(k), \quad U_K(k) = U_K(-k), \tag{21}$$

where k ranges over a Brillouin zone F appropriately shifted so as to incorporate the periodic boundary condition. Equation (20) becomes

$$[\omega - \epsilon_K(k)]U_K(k) = \frac{1}{N}\sum_{k'\in F} V_K(k,k')U_K(k'). \tag{22}$$

The sum in k' goes now over only the positive half $\bar{F}$ of the Brillouin zone. Also,

$$\begin{aligned}\epsilon_K(k) = 4JS[1 + \alpha - \cos\tfrac{1}{2}K\cos k \\ - \alpha\cos K\cos 2k].\end{aligned} \tag{23}$$

$\epsilon_K(k)$ is the energy of the two free-spin waves of the type (11), and it forms a continuum for each value of K. The interaction is

$$\begin{aligned}V_K(k,k') = 2J[\cos k(\cos\tfrac{1}{2}K - \cos k') \\ + \alpha\cos 2k(\cos K - \cos 2k')].\end{aligned} \tag{24}$$

We shall henceforth discuss only $S = \frac{1}{2}$ in detail and look for bound states outside the continuum. Since the kernel $V_K(k,k')$ is separable in k and k', the solution to (22) is of the form

$$U_K(k) = c_1[\cos k/D_K(k,\omega)] + c_2[\cos 2k/D_K(k,\omega)], \tag{25}$$

$$D_K(k,\omega) = \omega - \epsilon_K(k). \tag{26}$$

The Fourier transform of $U_K(k)$ gives the wavefunction in the coordinate space; it has quite a complicated structure. Substituting (25) into (22), we get the eigenvalue equation for the bound state as

$$\begin{vmatrix} 1 - I_{11} & I_{12} \\ I_{21} & 1 - I_{22} \end{vmatrix} = 0. \tag{27}$$

The I's are certain integrals when we replace the summation over k by integration:

$$I_{11} = \frac{2J}{\pi}\int_0^\pi dk\,\frac{(\cos\tfrac{1}{2}K - \cos k)\cos k}{D_K(k,\omega)}, \tag{28}$$

$$I_{12} = -\frac{2J}{\pi}\int_0^\pi dk\,\frac{(\cos\tfrac{1}{2}K - \cos k)\cos 2k}{D_K(k,\omega)}, \tag{29}$$

$$I_{21} = -\frac{2J}{\pi}\alpha\int_0^\pi dk\,\frac{(\cos K - \cos 2k)\cos k}{D_K(k,\omega)}, \tag{30}$$

$$I_{22} = \frac{2J\alpha}{\pi}\int_0^\pi dk\,\frac{(\cos K - \cos 2k)\cos 2k}{D_K(k,\omega)}. \tag{31}$$

Putting $\alpha = 0$, we recover the term $(1 - I_{11})$ alone, which gives the Bethe result. Even for a linear chain we have a more elaborate bound-state condition which, in general, has to be analyzed numerically.

III. BOUND STATES

The situation for $K = \pi$ can be treated analytically and it reveals the most interesting features of the problem. Consider first $K = \pi$ and $\alpha = 0$. Equation (27) reduces to

$$1 + \frac{2J}{\pi}\int_0^{\pi} dk \frac{\cos^2 k}{\omega - 2J} = 0.$$

Therefore, $\omega = J$. For general $\alpha > 0$, the continuum $\epsilon_K(k) = 2J(1 + \alpha) + 2J\alpha \cos 2k$; and the continuum extends from $2J$ upward to $2J(1 + 2\alpha)$.

The integrals (28)–(31) are very singularly behaved functions of α. Let

$$D_\pi(k, \omega) = \omega - \epsilon_\pi(k) = -2J\alpha(t + \cos 2k) \quad (32)$$

with

$$t = 1 + \alpha^{-1}[1 - (\omega/2J)]. \quad (33)$$

In (32) and (33) we assume that $\alpha \neq 0$. Notice that, as long as $\omega/2J < 1$ for $\alpha > 0$, $t > 1$. Consider $\alpha > 0$ from now on. Then, with the help of

$$I = \int_0^{\pi} \frac{dx}{(t + \cos x)} = \frac{\pi \operatorname{sgn} t}{(t^2 - 1)^{\frac{1}{2}}}, \quad |t| > 1, \quad (34)$$

and other elementary integrals, we get

$$I_{11} = \tfrac{1}{2}\alpha^{-1}[1 - (t - 1)^{\frac{1}{2}}/(t + 1)^{\frac{1}{2}}],$$
$$I_{12} = 0,$$
$$I_{22} = (1 - t)[1 - t/(t^2 - 1)^{\frac{1}{2}}].$$

Hence the bound states are solutions of the equation

$$F(\omega, \alpha) = \{1 - \tfrac{1}{2}\alpha^{-1}[1 - (t - 1)^{\frac{1}{2}}/(t + 1)^{\frac{1}{2}}]\} \times \{1 - (1 - t)[1 - t/(t^2 - 1)^{\frac{1}{2}}]\} = 0. \quad (35)$$

The second factor can be zero at $t = 0$ and 1, which are not in the allowed region. The first factor gives an acceptable solution:

$$t = [1 + (1 - 2\alpha)^2]/[1 - (1 - 2\alpha)^2]. \quad (36)$$

Hence the bound-state energy is

$$\omega_B = 2J\left(1 - \frac{1}{2}\frac{(1 - 2\alpha)^2}{1 - \alpha}\right). \quad (37)$$

The solution reduces to the correct value at $\alpha = 0$, and the bound-state energy goes on rising with α toward the continuum until, at $\alpha = 0.5$, the bound state reaches the edge of the continuum. The significance of $\alpha = 0.5$ is not hard to see. The maximum attraction of the first term in $V_\pi(k, k')$ is $-4JS(k = 0, k' = 0)$; this can be counterbalanced exactly by a contribution of the second term $8JS\alpha$ for $\alpha = 0.5$, thus destroying the attractive nature of the interaction. This argument has obvious generalizations for $K \neq \pi$.

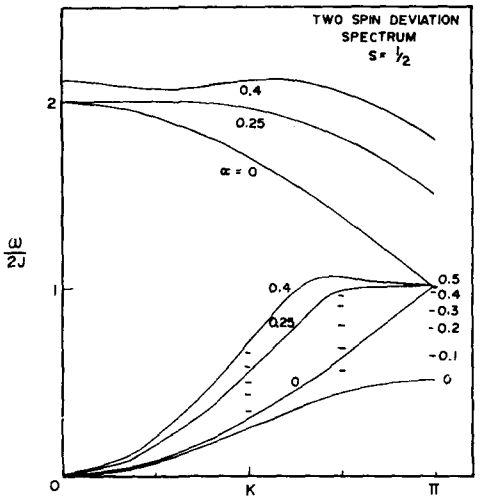

FIG. 2. The continuum and bound states for two spin deviations ($\alpha \geq 0$). The upper and lower boundaries of the continuum for $\alpha = 0$, 0.25, 0.4 are drawn. The bound states increase in energy with α from 0 upward.

Although the appearance of (37) seems to allow a well-defined ω_B for negative α by a series expansion for small α, this is easily ruled out. For negative α, $t > 1$ for $\omega > 2J$, but the expansion gives $\omega < 2J$, which is a contradiction. The point is that the integrals I_{ij} were evaluated for $t > 1$ and $\alpha > 0$, and t does not have any power series in α around $\alpha = 0$.

For $K = \pi/2$, one can again do the integrals analytically, but the bound state condition yields a complicated polynomial whose highest term has a multiplier in α^2, thus revealing again the singular nature of $\alpha = 0$. We have numerically evaluated the bound state energy at $K = \pi/2$ and $K = 3\pi/4$ for α up to 0.5. These points are indicated in Fig. 2. The bound state exists for $\alpha \geq 0.5$ for smaller values of K. The merging into the continuum starts from $K = \pi$ at $\alpha = 0.5$; the corresponding value of K diminishes as α keeps on increasing. The existence of the bound state is therefore a somewhat delicate function of the strength of the next-nearest-neighbor interaction.

For J positive and α negative, the continuum begins to spread below the boundary for $\alpha = 0$. For $\alpha < -\frac{1}{4}$, a part of the two-particle continuum definitely lies lower in energy than the completely aligned state. However, we have not found any bound state in this case.

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Some Asymptotic Behavior of Stieltjes Transforms

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We consider an integrable function $g(t)$ which behaves as $\zeta t^{-\alpha}$ when t tends to infinity (ζ is a finite number) for $0 < \alpha < 1$, and show that its Stieltjes transform has the same behavior when $|z|$ approaches infinity and provided that z is in the sector $|\arg z| < \pi - \delta$, where $\pi > \delta > 0$. (Theorem 1). In addition, we study the cases of α equal to zero, one, and larger than one (Theorems 2–4). Our results contain those of L. Lanz and G. M. Prosperi [Nuovo Cimento **33**, 201 (1964)] and those of W. S. Woolcock [J. Math. Phys. **8**, 1270 (1967)]. They are proved in a direct manner, using a theorem of D. V. Widder [*The Laplace Transform*,(Princeton University Press, Princeton, N.J., 1959), fifth printing, p. 329] and the regularity of the integral transforms that arise.

First we establish a lemma.

Lemma: Let t be a real variable, z a complex variable, ζ and A finite numbers, and let S denote a region in the complex plane. If

$$\int_0^\infty |k(z, t)|\, dt < M, \quad M \text{ is independent of } z \in S, \quad (1)$$

$$\int_0^{t_0} |k(z, t)|\, dt \to 0, \quad \text{for} \quad |z| \to \infty, \quad z \in S, \quad (2)$$

for every finite-positive t_0, and if

$$\int_0^\infty k(z, t)\, dt \to A \quad \text{for} \quad |z| \to \infty, \quad z \in S, \quad (3)$$

then

$$\int_0^\infty k(z, t)g(t)\, dt$$

is a regular transformation, i.e.,

$$g(t) \xrightarrow[t\to\infty]{} \zeta \Rightarrow \int_0^\infty k(z, t)g(t)\, dt \to A\zeta,$$

$$\text{for} \quad |z| \to \infty \quad \text{and} \quad z \in S,$$

whenever

$$\int_0^\infty k(z, t)g(t)\, dt \quad \text{exists for} \quad z \in S.$$

Proof: The proof of this lemma is similar to that of the case of a real variable z. (See, for example, Ref. 1.) In fact, according to Eq. (3), it is enough to show that

$$g(t) \xrightarrow[t\to\infty]{} 0 \Rightarrow \int_0^\infty k(z, t)g(t)\, dt \to 0,$$

$$\text{for} \quad |z| \to \infty \quad \text{and} \quad z \in S. \quad (4)$$

We know that for every $\epsilon > 0$ there exist z_0 and $t_0(\epsilon)$ such that

$$\int_0^{t_0} |k(z, t)|\, dt < \epsilon, \quad \text{for every} \quad z, |z| > |z_0|, \quad (5)$$

and

$$|g(t)| < \epsilon, \quad \text{for every} \quad t > t_0. \quad (6)$$

We have by (2) and (5):

$$\int_0^{t_0} |k(z, t)g(t)|\, dt \leq \epsilon \cdot \sup_{0 \leq t < \infty} |g(t)|,$$

$$\text{for} \quad z, |z| > |z_0|, \quad (7)$$

and by (1) and (6):

$$\int_{t_0}^\infty |k(z, t)g(t)|\, dt \leq \epsilon \cdot \int_{t_0}^\infty |k(z, t)|\, dt$$

$$\leq \epsilon \cdot \sup_{z\in S} \int_0^\infty |k(z, t)|\, dt. \quad (8)$$

The conclusion (4) follows from (7) and (8).

In the following we shall always denote by S a sector defined by $|\arg z| < \pi - \delta$, where $\pi > \delta > 0$.

Using the previous lemma we can now establish the following theorem.

Theorem 1: Let $g(t)$ be an integrable function in the ordinary sense in any finite interval. If

$$f(z) \overset{\text{DEF}}{=} \int_0^\infty \frac{g(t)\, dt}{z + t} \quad (9)$$

converges for a point $z = z_0$ which is not on the negative real axis and if $1 > \alpha > 0$, then

$$t^\alpha g(t) \xrightarrow[t\to\infty]{} \zeta \Rightarrow z^\alpha f(z) \to \pi\zeta/\sin(\alpha\pi),$$

$$z \in S \quad \text{and} \quad |z| \to \infty. \quad (10)$$

Proof: Using a theorem due to Widder,[2] stating that if the integral (9) converges for a point $z = z_0$ not on the negative real axis, then

$$\int_0^t g(u)\, du = o(t) \quad (t \to \infty),$$

[1] G. H. Hardy, *Divergent Series* (Oxford, Clarendon Press, 1949).

[2] D. V. Widder, *The Laplace Transform* (Princeton University Press, Princeton, N.J., fifth printing, 1959).

we find by integration by parts that

$$f(z) = \int_0^\infty \frac{G(t)}{(z+t)^2}\,dt, \quad z \in S, \tag{11}$$

where

$$G(t) = \int_0^t g(u)\,du, \quad t \geq 0.$$

Writing

$$t^{\alpha-1}G(t) = t^{\alpha-1}\int_0^t u^{-\alpha}u^{\alpha}g(u)\,du,$$

and using the regularity of the kernel

$$a(t,u) = \begin{cases} t^{\alpha-1}u^{-\alpha}, & t \geq u > 0, \\ 0, & u > t, \end{cases}$$

for $\alpha < 1$, we get

$$t^{\alpha}g(t) \to \zeta \Rightarrow t^{\alpha-1}G(t) \to \zeta/(1-\alpha), \quad t \to \infty. \tag{12}$$

By (11) we have

$$z^{\alpha}f(z) = \int_0^\infty k(z,t)G(t)\cdot t^{\alpha-1}\,dt,$$

where

$$k(z,t) = z^{\alpha}t^{1-\alpha}/(z+t)^2. \tag{13}$$

The kernel (13) is regular for $z \in S$ and $1 > \alpha > 0$. Indeed,

$$\int_0^\infty k(z,t)\,dt = \frac{\pi(1-\alpha)}{\sin(\pi\alpha)}, \quad z \in S \quad \text{and} \quad 0 < \alpha < 1, \tag{14}$$

(see, for example, Ref. 3) and therefore the kernel (13) satisfies (3).

By (14) it follows that (13) also satisfies (1) for every positive value of z. On the other hand, denoting by x and y the real and imaginary parts of z, we have for $y \neq 0$:

$$|z|^{\alpha}\int_0^\infty \frac{t^{1-\alpha}}{|z+t|^2}\,dt = \frac{\pi}{\sin(\pi\alpha)}\cdot\frac{\sin\{(1-\alpha)\arg z\}}{\sin(\arg z)}. \tag{15}$$

(See, for example, Ref. 4.)

From (15) it follows that

$$|z|^{\alpha}\int_0^\infty \frac{t^{1-\alpha}}{|z+t|^{\alpha}}\,dt = O(1),$$
$$y \neq 0, \quad z \in S \quad \text{and} \quad |z| \to \infty.$$

Finally, it is easily seen that (13) satisfies (2) for $z > 0$, and $y \neq 0$; we have

$$|z|^{\alpha}\int_0^{t_0} \frac{t^{1-\alpha}}{|z+t|^2}\,dt \leq |z|^{\alpha}\cdot t^{1-\alpha}\int_0^{t_0}\frac{dt}{(t+x)^2+y^2}$$
$$= \frac{|z|^{\alpha}t_0^{1-\alpha}}{y}\cdot\arctan\left(\frac{y\cdot t_0}{z^2+x\cdot t_0}\right)$$
$$= O\left(\frac{1}{|z|^{2-\alpha}}\right), \quad z \in S \quad \text{and} \quad |z| \to \infty.$$

[3] W. Gröbner and N. Hofreiter, *Integraltafel, Zweiter Teil: Bestimmte Integrale* (Springer-Verlag, Wien, 1966), p. 177.

[4] Reference 3, p. 184.

Hence the kernel (13) satisfies the three conditions of the previous lemma and is therefore regular. It follows that

$$t^{\alpha-1}G(t) \xrightarrow[t\to\infty]{} \zeta/(1-\alpha) \Rightarrow z^{\alpha}f(z) \to \frac{\pi\zeta}{\sin(\pi\alpha)},$$
$$\text{for} \quad z \in S, \quad |z| \to \infty, \quad \text{and} \quad 1 > \alpha > 0.$$

The conclusion (10) follows from the last relation and from (12).

Theorem 2: $\alpha = 1$.

If

$$f(z) = \int_0^\infty \frac{g(t)}{z+t}\,dt$$

converges for a point $z = z_0$ not on the real negative axis, then

$$t\cdot g(t) \xrightarrow[t\to\infty]{} 0 \Rightarrow \frac{zf(z)}{\log z} \to 0,$$
$$\text{for} \quad z \in S \quad \text{and} \quad |z| \to \infty.$$

Proof: Let $t_0 > 0$ and

$$\psi(x) = \int_x^\infty g(t)/t\cdot dt, \quad x > 0.$$

Integration by parts yields

$$f(z) = \int_0^{t_0}\frac{g(t)\,dt}{z+t} + \int_{t_0}^\infty \frac{g(t)\,dt}{z+t}$$
$$= \int_0^{t_0}\frac{g(t)\,dt}{z+t} + \frac{t_0}{z+t_0}\psi(t_0) + z\int_{t_0}^\infty \frac{\psi(t)\,dt}{(z+t)^2}$$
$$= z\int_{t_0}^\infty \frac{\psi(t)\,dt}{(z+t)^2} + O\left(\frac{1}{|z|}\right),$$
$$\text{for} \quad z \in S \quad \text{and} \quad |z| \to \infty.$$

As

$$g(t) = o\left(\frac{1}{t}\right) \Rightarrow \psi(t) = o\left(\frac{1}{t}\right), \quad t \to \infty,$$

it is enough to show that, for any finite number $t_0 > 0$, we have

$$z\int_{t_0}^\infty \frac{dt}{t\,|z+t|^2} = O\left(\frac{\log|z|}{|z|}\right),$$
$$\text{for} \quad z \in S \quad \text{and} \quad |z| \to \infty.$$

The last relation is checked by integration.

Theorem 3: $\alpha = 0$.

If the integral (9) converges for a point $z = z_0$ not on the negative real axis, then

$$f(z) \to 0, \quad \text{for} \quad z \in S \quad \text{and} \quad |z| \to \infty. \tag{16}$$

Proof: The proof is similar to that of Widder's for a real variable z (see Ref. 5). In fact, using the auxiliary function

$$H(t) = \int_0^t \frac{g(u)}{1+u}\,du \quad (t \geq 0),$$

we obtain by integration by parts

$$f(z) = \int_0^\infty H'(t) \cdot \frac{1+t}{z+t} \cdot dt$$
$$= f(1) + (1-z)\int_0^\infty \frac{H(t)\,dt}{(z+t)^2}. \tag{17}$$

As $H(t) \xrightarrow[t\to\infty]{} f(1)$ [see Eq. (9)], we have by the regularity of the kernel

$$k(z,t) = \frac{z}{(z+t)^2}, \quad z \in S,$$
$$\int_0^\infty \frac{H(t)\,dt}{(z+t)^2} = O\left(\frac{1}{|z|}\right) \tag{18}$$

and

$$z\int_0^\infty \frac{H(t)\,dt}{(z+t)^2} \to f(1), \quad \text{for} \quad z \in S \quad \text{and} \quad |z| \to \infty. \tag{19}$$

The conclusion (16) follows now from (17) to (19).

[5] Reference 2, p. 333.

Theorem 4: $\alpha > 1$.

Let $g(t)$ be an integrable function in the ordinary sense in any finite interval, and let $\alpha > 1$.

If

$$g(t) = o(t^{-\alpha}), \quad t \to \infty, \tag{20}$$

then

$$\lim_{\substack{|z|\to\infty \\ z\in S}} \{zf(z)\} = \int_0^\infty g(t)\,dt,$$

where $f(z)$ is defined by (9).

Proof: As

$$g(t) = z \cdot \frac{g(t)}{z+t} + t \cdot \frac{g(t)}{z+t},$$

we have

$$\int_0^\infty t\,\frac{g(t)\,dt}{z+t} = \int_0^\infty g(t)\,dt - zf(z), \quad z \in S,$$

and it is sufficient to show that

$$h(z) \overset{\text{DEF}}{=} \int_0^\infty t \cdot \frac{g(t)\,dt}{z+t}$$

exists for $z \in S$ and tends to zero, then $|z| \to \infty$. Since by (20), $h(z)$ exists for such values of z, the conclusion follows from Theorem 3 applied to the function $h(z)$.

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Bethe–Salpeter Equation

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We treat the Bethe–Salpeter equation as a problem in singular integral equations. As such, it has three outstanding features: its algebraic structure, the fixed propagator singularities in the direct channel, and the possible singularities in the potential, which are usually moving singularities. We exploit the algebraic structure in order to give insight into the possible correctness classes for the equation. We give explicit prescriptions for the removal of fixed singularities in a wide class of equations. We show under what circumstances these prescriptions can be adapted to maintain such desirable features as symmetry of the kernel. Moving singularities arise in physically realistic kernels; they are the crossed-channel singularities. The basic mathematics of such singularities is well known and is related to the Riemann–Hilbert problem, but this is useless in off-shell methods because it cannot cope with the integration over the space parts of 4-momenta. Instead, we adopt a method (proposed by one of us elsewhere) based on analyticity in energy variables. The resulting formalism is too complicated to be applied in full generality. We therefore consider the example of the single-particle exchange potential in detail, and show how the moving singularities can be eliminated, exhibiting the resulting equations explicitly in a form to which our theory of fixed singularities can immediately be applied. All our arguments are exact.

1. INTRODUCTION

1.1. Summary and Review of Previous Work

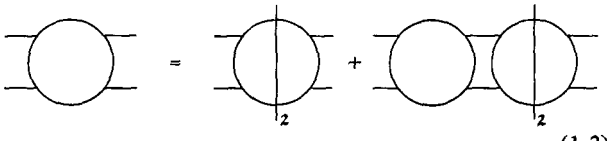
The Bethe–Salpeter equation[1] is essentially a linear off-shell equation for the (two-body) T matrix:

$$T = V + VGT, \tag{1.1}$$

where V is a "potential" and G is a given Green's function. The potential V may be given, or may be an unknown determined by a further equation. Equations of the general form (1.1) arise in several ways: from attempts to sum various classes of perturbation diagrams,[1] for instance, in the ladder or single-particle exchange approximation

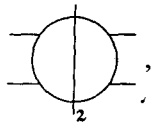
$V =$  , (1.2)

or in quantum electrodynamics.[2] In a general Green's function treatment of quantum field theory,[3] such an equation as



(1.3)

of the precise form (1.1), arises through considerations of charge renormalization, the object

$V =$  , (1.4)

acting as a potential. By this we mean that if one wants to obtain approximate equations reflecting, say, dominance of single-particle exchange in a crossed channel, one again substitutes (1.2). This single-particle (or its generalization to many-particle) exchange contribution to V may also be used to obtain a bootstrap structure.[4–6] In general, Eq. (1.3) is the expression of complete unitarity in the direct channel.[3]

Equations like (1.1) also arise[7] from the separable approximation to a relativistic generalization[8] of the Faddeev equations.[9]

Attempts at exact numerical calculations have been made in the ladder approximation for bound states,[10]

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[1] Y. Nambu, Progr. Theoret. Phys. (Kyoto) **5**, 614 (1950); M. Gell-Mann and F. E. Low, Phys. Rev. **84**, 350 (1951); E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951); J. Schwinger, Proc. Natl. Acad. Sci. U.S. **37**, 452, 455 (1951).

[2] K. Johnson, M. Baker, and R. S. Willey, Phys. Rev. **136**, B1111 (1965); R. S. Willey, Phys. Rev. **153**, 1364 (1967). Earlier references are given in the first paper of Ref. 11 below.

[3] J. G. Taylor, Nuovo Cimento Suppl. **1**, 857 (1963).

[4] M. M. Broido and J. G. Taylor, Phys. Rev. **147**, 993 (1966).

[5] Reference 3, p. 1026; Ref. 4, p. 1006; W. Güttinger, Nuovo Cimento **36**, 968 (1965); T. Yoshimura, Nuovo Cimento **39**, 984 (1965); S. N. Biswas and L. A. P. Balazs, Phys. Rev. **156**, 1511 (1967); D. Bondyopadhyay, S. N. Biswas, and R. P. Saxena, Phys. Rev. **160**, 1272 (1967).

[6] M. M. Broido, J. Math. Phys. **6**, 1702 (1965).

[7] H. Cohen, A. Pagnamenta, and J. G. Taylor (unpublished).

[8] J. G. Taylor, Phys. Rev. **150**, 1321 (1966).

[9] L. D. Faddeev, *Quantum Theory of Scattering for 3-particle Systems*, A.E.R.E. Harwell translation, 1964 (unpublished) and references quoted there.

[10] C. Schwartz, Phys. Rev. **137**, B717 (1965). In the quark model, with scalar mesons as bound states of scalar quarks, the bound-state Bethe–Salpeter calculation of D. Holdsworth has shed light on the nature of the quark–quark interaction; see comments by R. H. Dalitz in *Proceedings of the XIII'th International Conference on High Energy Physics, Berkeley 1966* (University of California Press, Berkeley, 1967).

elastic-region phase shifts,[11] and for the region between the first and second inelastic thresholds.[12] Also in the ladder approximation, calculations have been performed with approximate kernels.[13] In the form arising from the relativistic Faddeev equations, approximate calculations have also been carried out.[14] Padé approximants have been applied to the computation problem.[14a]

The Bethe–Salpeter equation may be considered either in differential or integral form. As a differential equation it is of fourth order, but the boundary conditions in the bound-state problem are simple enough that it is worth using for bound-state computations.[10] Some progress has also been made towards a general analytic discussion of the differential equation in the Riemannian formulation of the boundary-value problem,[14b] but this formulation does not help to elucidate the bound-state structure. We prefer to treat the momentum-space integral equation for two reasons. First of all, it is most closely related to the physical interpretation; it is easiest for considering the role of unitarity. Secondly, the Bethe–Salpeter equation is, after all, only the lowest of a hierarchy of Green's function equations[3] describing the momentum-space structure of multiparticle processes, and our eventual hope must be to devise methods for dealing with all of these. From now on, whenever we use the phrase "Bethe–Salpeter equation," we will mean the momentum-space integral equation.

Experience indicates that there are two main difficulties in using the BS equation:

(1) singularities in the Green's function G;
(2) singularities in the kernel V.

Since the natural method of dealing with any singular integral equation is to reduce it to a Fredholm equation, there will be the following further features to consider:

(3) the special algebraic structure of the equation;
(4) the need in certain discussions to have kernels representing Hermitian operators, and related features involving the Feynman $i\epsilon$ in the singular denominators.

Before we embark on a detailed treatment of the equation, let us outline the effects of these four features.

In practice, one is always considering a two-particle BS equation in which the Green's function is the product of two propagators, usually free. This is the case at which most of the work in this paper is aimed. The removal of the direct-channel propagator singularities, then, is a *general* problem concerning many classes of Bethe–Salpeter equation. It has been considered by one of us elsewhere[15] by a kind of Taylor expansion about the mass shell (a more sophisticated form of subtraction method). In this paper we use a different, more general expansion method.

There exists a further general method for the removal of singularities, that of analytic continuation in the energy variables ("generalized Wick rotations").[16,17] We use that method here for the removal of moving singularities.

The removal of singularities in the kernel V is important for computation and for physical argument, but it is not such a general problem. It has been considered generally in connection with the removal of propagator singularities by generalized Wick rotations[18] and specifically, for computational reasons, in many of the above-mentioned papers.

We note that the general problem of the removal of fixed singularities from integral equations does not seem to have received any attention in the mathematical literature. For instance, the book of Muskhelishvili[19] considers only singular integrals of the type

$$\int \frac{K(x, y)f(y)}{x - y}\, dy, \tag{1.5}$$

related to the Riemann–Hilbert problem in analytic function theory. For this reason and others which we discuss below, we will be able to make scarcely any use of the classical literature on singular integral equations.

The purpose of this paper is to give a general account of the methods by which a BS equation may be

[11] C. Schwartz and C. Zemach, Phys. Rev. **141**, 1454 (1966); R. W. Haymaker, Phys. Rev. Letters **18**, 968 (1967).

[12] M. Levine, J. Tjon, and J. Wright, Phys. Rev. Letters **16**, 962 (1966); Phys. Rev. **154**, 1433 (1967). These authors have also shown [Phys. Rev. **157**, 1416 (1967)] that an ansatz for the complete propagator improves the unitarity behavior between the three-body and four-body thresholds; see also R. M. Saenger, Phys. Rev. **159**, 1433 (1967). Although we do not consider using a complete propagator in this paper, we observe that this type of ansatz can very easily be included into the general methods we discuss.

[13] R. Blankenbecler and R. Sugar, Phys. Rev. **142**, 1051 (1966).

[14] See Ref. 7 and also H. Cohen, A. Pagnamenta and J. G. Taylor, Nuovo Cimento **50**, 586 (1967).

[14a] R. W. Haymaker, Phys. Rev. **165**, 1790 (1968).

[14b] J. Honerkamp, "Lösung der Bethe–Salpeter-Gleiching mit Hilfe der Riemann'schen Methode," Institut für Theoretische Physik, Hamburg preprint, 1967.

[15] See paper 5 of Ref. 3.

[16] J. G. Taylor, Phys. Rev. **136**, B1134 (1964).

[17] This energy-analytic representation has been applied to the Green's function equations describing many-particle scattering and production processes by J. G. Taylor, *Boulder Summer Institute Lectures 1966*, M. Guenin, ed. (Gordon and Breach Science Publishers, Inc., New York, 1967). It has been used to discuss the $^3P_1$ state of nucleon–nucleon scattering by H. Ito *et al.*, Progr. Theoret. Phys. (Kyoto) **37**, 372 (1967).

[18] A. Pagnamenta and J. G. Taylor, Phys. Rev. Letters **17**, 218 (1966).

[19] N. I. Muskhelishvili, *Singular Integral Equations* (Moscow, 1946) [(English translation: Noordhoff, Groningen, 1953)].

reduced to the standard Fredholm form, having regard to the features (1)–(4) mentioned above. The organization of the paper is as follows:

Algebraic generalities concerning the BS equation are dealt with in subsection 1.2. We will see that they have a considerable effect on the choice of possible correctness classes (which are classes of functions in which the problem of solving the BS equation is correctly posed, i.e., makes sense).

The connection between unitarity and the reality of the eigenvalues of the kernel is discussed in subsection 1.3.

In Sec. 2 we give detailed prescriptions for removing fixed singularities from the kernels of integral equations. These prescriptions apply to a far wider class of equations than the BS equation, and they are presented with appropriate generality. They are essentially *algebraic* in nature; nevertheless, the resulting singularity free integral equations must satisfy certain well-known analytic conditions in order that Fredholm theory may apply, and these are reflected in certain continuity and integrability conditions on the objects appearing in the original equations.

In Sec. 3, these methods are applied to a study of the general field-theoretic BS equation (1.3) in the case where the potential V does not have crossed-channel singularities. Our methods succeed in removing the singularities. This can be done in such a way as to preserve the symmetry property required for the analysis of more complex problems (see Ref. 6), but we do not pursue this topic here.

Realistic problems will have, in addition, crossed-channel singularities. These give rise to moving singularities which cannot be dealt with directly by the methods of Sec. 2. The classical methods associated with the expression (1.5) are useless for elementary particle physics because they cannot take into account the integration over the space components. For this reason we present, in Sec. 4, an appropriate version of the method of generalized Wick rotations. We cannot hope to give a completely general account of the application of this method to the BS equation; the situation is too complicated. But, in Sec. 5, we do present a complete and explicit treatment of the one-particle exchange problem [Eq. (1.2)], showing how the generalized Wick rotation does remove the moving singularity, and we exhibit the equation in a form to which the considerations of Sec. 2 apply. Although we do not attempt numerical computation in the present paper, this treatment shows transparently enough how all the technical problems encountered in earlier work can be overcome *without making further approximations* (i.e., beyond the one-particle exchange approximation). The generalization to the simultaneous exchange of several particles is too complex to give here, but presents no new difficulties of principle. Since other contributions to the "exchange potential" are likely to be less singular than these, we have actually shown how to deal with a very large class of potentials. In other words, the one-particle exchange gives the "dominant" part of the potential in the sense of Muskhelishvili.[19]

The following problems are not treated in this paper: computational problems *per se*; pole structure and renormalization of the equation; the generalization to systems with spin; the problem of determining the "potential" (beyond the one-particle exchange approximation).

1.2. Algebraic Generalities

Elsewhere[20] one of us has dealt quite generally with the algebraic properties of the BS equation. By using properties of certain types of BS equations, this discussion can be taken further. In the case where the T and V of (1.1) are in some sense drawn from the same class E_0 [e.g., of four-point functions, in the case of Eq. (1.3)], the mapping

$$(T, V) \to VGT,$$

gives rise to a *multiplication* on E_0.[21] This E_0 will clearly become a *ring*, and indeed in all physical cases, an *algebra* (over the complex numbers). Suppose we denote the multiplication by $*$. Then (1.1) is equivalent to

$$T - V - V * T = 0, \tag{1.6}$$

so that T and $-V$ are *quasi-inverses* for $*$. If we add an identity I to E_0, we can put

$$(I - V) * (I + T) = I, \tag{1.7}$$

so that $I - V$ is a left inverse of $I + T$; if $*$ is a *commutative* multiplication, i.e., $V * T = T * V$, as is the case with Eq. (1.3), then $I - V$ and $I + T$ are simply *inverses* and we can solve (1.1) unambiguously in the form

$$T = (I - V)^{-1} - I. \tag{1.8}$$

It should be emphasized that this is a rigorous, uniquely defined procedure, not merely a formal hand-waving. Of course, it will be difficult to compute explicitly the expressions we have just written down. This is why we wish to remove the singularities: Fredholm theory then gives us a comparatively explicit method for this computation. Moreover, we wish to

[20] M. M. Broido, "Equations which are Relations on an Algebraic Structure" (unpublished).

[21] E_0 is what we called the *solution class* in Ref. 20.

do this in such a way as to preserve these desirable algebraic properties. We do not know of any existing treatment of the BS equation where this happens.

Abstractly, the problem in the commutative case is to show that one of the factors on the left-hand side of (1.7) which is given, possesses an inverse in E_0. The existence of this inverse is thus a *necessary and sufficient* condition for the existence *and uniqueness* of the solution to the original BS equation.

In the noncommutative case, the most general necessary condition for existence on Eq. (1.7) is the existence of the appropriate one-sided inverse. One-sided inverses are not unique in general, so this will not give a uniqueness theorem.

The most important physical examples are commutative [e.g., Eq. (1.3)].

The most general Fredholm equations are of the form

$$a = b + Ka, \tag{1.9}$$

$$A = B + KA, \tag{1.10}$$

where K is a given completely continuous linear operator on a Hilbert space, b (B) a given vector (operator), and a (A) an unknown vector (operator). Then if $I - K$ is invertible, the solutions are

$$a = (I - K)^{-1}b, \tag{1.11}$$

$$A = (I - K)^{-1}B. \tag{1.12}$$

Otherwise we have the Fredholm alternative for appropriate b,B (at least in the case of Hermitian K); this alternative is not, in general, unique. We note that the Fredholm alternative is obtained by considering the inversion of $(I - K)$ in a certain subspace of the original Hilbert space, so in the case of (1.10), it can be regarded as arising from a different choice of E_0.

Equation (1.10) with $B = K$ has the same algebraic structure as the BS equation. The Fredholm alternative is irrelevant in this case. On the other hand, we see that the condition $B = K$ has nothing to do with the basic form of the solution when we write it by Eq. (1.12). Thus we can afford to transform (1.6) into the apparently less favorable form (1.10), provided we maintain the invertibility.

The discussion we have given so far assumes that the operation is defined for any two members of the solution class E_0, and leads to another member of this class. This assumption is somewhat stronger than what one most obviously requires (namely, that the product $V * T$ is defined). One can imagine slightly less restrictive conditions—for instance, that E_0 is a given vector space, but that the product $V * T$ is defined for all $T \in E_0$ only when V is restricted to some subset $E_1 \subset E_0$ (say). This is the situation which arises when one tries to iterate the first-order perturbation term in the Green's function equations of field theory.[3] In this situation, the class E_1 is usually an algebra. Clearly, if we seek a solution with V in E_1 but T not in E_1, neither can $V * T$ be in E_1. Analysis of special cases of some physical interest[22] suggests that this apparent generalization will not lead to anything new.

We also see that our above assumptions arose because, having an equation with an algebraic multiplication operation in it, we considered correctness classes which are rings of functions rather than rings of operators. We can finally end up with the multiplicative structure of a ring of operators. For this reason it seems to us that the use of algebraic structures of double internal composition (rings, algebras) is quite essential in any deeper study of the BS equation.[23]

The argument which we have given so far assumed that the multiplication $*$ is fixed once and for all. Although we will not consider this in the present paper, we observe that it may be convenient to change the form of multiplication by absorbing parts of the Green's function G into the kernel or otherwise. In this way, one may be able to cause a damping in TGV to become apparent, or to achieve other desirable results. Such a procedure is used in connection with the Lippmann–Schwinger equation for singular potentials elsewhere.[24]

1.3. Reality of Eigenvalues and the Feynman $i\epsilon$ Prescription

In this subsection we review, in a thoroughly intuitive way, the connection between the requirements of Fredholm theory (particularly hermiticity of the operators represented by the potential V and the scattering amplitude T), and the use of the Feynman $i\epsilon$ prescription in the propagators. Since these arguments are essentially of a physical nature, we present them specifically in terms of the physical problem, Eq. (1.3). We denote the four-momentum in the direct channel by p, $s = p^2$, $\mathbf{p} = (p_1p_2p_3)$. The convolutive multiplication in (1.3) does not involve the variable s, so we may write

$$T(s) = V(s) + \rho(s)[V(s) * T(s)], \tag{1.13}$$

where $\rho(s)$ is a kinematic factor which will, in general, contain a multiplicative (coupling) constant. Thus, in addition to the general algebraic considerations of the previous subsection, we must consider what is the

[22] See Ref. 3, paper 4.

[23] It will be found helpful to compare this discussion with the more general one given in Ref. 20. Although arguments pertaining to the BS equation are given in Ref. 20, those of the present paper go much further.

[24] H. H. Aly and J. G. Taylor, J. Math. Phys. (to be published).

effect of the s-dependence made explicit in Eq. (1.13) and, in particular, of the kinematic factor $\rho(s)$.

In general, there will be values s' of s for which $\lambda = [\rho(s')]^{-1}$ is an eigenvalue of the operator V. Under these circumstances, the algebraic arguments of the previous subsection show that (1.13) cannot have a solution as it stands. What happens physically is, of course, well-known; we have a bound state in the direct channel. Mathematically, this is expressed by the existence of an eigenvector $T(s')$:

$$V(s') * T(s') = \lambda T(s'). \tag{1.14}$$

In general terms, the compactness of the operator $V(s)$ is enough to ensure the existence of this eigenvector, because a compact operator has only isolated spectral points (apart perhaps from zero, i.e., apart from the singularities of the kinematic factor), and these are necessarily eigenvalues. How does one reconcile this with Eq. (1.13)? The answer is again well known: there must be a pole in $T(s)$ which makes the $V(s)$ term by itself negligible. We easily convince ourselves that there is no other possibility. Thus for these exceptional values of s, the original Bethe–Salpeter structure disappears; the equation becomes homogeneous. This, of course, is exactly the condition for a bound state. In the center-of-mass system, we will have $(s')^{\frac{1}{2}} = p_0 = \mu$, say, which will give us the mass of the bound state.

Let m denote the mass of the incoming particles (the argument is easily generalized to particles with different masses). Then, for $p_0 < 2m$, the Feynman $i\epsilon$ in the intermediate propagators does not contribute. Hence we are dealing with a real integral equation and the eigenvalues must be real. On the other hand, for $p_0 > 2m$, there can be no eigenvalues, as is well known; for they would contradict unitarity. (Suppose we had an S-wave pole. We have

$$T \sim \frac{\Gamma}{p_0 - \mu},$$

$$|T|^2 \sim \frac{\Gamma}{|p_0 - \mu|^2},$$

$$\operatorname{Im} T \sim \Gamma \delta(p_0 - \mu),$$

contradicting the unitarity requirement $\operatorname{Im} T = |T|^2$.) Thus we have shown that the Feynman $i\epsilon$ will not interfere with the reality of the spectrum of V.

Compactness is not strictly necessary in the above argument. What concerns us is the point nature of the spectrum. But in this type of problem we normally handle square-summable functions (Sec. 2) which automatically give rise to compact operators. Let us briefly consider what kind of kernels give rise to operators which are continuous, but not completely continuous. By standard techniques of Fourier analysis, we can reduce this problem to that of double sequences $\{a_{ij}\}$. Square-summability of the kernel corresponds to $\sum_{ij} |a_{ij}|^2 < \infty$. For continuity,

$$\sup_j \sum_i |a_{ij}|^2 < \infty,$$

is necessary and sufficient. Unfortunately, the latter condition is inconveniently asymmetric and does not seem to have any simple interpretation in terms of the original kernel.

To get a Hermitian operator out is much more difficult. The only general condition which we can exploit is the symmetry of T in all variables (which arises from field theory). Unfortunately, this does not correspond to hermiticity in the normal Hilbert space sense, which requires rather a property of the form $U(x, y) = \bar{U}(y, x)$ (the bar denotes complex conjugation). We discuss this problem in more detail in Sec. 3.

1.4. Continuity Conditions

A function $\phi(x)$ of a single real variable is said to *satisfy the Hölder condition* $H(\mu)$ if, for some constant C,

$$|\phi(x_1) - \phi(x_2)| < C\,|x_1 - x_2|^{\mu},$$

for all x_1, x_2. In the case of moving singularities (1.5), such conditions have to be applied over the whole range of x.[19] We will be dealing largely with fixed "propagator" singularities at $x = a$ (say), and will impose Hölder conditions only *in some neighborhood of this point* in such cases (even where not explicitly stated). In the case of functions of two (or more) variables, we can talk about a Hölder condition $H(\mu, \nu)$, say, corresponding to

$$|\phi(x_1, y_1) - \phi(x_2, y_2)| < C\,|x_1 - x_2|^{\mu} + D\,|y_1 - y_2|^{\nu},$$

and so forth. In this paper, functions of several variables will, in general, be required to satisfy Hölder conditions in each variable separately (in some neighborhood of some fixed point) and also higher-order Hölder conditions where several variables are all near their singular points. The precise Hölder conditions to be used will generally be obvious, but will be spelled out in detail if they are not.

2. SOME CLASSES OF SINGULARITY-REMOVING TRANSFORMATIONS

2.1. Functions of a Single Variable

In this subsection we will consider how to remove the singularity from such an integral equation as

$$f(x) = g(x) + \int \frac{K(x, y) f(y)\, dy}{y - a}, \tag{2.1}$$

(in this and similar equations we will uniformly add $+i\epsilon$ to the denominator if necessary), where f and g are functions of a single variable x. We wish, then to reduce Eq. (2.1) to the form

$$f'(x) = g'(x) + \int K'(x, y)f'(y)\,dy, \tag{2.2}$$

where the kernel K' is to be sufficiently smooth that the standard Fredholm techniques can be applied. One of us has discussed this problem elsewhere[15] and has pointed out that the essential step is to expand the functions about the singular point $x = a$. Previously[15] we simply took the Taylor expansion of $f(x)$

$$f(x) = f(a) + (x - a)f'(x), \tag{2.3}$$

and showed that the reduction can indeed be accomplished by putting

$$g(x) = \frac{1 - K_0(x)}{1 - K_0(a)}\,g(a) + (x - a)g'(x), \tag{2.4}$$

and

$$K(x, y) = \frac{1 - K_0(x)}{1 - K_0(a)}\,K(a, y) + (x - a)K'(x, y), \tag{2.5}$$

where

$$K_0(x) = \int \frac{K(x, y)}{y - a}\,dy. \tag{2.6}$$

Such a treatment is perfectly sufficient for simple linear Bethe–Salpeter equations with given kernel $K(x, y)$. However, the transformation absorbs the singularity entirely into the unknown function $f(x)$ [since (2.5) transforms $K(x, y)$ only in the first variable, which is not integrated over in (2.1)]. As we discussed in a general way in the Introduction, this feature makes it impossible to generalize the transformation (2.3)–(2.6) to such an equation ("equation in kernel functions") as

$$f(x, y) = g(x, y) + \int \frac{K(x, z)f(z, y)\,dz}{z - a}, \tag{2.7}$$

without introducing an asymmetry between the two variables, which makes it very difficult to see what is going on. The problem of a consistent removal of singularities from singular integral equations is certain to be an important one also in a general Green's function treatment of quantum field theory.[3] For these reasons we will consider from the outset a more symmetrical class of transformations. In order to maintain a reasonable balance between simplicity and generality, we will return to the form (2.1) and will consider the following rather general transformation of the functions appearing in it:

$$\begin{aligned} f(x) &= F(x)f(a) + (x - a)^{\frac{1}{2}}f'(x), \\ g(x) &= G(x)g(a) + (x - a)^{\frac{1}{2}}g'(x), \\ K(x, y) &= K_1(x)K(a, y) + K(x, a)K_2(y) \\ &\quad - K_1(x)K_2(y)K(a, a) + (x - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}}K'(x, y). \end{aligned} \tag{2.8}$$

By retaining different functions $F(x)$, $G(x)$, $K_1(x)$, $K_2(x)$, we have still not achieved complete symmetry; but by using square roots we have "divided" the singularity between the two functions under the integral sign in (2.1). We could have achieved a little more generality by using arbitrary smooth functions having $x^{\frac{1}{2}}$-type zeros at $x = a$, and obtained some damping of the resulting integrals; this generalization is easily made when necessary and we will not pursue it in detail. The retention of four different transformation functions will clarify the origin of various cancellations which occur and, as we will see, will have other valuable features which justify the extra complication of the treatment.

Notice that if the singularity is to be effectively removed by the transformation (2.8), we must require that

$$\lim_{x\to a} F(x) = \lim_{x\to a} G(x) = \lim_{x\to a} K_1(x) = \lim_{x\to a} K_2(x) = 1, \tag{2.9}$$

and that, around $x = a$, continuity conditions of the Hölder type (Sec. 1.4) apply, to which we return later.

When (2.9) holds, separate first-order variations in the independent variables are taken care of by cancellation between pairs of the terms in the expansion for $K(x, y)$.

In attempting to obtain Eq. (2.2), we will wish to evaluate the integral

$$I[K', f'] \equiv \int K'(x, y)f'(y)\,dy, \tag{2.10}$$

which will be aided by a general notation for singular integrals:

$$P(x, \overline{y)Q(y, z)} \equiv \int \frac{P(x, y)Q(y, z)\,dy}{y - a}. \tag{2.11}$$

We obtain

$$\begin{aligned} &(x - a)^{\frac{1}{2}}I[K', f'] \\ &\quad = K(x, \overline{y)f(y)} - K(x, \overline{y)F(y)}f(a) \\ &\qquad - K_1(x)K(a, \overline{y)f(y)} + K_1(x)K(a, \overline{y)F(y)}f(a) \\ &\qquad - K(x, a)K_2(\overline{y)f(y)} + K(x, a)K_2(\overline{y)F(y)}f(a) \\ &\qquad + K_1(x)K_2(\overline{y)f(y)}K(a, a) \\ &\qquad - K_1(x)K_2(\overline{y)F(y)}f(a)K(a, a). \end{aligned} \tag{2.12}$$

We want this to be equal to the expression

$$(x-a)^{\frac{1}{2}}(f'(x)-g'(x))$$
$$\equiv f(x)-g(x)-(F(x)f(a)-G(x)g(a)). \quad (2.13)$$

It would be too complicated to discuss the most general way in which this could happen. However, we note that even without using Eq. (2.1), the last six terms cancel in horizontal pairs if we impose these simple restrictions on the transformation functions:

$$K(a,\overline{y)f(y)}=K(a,\overline{y)F(y)}f(a),$$
$$K_2\overline{(y)f(y)}=K_2\overline{(y)F(y)}f(a), \quad (2.14)$$

which we will do from now on. In this case the use of (2.1) gives

$$(x-a)^{\frac{1}{2}}I[K',f']=f(x)-g(x)-K(x,\overline{y)F(y)}f(a). \quad (2.15)$$

In order for (2.2) to hold, this must be equal to

$$(x-a)^{\frac{1}{2}}(f'(x)-g'(x))$$
$$=f(x)-g(x)-F(x)f(a)+G(x)g(a).$$

so that we want F and G to satisfy the integral equation

$$F(x)f(a)=G(x)g(a)+f(a)K(x,\overline{y)F(y)}. \quad (2.16)$$

At $x=a$, this reads

$$f(a)=g(a)+f(a)K(a,\overline{y)F(y)}, \quad (2.17)$$

whereas the original equation (2.1) reads, at $x=a$,

$$(a)=g(a)+K(a,\overline{y)f(y)} \quad (2.18)$$
$$\equiv g(a)+f(a)K(a,\overline{y)F(y)}+\int\frac{K(a,y)f'(y)}{(y-a)^{\frac{1}{2}}}\,dy. \quad (2.19)$$

In order that (2.17) and (2.19) shall be consistent, we must have

$$\int\frac{K(a,y)f'(y)\,dy}{(y-a)^{\frac{1}{2}}}=0. \quad (2.20)$$

Once we have ensured (2.20), the first cancellation condition of (2.14) will hold, provided that Eq. (2.1) holds at $x=a$. We will show later how to ensure (2.20). Then we can *calculate* $f(a)$ by (2.17). Having done this, we can calculate a $G(x)$ satisfying (2.16), with $G(a)=1$, by

$$G(x)=\frac{F(x)-K(x,\overline{y)F(y)}}{1-K(a,\overline{y)F(y)}}. \quad (2.21)$$

Similarly, for any K_2 of the form

$$K_2(x)=\frac{K''(\overline{z)K(z,x)}}{K''(\overline{z)K(z,a)}}, \quad (2.22)$$

the second of the cancellation conditions (2.14), together with (2.1) (this time for all x), is equivalent to

$$\int\frac{K_2(y)f'(y)\,dy}{(y-a)^{\frac{1}{2}}}=0. \quad (2.23)$$

These considerations may be summed up in the following:

Theorem 1: Provided suitable summability and continuity conditions hold, the transformation (2.8) may be used to reduce the singular integral equation (2.1) to the Fredholm form (2.2) in which the singularity is absent. We must pick F so that the conditions (2.9) and (2.20) hold, and must define G by (2.21); K_1 and K_2 are arbitrary, except that F, G, K_1, and K_2 must satisfy (2.9).

Theorems of this kind establish a correspondence between the original singular equation [such as (2.1)] and a certain *class* of Fredholm equations of the form (2.2). In order to make this correspondence more precise, we may try to answer the following questions:

A. Which of the functions F, G, K_1, K_2 can be chosen arbitrarily, and how must the others be specified, in order to set up an *equivalence* between the singular equation (2.1) and the Fredholm equation (2.2)?

B. Assuming now that the equivalence has been set up for one choice of arbitrary functions and that the Fredholm equation then has a unique solution (so that the singular equation has a well-defined solution), do we get the same solution to the singular equation by taking a different choice of the arbitrary functions permissible under A above?

In order to get an *existence* theorem for the equation, it is sufficient to give one (perhaps) special answer to question A, for this reduces the existence problem to that for Fredholm kernels, which is well-understood. If for some particular choice of K_1 and K_2 the operator-kernel $(1-K')$ is invertible, the answer to problem A will furnish us with a solution to the singular integral equation. If for this particular choice of K_1 and K_2, $(1-K')$ is not invertible, we may still consider whether it might be invertible for another choice of K_1 and K_2. Thus this method is capable of yielding an existence theorem, but not (at least in its present form) a precise *non*existence theorem.

Furthermore, it may be that the Fredholm equation *has* solutions, but that these are not unique. Now this can only happen if the homogeneous Fredholm equation has a solution. In the Bethe–Salpeter equation, we expect this situation to arise where there are bound states and resonances. Naturally, if the homogeneous Fredholm equation *does* have a solution, we will want to inquire whether this could give rise to a solution of the *inhomogeneous* singular equation. In our symbols, can we have $g'=0$ but $g\neq 0$? We

cannot answer this question in full generality; but it is clear that such a situation cannot arise through the cancellation of the last six terms of (2.12). For now (2.16) is, for all practical purposes, equivalent to the original integral equation—instead of computing $G(x)$ from it, we must compute $F(x)$ from it. In other words, the expansion (2.8) has not simplified the problem. For the moment we assume that this oddity can be ignored.

These remarks should be taken as a guide to what can reasonably be expected of the present method. From now on we will restrict ourselves to the choice

$$K_2(x) = K(a, x)/K(a, a). \tag{2.24}$$

This is motivated partly by features of the two-dimensional case which we will observe in the next subsection. At the cost of abandoning any choice in the kernel K', it simplifies the expansion of K to

$$K(x, y) = \frac{K(x, a)K(a, y)}{K(a, a)} + (x - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}}K'(x, y). \tag{2.25}$$

It also simplifies the two cancellation conditions, making them equivalent. Thus we have no need to refer further to (2.23).

The task of dealing with problem A [within the limits of (2.24)] has now been reduced to showing how $F(x)$ can be used to ensure that (2.20) holds. For this purpose we take any function $H(x)$, vanishing at $x = a$, and define

$$F(u, x) = 1 + u(x - a) + H(x). \tag{2.26}$$

Now we suppose that $(1 - K')$ has an inverse, without which, as we remarked earlier, we cannot hope to get any definite result at all. Under these circumstances, by defining a "trial" G by

$$G(u, x) = \frac{F(u, x) - K(x, \overline{y)F(u, y)}}{1 - K(a, \overline{y)F(u, y)}}, \tag{2.27}$$

we obtain a "trial" $g'(u, y)$ by

$$g'(u, x) = (x - a)^{\frac{1}{2}}[G(u, x)g(a) - g(x)], \tag{2.28}$$

giving a "trial" $f'(x)$ by

$$f'(x) = \int (1 - K')^{-1}(x, y)g'(u, y)\, dy.$$

Now we can consider the expression

$$\mathfrak{L}(u) = \frac{K(a, y)(1 - K')^{-1}(y, x)g'(u, x)\, dy\, dx}{(y - a)^{\frac{1}{2}}}. \tag{2.29}$$

$\mathfrak{L}(u)$ is a well-defined, *fractional-linear* function of u—say

$$\mathfrak{L}(u) = \frac{A + Bu}{C + Du}. \tag{2.30}$$

Thus the equation $\mathfrak{L}(u) = 0$ will have a *unique* solution u_0, say (provided $B \neq 0$—this is not difficult to ensure); and so if we define $F(x)$ by

$$F(x) = F(u_0, x), \tag{2.31}$$

condition (2.20) holds and so *the cancellation conditions* (2.14) *hold.*

This completes the proof of the existence theorem for the singular equation when the Fredholm kernel K', given by (2.25), is such that $(1 - K')$ is invertible.

We have shown that $F(x)$ still contains the arbitrary component $H(x)$ [in Eq. (2.26)]. The form of uniqueness problem set up under B above may now be formulated more precisely:

Suppose we take two *different* functions $H_1(x)$ and $H_2(x)$, giving solutions $u_{0,1}$ and $u_{0,2}$ of (2.30), etc., and calculate solutions $f_1(x), f_2(x)$ of the singular equation. Are these solutions identical?

We will now show, under the same assumptions as before, that they are indeed identical. Thus the arbitrariness of H does not lead to any lack of uniqueness of the solution.

We will do this by calculating the expression $(1 - K')f^-$, where

$$f^-(x) = \frac{f_1(x) - f_2(x)}{(x - a)^{\frac{1}{2}}}. \tag{2.32}$$

Indeed, writing

$$F^-(x) = \frac{F_1(x)f_1(a) - F_2(x)f_2(a)}{(x - a)^{\frac{1}{2}}}, \tag{2.33}$$

and using the fact that f_1' and f_2' solve the Fredholm equations, we have

$$(1 - K')f^- = (1 - K')F^- + g_1' - g_2'. \tag{2.34}$$

The right-hand side of (2.34) can be calculated explicitly. By using the expansions of g and K, we get

$$\int \frac{K'(x, y)}{(y - a)^{\frac{1}{2}}}[F_1(y)f_1(a) - F_2(y)f_2(a)]\, dy = (x - a)^{-\frac{1}{2}}\left\{\left[K(x, \overline{y)F_1(y)} - \frac{K(x, a)}{K(a, a)}K(a, \overline{y)F_1(y)}\right]f_1(a) - \left[K(x, \overline{y)F_2(y)} - \frac{K(x, a)}{K(a, a)}K(a, \overline{y)F_2(y)}\right]f_2(a)\right\}$$

and

$$g_1'(x) - g_2'(x) = -\frac{g(a)}{(x - a)^{\frac{1}{2}}}\left\{\frac{F_1(x) - K(x, \overline{y)F_1(y)}}{1 - K(a, \overline{y)F_1(y)}} - \frac{F_2(x) - K(x, \overline{y)F_2(y)}}{1 - K(a, \overline{y)F_2(y)}}\right\}.$$

We see that almost everything cancels to give

$$(1 - K')f^- = -\frac{K(x, a)}{K(a, a)} g(a)[f_1(a) - f_2(a)]. \quad (2.35)$$

Now we argue that, since $(1 - K')$ is invertible, $(1 - K')f^- = 0$ is equivalent to $f^- = 0$ (which is what we want to prove). Thus we only have to show that $f_1(a) = f_2(a)$. But $f_1(x)$ and $f_2(x)$ are, by construction, solutions of (2.1). We can expand $f_2(x)$ by using F_1 (rather than F_2). From the construction of F_1, the condition (2.20) holds. But it is now equivalent to $f_2(a) = g(a)[1 - K(a, y)\overline{F_1(y)}]^{-1}$, i.e., to precisely the expression used to calculate $f_1(a)$ [compare (2.16)]. That is to say, the fact that f_2 is a solution has been used to show that $f_2(a) = f_1(a)$. As we remarked, (2.35) now shows that $f_2(x) = f_1(x)$ everywhere.

Q.E.D.

To sum up, we have given a complete treatment of the case $K_2(x) = K(a, x)/K(a, a)$. We have shown that if the kernel $1 - K'$ arising from this choice is invertible (so that the Fredholm equation has a unique solution), then the original singular equation also has a *unique* solution independent of the arbitrariness in the choice of $F(x)$ by Eq. (2.31).

The general method of dealing with other functions K_2 of the form (2.23) is clear (take another term in the Taylor expansion of $F(x)$ about $x = a$). We will not go into details here. Generally, we see that we are very far from the powerful uniqueness theorem (Fredholm alternative) available for Fredholm equations. This uniqueness problem is clearly important for applications, particularly where numerical computation is contemplated, and we will deal with it more fully elsewhere. On the other hand, we believe that we have now achieved a reasonably satisfactory existence result.

We turn now to a more detailed discussion of the square summability and continuity conditions at $x = a$, required for the application of Theorems 1 and 2.

In the problem of Eq. (2.1), there will be no nonintegrable singularities around $x = a$ provided, say, that $f(x)$ and $g(x)$ satisfy Hölder conditions $H(\mu)$ at $x = a$ with $\mu \geq \frac{1}{2}$, and that $K(x, y)$ satisfies a Hölder condition $H(\mu, \mu)$ at $(x, y) = (a, a)$ with $\mu \geq \frac{1}{2}$ [these conditions arise from Eq. (2.8)], and provided also that the arbitrary functions F, K_1 are $H(\mu)$ at $x = a$ [this arises from (2.12)]. (As we will see later, although weaker Hölder conditions can be given, there is no point in going into more detail.) Again, a symmetrical treatment will also impose Hölder conditions on the other functions G, K_2.

The integrals in (2.12) will then converge, for instance, provided that the following functions are square-summable at infinity in y, when multiplied by $y^{\frac{1}{2}}$:

$$K(x, y); \quad F(y); \quad f(y); \quad K_2(y).$$

These conditions already ensure that $f'(x)$ is a square-summable function. The function $g'(x)$ will be square-summable provided that in addition, $x^{\frac{1}{2}}g(x)$ and $x^{\frac{1}{2}}G(x)$ are square-summable at infinity. Finally, $K'(x, y)$ will be double-square-summable provided that $x^{\frac{1}{2}}K_1(x)$ and $x^{\frac{1}{2}}K(x, a)$ are square-summable at infinity, and that $x^{\frac{1}{2}}y^{\frac{1}{2}}K(x, y)$ is double-square-summable at infinity. Again, these are by no means the weakest conditions that can be imposed, if one is willing to go to enough trouble, but they have the merit of allowing a completely symmetric treatment. One may consider relaxing these conditions in a different way on g and f, but in the case of the Bethe–Salpeter equation, the considerations of Sec. 1.2 apply and make it unlikely that this will lead to greater generality.

In this situation, then, Eq. (2.2) can be handled by the usual methods of Fredholm theory, and will give a square-summable solution $f'(x)$, so that the function

$$\frac{f(x) - F(x)f(a)}{(x - a)^{\frac{1}{2}}},$$

will be square-summable; the singularity is not getting worse.

Now suppose that all the conditions on the kernel K hold. Then K' defines a transformation which we will also label K', from $L^2(-\infty, \infty)$ into itself, with norm

$$\|K'\|^2 = \int |K'(x, y)|^2 \, dx \, dy,$$

so that then we may extend the treatment to *any* functions f, g such that f', g' are square-summable, regardless of whether or not the Hölder conditions apply.

The further paragraphs of this section will be concerned with generalizations of the procedure of Theorem 1 to the following situations:

Sec. 2.2: equations between kernel functions;

Sec. 2.3: equations with singularities in two intermediate variables;

Sec. 2.4: equations with several singularities in each intermediate variable;

Sec. 2.5: further generalizations.

2.2. Equations Between Kernel Functions

We now consider how to transform Eq. (2.7) in a fashion reasonably symmetrical between the two variables. In principle, we use transformation equations for all three functions similar to those for

$K(x, y)$ in (2.8). The case $G = K_1$ must be used if we wish to have $g = K$ in (2.7). If we wish to regard the multiplication in (2.7) as giving rise to an algebra structure on the class of kernels (Sec. 1.2), we must have K_1, K_2, etc. Notice that the transformation will never be a homomorphism of such an algebra structure, since it is dependent on the special kernel K. However, we may obtain a homomorphism of the algebra generated by K, etc. But in general, if we wish to use the algebra structure defined by the equations, we must use that of the *transformed* equations.

We want to transform both sets of variables at once. Now it is simply not true that the transformation (2.8) takes the integral in (2.7) into the form

$$J[K', f'] \equiv \int K'(x, z) f'(z, y)\, dz. \tag{2.36}$$

This works only for the special kernel K of Eq. (2.1). For this reason we have to write down transformation equations analogous to (2.8) for three functions each of two variables, and calculate the integral (2.20). We take, then, the transformations

$$\begin{aligned} f(x, y) &= F_1(x) f(a, y) + f(x, a) F_2(y) - F_1(x) F_2(y) f(a, a) + (x - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}} f'(x, y), \\ g(x, y) &= G_1(x) g(a, y) + g(x, a) G_2(y) - G_1(x) G_2(y) g(a, a) + (x - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}} g'(x, y), \\ K(x, y) &= K_1(x) K(a, y) + K(x, a) K_2(y) - K_1(x) K_2(y) K(a, a) + (x - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}} K'(x, y), \end{aligned} \tag{2.37}$$

giving the following expression:

$$\begin{aligned} &(x - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}} J[K', f'] \\ &= + K(x, \overline{z) f(z}, y) - K(x, \overline{z) F_1(z}) f(a, y) - K(x, \overline{z) f(z}, a) F_2(y) + K(x, \overline{z) F_1(z}) F_2(y) f(a, a) \\ &\quad - K_1(x) K(a, \overline{z) f(z}, y) + K_1(x) K(a, \overline{z) F_1(z}) f(a, y) + K_1(x) K(a, \overline{z) f(z}, a) F_2(y) - K_1(x) K(a, \overline{z) F_1(z}) F_2(y) f(a, a) \\ &\quad - K(x, a) K_2(\overline{z) f(z}, y) + K(x, a) K_2(\overline{z) F_1(z}) f(a, y) + K(x, a) K_2(\overline{z) f(z}, a) F_2(y) - K(x, a) K_2(\overline{z) F_1(z}) F_2(y) f(a, a) \\ &\quad + K(a, a)[K_1(x) K_2(\overline{z) f(z}, y) + K_1(x) K_2(\overline{z) F_1(z}) f(a, y) - K_1(x) K_2(\overline{z) f(z}, a) F_2(y) + K_1(x) K_2(\overline{z) F_1(z}) F_2(y) f(a, a)]. \end{aligned} \tag{2.38}$$

As before, we can remove everything except the top row by imposing on the arbitrary functions the cancellation conditions

$$K(a, \overline{z) f^*(z}, y) = K(a, \overline{z) F_1(z}) f^*(a, y), \tag{2.39}$$

$$K_2(\overline{z) f^*(z}, y) = K_2(\overline{z) F_1(z}) f^*(a, y), \tag{2.40}$$

where

$$f^*(x, y) = f(x, y) - f(x, a) F_2(y). \tag{2.41}$$

The original singular equation reads, at $x = a$,

$$\begin{aligned} f(a, y) &= g(a, y) + K(a, \overline{z) f(z}, y) && (2.42) \\ &\equiv g(a, y) + K(a, \overline{z) f^*(z}, y) \\ &\qquad + K(a, \overline{z) f(z}, a) F_2(y), && (2.43) \end{aligned}$$

and expansion of $f(z, y)$ in (2.42) yields

$$\begin{aligned} f(a, y) = g(a, y) &+ K(a, \overline{z) F_1(z}) f^*(a, y) \\ &+ K(a, \overline{z) f(z}, a) F_2(y) \\ &+ (y - a)^{\frac{1}{2}} \int \frac{K(a, z) f'(z, y)\, dy}{(z - a)^{\frac{1}{2}}}. \end{aligned} \tag{2.44}$$

Suppose we can choose the arbitrary functions so that

$$\int \frac{K(a, z) f'(z, y)\, dy}{(z - a)^{\frac{1}{2}}} = 0. \tag{2.45}$$

(We will show later how this can be done.) Then comparison of (2.44) with (2.43) shows that the first cancellation condition (2.39) will hold.

Now we suppose further that the one-dimensional problem

$$f(x, a) = g(x, a) + K(x, \overline{y) f(y}, a), \tag{2.46}$$

has been solved by the method of the previous subsection. Knowing $f(x, a)$, we can compute $f(a, y)$ from (2.44) (dropping the last term). Now we return to the residual terms remaining when the cancellation conditions (2.34–40) are fulfilled. In order to ensure that Eq. (2.7) reduces to the form

$$f'(x, y) = g'(x, y) + \int K'(x, z) f'(z, y)\, dy, \tag{2.47}$$

the following relation must hold between the residual terms [compare (2.16)]:

$$\begin{aligned} &F_1(x) f^*(a, y) - G_1(x) g^*(a, y) + f(x, a) F_2(y) \\ &\qquad - g(x, a) G_2(y) - G_1(x) g(a, a)[F_2(y) - G_2(y)] \\ &= K(x, \overline{z) f(z}, a) F_2(y) + K(x, \overline{z) F_1(z}) f^*(a, y), \end{aligned} \tag{2.48}$$

where (*sic*)

$$g^*(x, y) = g(x, y) - g(x, a) F_2(y). \tag{2.49}$$

By using (2.46), we can rewrite (2.48) in the form

$$F_1(x)f^*(a, y) - G_1(x)g^*(a, y) = [g(x, a) - G_1(x)g(a, a)][F_2(x) - G_2(x)] + K(x, \overline{z)F_1(z)}f^*(a, y). \quad (2.50)$$

We note that since the condition (2.45) is assumed here to hold, (2.50) becomes, at $x = a$, the *identity*

$$f^*(a, y) = g^*(a, y) + K(a, \overline{z)F_1(z)}f^*(a, y).$$

Substituting back into (2.50), we see that (2.50) follows from the following two explicit restrictions on the arbitrary functions:

$$F_2(x) = G_2(x), \quad (2.51)$$

$$G_1(x) = \frac{F_1(x) - K(x, \overline{z)F_1(z)}}{1 - K(a, \overline{z)F_1(z)}}, \quad (2.52)$$

[compare this latter with (2.21)]. Thus the residual condition holds when (2.41–42) hold, and we can go on to show how the cancellation conditions may be made to hold.

We will do this in detail only for the special case where

$$K_2(x) = K(a, x)/K(a, a), \quad (2.53)$$

just as in Sec. 2.1. Then the two cancellation conditions (2.19–20) are identical. We now show how, by the choice of G_2 [upon which there is as yet no restriction if we regard (2.51) as a formula giving F_2], (2.45) can be ensured. We write

$$g'(x, y) = \frac{g^{**}(x, y) - g^{**}(x, a)G_2(y)}{(y - a)^{\frac{1}{2}}}, \quad (2.54)$$

where

$$g^{**}(x, y) = \frac{g(x, y) - G_1(x)g(a, y)}{(x - a)^{\frac{1}{2}}}. \quad (2.55)$$

As usual we suppose that the kernel $(1 - K')$ is invertible, with the inverse represented by a function (or distribution—the difference is unimportant here), $L(x, y)$ say. Then, if $f'(x, y)$ is the unique solution of (2.47), so that $f' = Lg'$, we have

$$\int \frac{K(a, z)f'(z, y)\,dz}{(z - a)^{\frac{1}{2}}} = \iint \frac{K(a, z)L(z, w)g^{**}(w, y) - g^{**}(w, a)G_2(y)\,dz\,dw}{(z - a)^{\frac{1}{2}}(y - a)^{\frac{1}{2}}}. \quad (2.56)$$

Thus (2.45) will hold if we make the following choice of G_2:

$$G_2(x) = \iint \frac{K(a, z)L(z, w)g^{**}(w, x)\,dz\,dw}{(z - a)^{\frac{1}{2}}} \Big/ \iint \frac{K(a, z)L(z, w)g^{**}(w, a)\,dz\,dw}{(z - a)^{\frac{1}{2}}}. \quad (2.57)$$

We note that $G_2(a) = 1$ automatically for this choice. We must make sure that the denominator of (2.57) does not vanish; one sees easily that this essentially means *not* using F_1 for the expansion of $f(x, a)$ when solving (2.46), but by using another expansion function and appealing to the uniqueness theorem proven in Sec. 2.1.

This sequence of constructions may be summed up as follows:

If the K' arising from the choice $K_2(x) = K(x, a)/K(a, a)$ is such that $(1 - K')$ is invertible, we may choose F_1 arbitrarily [subject to $F_1(a) = 1$]; G_1 is defined by (2.52), and G_2 is defined in terms of G_1 and (implicitly) K_2 by (2.57). Then (2.45) holds. Take $F_2 = G_2$. Then $f(a, y)$ may be computed by first solving (2.46) [our assumption on $(1 - K')$ assures us that there is a unique solution $f(x, a)$] and then using (2.44–45). Then the residual condition (2.48) is assured, and the singular equation is reduced to the Fredholm equation. Conversely, with the same choices, the solution f' of the Fredholm equation gives rise to a solution $f(x, y)$ of the singular equation [computed by (2.37)].

We will not state a formal uniqueness result corresponding to that of Sec. 2.1, but will defer this rather complicated question to a future publication. A formal summing up of the existence results is provided by the following two statements:

Theorem 2: Provided that suitable continuity and square summability conditions hold, the expansion (2.37) reduces the singular integral equation (2.42) to the Fredholm form (2.47), if the arbitrary functions F_i, G_i, K_i $(i = 1, 2)$ are chosen so as to satisfy the cancellation conditions (2.39)–(2.40) and the residual condition (2.48).

Theorem 3: In theorem 2, take $K_2(x) = K(a, x)/K(a, a)$. K_1 is now redundant. Suppose the resulting kernel

$$K'(x, y) = [(x - a)(y - a)]^{-\frac{1}{2}} \times \left[K(x, y) - \frac{K(x, a)K(a, y)}{K(a, a)}\right],$$

is such that $(1 - K')$ is invertible. Then there exists a choice of arbitrary functions for which the cancellation and residual conditions are satisfied, so that the singular equation possesses a solution.

We note that these methods do not allow us to preserve directly the *commutativity* property

$$K(x, \overline{y)f(y}, z) = f(x, \overline{y)K(y}, z), \quad (2.58)$$

of the equation (where it holds). That is, if (2.58) is

known to hold, we cannot ensure *directly* that the Fredholm equation has the corresponding property

$$\int K'(x, y)f'(y, z)\,dy = \int f'(x, y)K'(y, z)\,dy. \quad (2.59)$$

We cannot *at the same time and by the same methods* cause the equation

$$f(x, y) = g(x, y) + f(x, \overline{z)K(z}, y), \quad (2.60)$$

to imply

$$f'(x, y) = g(x, y) + \int f'(x, z)K'(z, y)\,dz. \quad (2.61)$$

This is because the cancellation condition required to pass from (2.60) to (2.61) by our methods is

$$\int \frac{f'(x, z)K(z, a)\,dz}{(z-a)^{\frac{1}{2}}} = 0, \quad (2.62)$$

and would have to be ensured by judicious choice of G_1. But we are not at liberty to fix G_1 *ab initio* because we could not then solve (2.52) for F_1.

This commutativity is most interesting in the "reciprocal kernel" case whose algebraic properties are mentioned in the Introduction, i.e., the case $g(x, y) = K(x, y)$. Our treatment does not preserve this property [$g'(x, y) \neq K'(x, y)$]. Where the commutativity property is important, it seems indicated to give a treatment along the present lines using the expansions

$$\begin{aligned} f(x, y) &= F_1(x)f(a, y) + f(x, a)F_2(y) \\ &\quad - F_1(x)F_2(y)f(a, a) \\ &\quad + (x-a)^{\frac{1}{2}}(y-a)^{\frac{1}{2}}f'(x, y), \\ g(x, y) &= \frac{g(x, a)g(a, y)}{g(a, a)} \\ &\quad + (x-a)^{\frac{1}{2}}(y-a)^{\frac{1}{2}}g'(x, y), \\ K(x, y) &= \frac{K(x, a)K(a, y)}{K(a, a)} \\ &\quad + (x-a)^{\frac{1}{2}}(y-a)^{\frac{1}{2}}K'(x, y). \end{aligned} \quad (2.63)$$

[Note that this type of expansion, $F_2(y) = f(a, y)/f(a, a)$, will not do for $f(x, y)$ since it leads to a nonlinear problem.] We leave details to the reader.

Now let us return briefly to our original expansion method (2.37) and see what happens when we take for K_2 some function other than $K(a, y)/K(a, a)$. We take for K_2 the form (2.22), where $K''(x)$ is as yet undetermined. We introduce the notation

$$\bar{f}(y) = K''(\overline{z)f(z}, y), \quad \text{etc.}, \quad (2.64)$$

$$\bar{F}_1 = K''(\overline{z)F_1(z}), \quad \text{etc.}, \quad (2.65)$$

so that

$$K''(\overline{z)K(z}, a) = \bar{K}(a).$$

Inserting this definition of K_2 into the last transformation equation (2.37), we obtain

$$0 = \bar{K}_1(K(a, y) - K_2(y)K(a, a)) - (y-a)^{\frac{1}{2}}\int \frac{K''(z)K'(z, y)\,dz}{(z-a)^{\frac{1}{2}}}. \quad (2.66)$$

Since the second cancellation condition (2.40) is equivalent to

$$\int \frac{K_2(z)f'(z, y)\,dz}{(z-a)^{\frac{1}{2}}} = 0, \quad (2.67)$$

(2.66) tells us that it is also equivalent to

$$\bar{K}_1 \int \frac{K(a, z)f'(z, y)\,dz}{(z-a)^{\frac{1}{2}}} = (y-a)^{\frac{1}{2}} \iint \frac{K''(u)K'(u, z)f'(z, y)\,du\,dz}{(u-a)^{\frac{1}{2}}(z-a)^{\frac{1}{2}}}, \quad (2.68)$$

always provided that

$$\bar{K}_1 K(a, a) \neq 0. \quad (2.69)$$

But if the first cancellation condition (2.39) is satisfied, the left-hand side of (2.68) vanishes. Thus the second cancellation condition (2.40) will automatically be satisfied at $y = a$; and it will be satisfied for all y provided that the double integral in (2.68) vanishes (identically in y). This is a condition on a function of one variable, and hence we are not losing much by looking for the particular case where

$$\int \frac{K''(u)K'(u, y)\,du}{(u-a)^{\frac{1}{2}}} = 0, \quad (2.70)$$

i.e.,

$$K_2(y)\bar{K}_1 K(a, a) = \bar{K}_1 K(a, y),$$

which determines K_2 uniquely:

$$K_2(y) = K(a, y)/K(a, a),$$

[so that $K''(y)$ is actually a distribution of a rather special sort]. No other choice of K_2 will allow the cancellation by a mechanism which depends on f' only through (2.39). The only other freedom we can use to make sure that (2.67) holds is that in K_2 itself. But (2.67) is *nonlinear in* K_2 (for K_2 enters implicitly also in $f' = Lg'$); this makes it very difficult to give an explicit condition on K_2 other than, of course, $K_2(x) = K(a, x)/K(a, a)$. Thus we will not consider this possibility further.

The constructions we have given are specialized not only in the sense that the mechanism used to ensure the residual condition (2.48) is specialized (however natural in appearance), but, more generally, in that we have caused the last three rows of (2.38) to vanish *separately* by the cancellation conditions (2.39–40). One may investigate whether this can be generalized so that the last three rows still vanish. We have done this, and it turns out that the only

alternative to the choice $K_2(x) = K(a, x)/K(a, a)$ leads to a homogeneous-linear constraint for K_2 which, in general, will have no solution. Since this apparent generalization thus leads nowhere, we omit the details.

Finally, we mention the possibility of using for kernel functions, a slightly different type of expansion more closely related to, but simpler than, the Taylor expansions used in Ref. 15. For instance, we may try

$$f(x, y) = f(a, a) + (x - a)f_1(x) + (y - a)f_2(y) + (x - a)(y - a)f'(x, y),$$
$$g(x, y) = g(a, a) + (x - a)g_1(x) + (y - a)g_2(y) + (x - a)(y - a)g'(x, y),$$
$$K(x, y) = K(a, a) + (x - a)K_1(x) + (y - a)K_2(y) + (x - a)(y - a)K'(x, y).$$

This leads to a system of *coupled* Fredholm equations, for which we will evidently have a uniqueness theorem. However, because of the limitations of our expansion, there is no hope of extending such a uniqueness theorem to functions which are not differentiable in x or y at a, but are still functions of the type (2.37).

2.3. Equations with Singularities in Two Intermediate Variables

The physical importance of this generalization is obvious.

We take as our basic equation

$$f(x) = g(x) + \int \frac{K(x, z_1, z_2)f(z_1, z_2)\, dz_1\, dz_2}{(z_1 - a)(z_2 - a)}, \quad (2.71)$$

where $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, etc. Equation (2.70) thus corresponds to a Bethe–Salpeter or similar equation in which two-particle intermediate states are exposed in the direct channel. However, we have not indicated the "kernel" nature of all the functions explicitly, so that we are generalizing Sec. 2.1 but not, as yet, Sec. 2.2. In Ref. 15 we used an expansion of the form

$$f(x_1, x_2) = g(x_1, x_2) + (x_1 - a)m_1(x_1) + (x_2 - a)m_2(x_2) + (x_1 - a)(x_2 - a)n(x), \quad (2.72)$$

in order to obtain equations between functions in certain L^p spaces. However, this time we use the more flexible procedures introduced in the previous sections. For simplicity, we will give a rather "asymmetric" treatment of (2.71) in which the x variable in K is left entirely alone, briefly indicate how the cancellations arise, and then sketch a more "symmetrical" treatment. As might be expected, the formulas rapidly become extremely cumbersome.

We use the expansions

$$\begin{aligned} f(x_1, x_2) &= F_1(x_1)F_2(x_2)f(a, a) - F_1(x_1)f(a, x_2) - F_2(x_2)f(x_1, a) + (x_1 - a)^{\frac{1}{2}}(x_2 - a)^{\frac{1}{2}}f'(x_1, x_2), \\ g(x_1, x_2) &= G_1(x_1)G_2(x_2)g(a, a) - G_1(x_1)g(a, x_2) - G_2(x_2)g(x_1, a) + (x_1 - a)^{\frac{1}{2}}(x_2 - a)^{\frac{1}{2}}g'(x_1, x_2), \\ K(x, y_1, y_2) &= K_1(y_1)K_2(y_2)K(x, a, a) - K_1(y_1)K(x, a, y_2) - K_2(y_2)K(x, y_1, a) + (y_1 - a)^{\frac{1}{2}}(y_2 - a)^{\frac{1}{2}}K'(x, y_1, y_2). \end{aligned} \quad (2.73)$$

Then, introducing the generalized integral notation

$$K(x, \overline{y)f(y)} = \int \frac{K(x, y_1y_2)f(y_1, y_2)\, dy_1\, dy_2}{(y_1 - a)(y_2 - a)}, \quad \text{etc.}, \quad I[K', f'] = \int K'(x, y_1, y_2)f'(y_1, y_2)\, dy_1\, dy_2, \quad \text{etc.},$$

we obtain the expression corresponding to (2.38):

$$\begin{aligned} &I[K,f'] \\ &= K(x, \overline{y)f(y)} - K(x, \overline{y_1, y_2)f(a, y_2)}F_1(y_1) - K(x, \overline{y_1, y_2)F_2(y_2)f(y_1, a)} + J(x, \overline{y_1,, y_2)F_1(y_1)F_2(y_2)}f(a, a) \\ &\quad - K(x, a, \overline{y_2)K_1(y_1)f(y_1, y_2)} + K(x, a, \overline{y_2)K_1(y_1)f(a, y_2)}F_1(y_1) + K(x, a, \overline{y_2)K_1(y_1)F_2(y_2)f(y_1, a)} - K(x, a, \overline{y_2)K_1(y_1)F_1(y_1)F_2(y_2)}f(a, a) \\ &\quad - K(x, \overline{y_1, a)K_2(y_2)f(y_1, y_2)} + K(x, \overline{y_1, a)K_2(y_2)f(a, y_2)}F_1(y_1) + K(x, \overline{y_1, a)K_2(y_2)F_2(y_2)f(y_1, a)} - K(x, \overline{y_1, a)K_2(y_2)F_1(y_1)F_2(y_2)}f(a, a) \\ &\quad + K(x, a, a)\{K_1(y_1)K_2(y_2)f(y_1, y_2) - K_1(y_1)K_2(y_2)F_1(y_1)f(a, y_2) - K_1(y_1)K_2(y_2)f(y_1, a)F_2(y_2) + K_1(y_1)K_2(y_2)F_1(y_1)F_2(y_2)f(a, a)\}. \end{aligned} \quad (2.74)$$

Here the second row will cancel identically if *either* of the relations

$$K(x, a, \overline{y_2)f(y_1, y_2)} = K(x, a, \overline{y_2)F_2(y_2)}f(y_1, a),$$
$$K_1(\overline{y_1)f(y_1, y_2)} = K_1(\overline{y_1)F_1(y_1)}f(a, y_2) \quad (2.75)$$

holds; the third will cancel identically if *either* of the relations

$$K(x, \overline{y_1, a)f(y_1, y_2)} = K(x, \overline{y_1, a)f_1(y_1)}f(a, y_2),$$
$$K_2(\overline{y_2)f(y_1, y_2)} = K_2(\overline{y_2)F_2(y_2)}f(y_1, a) \quad (2.76)$$

holds; finally, the vanishing of the fourth row may be ensured by a scalar condition which may be written in obvious notation

$$(K_1K_2f) - (K_1F_1)(K_2f) - (K_1f)(K_2F_2) + (K_1F_1)(K_2F_2) = 0,$$

with

$$(K_2f) = K_2(\overline{y_2)f(a, y_2)}, \quad \text{etc.}$$

Then the imposition of further conditions assuring that the integral equation can be written in

nonsingular form will follow the same general pattern as in previous cases.

A more "symmetric" treatment would take the following general course. In order to handle the rather complicated expressions, we introduce a matrix notation

$$X^\alpha(x) = \begin{pmatrix} & 1 & \\ & 1 & \\ & 1 & \\ (x_1 - a)^{\frac{1}{2}}(x_2 - a)^{\frac{1}{2}} & & \end{pmatrix},$$

$$F_\alpha(x) = (F_1(x_1)F_2(x_2)f(a, a), -F_1(x_1)f(a, x_2), -F_2(x_2)f(x_1, a), f'(x)),$$

so that the natural transformation

$$f(x) = F_1(x_1)F_2(x_2)f(a, a) - F_1(x)f(a, x_2) - F_2(x_2)f(x_1, a) + (x_1 - a)^{\frac{1}{2}}(x_2 - a)^{\frac{1}{2}}f'(x, y)$$

takes the form

$$f(x) = X^\alpha(x)F_\alpha(x). \tag{2.77}$$

Similarly, we write

$$g(x) = X^\alpha(x)G_\alpha(x) \tag{2.78}$$

and

$$K(x, y) = X^\alpha(x)K_{\alpha\beta}(x, y)X_\beta(y), \tag{2.79}$$

where the G_α in (2.78) is obvious and the matrix $K_{\alpha\beta}$ of (2.79) has the elements

$$K_{\alpha\beta}(x, y) = \begin{pmatrix} K^1(x_1)K^2(x_2)K_1(y_1)K_2(y_2)K(aaaa), & K^1(x_1)K^2(x_2)K_2(y_2)K(aay_1a), & K^1(x_1)K^2(x_2)K_1(y_1)K(aaay_2), & K^1(x_1)K^2(x_2)K(aay_1y_2), \\ K(x_1aaa)K^2(x_2)K_1(y_1)K_2(y_2), & K^2(x_2)K_2(y_2)K(x_1ay_2a), & K^2(x_2)K_1(y_1)K(x_1aay_2), & K^2(x_2)K(x_1ay_1y_2), \\ K^1(x_1)K(ax_2aa)K_1(y_1)K_2(y_2), & K^1(x_1)K_2(y_2)K(ax_2y_1a), & K^1(x_1)K_1(y_1)K(ax_2ay_2), & K^1(x_1)K(ax_2y_1y_2), \\ K(x_1x_2aa)K_1(y_1)K_2(y_2), & K_2(y_2)K(x_1x_2y_1a), & K_1(y_1)K(x_1x_2ay_2), & K'(x_1x_2y_1y_2), \end{pmatrix} \tag{2.80}$$

in which the K^s and K_s are the usual arbitrary functions and the $K(pqrs) = K(p, q, r, s)$ are the values of the original kernel K with appropriate independent variables held fixed at a, as indicated, and finally $K'(x_1x_2y_1y_2) = K'(x, y)$ is the function which is to appear in the transformed integral equation. The integral equation now takes the form

$$X^\alpha(x)[F_\alpha(x) - G_\alpha(x)] = \int X^\alpha(x)K_{\alpha\beta}(x, z) \times X^\beta(z)X^\gamma(z)F_\gamma(z)\,dz. \tag{2.81}$$

The conditions under which cancellations occur in this equation and under which it can be reduced to the nonsingular form

$$f'(x) = g'(x) + \int K'(x, z)f'(z)\,dz,$$

are again closely related to those of the previous sections and can be written down by the same methods used in Ref. 15. Here, however, the integral equations corresponding to the first three "components" of (2.81) are to be regarded as subsidiary conditions on the arbitrary functions. The details of these manipulations, as well as those where the full treatment of kernel functions is carried out, are left to the reader.

2.4. Several Singularities in Each Intermediate Variable

The characteristic complication with which we deal in this section arises when we consider, instead of Eq. (2.1), the equation

$$f(x) = g(x) + \int \frac{K(x, y)f(y)\,dy}{(y - a_1)(y - a_2)}, \tag{2.82}$$

with $a_1 \neq a_2$. We may say that there are two singularities in the intermediate variable y. Moreover, in an obvious sense, these singularities are *nonoverlapping*; they cannot occur simultaneously for any value of the variable y. In the case where there is only one intermediate variable, this situation is fairly general; the only further difficulty that can occur is exhibited by the equation

$$f(x) = g(x) + \int \frac{K(x, y)f(y)\,dy}{D(y)}, \tag{2.83}$$

where $D(y)$ may have zeros of order higher than one. As we have observed before, such singularities do not present anything of interest, since they must necessarily be cancelled by zeros of suitable order in the numerator if the integral is to be well defined.

A significantly more complicated situation may occur with two or more intermediate variables, however. Consider the equation

$$f(x_1, x_2) = g(x_1, x_2) + \int \frac{K(x_1x_2y_1y_2)f(y_1y_2)\,dy_1\,dy_2}{D(y_1, y_2)}, \tag{2.84}$$

where the denominator function $D(y_1, y_2)$ has certain zeros which we wish to eliminate. It may be that for general values of y_1, D has only first-order zeros in y_2 and vice versa; and yet for certain (y_1, y_2), D may have a higher-order zero. This complication already occurs for the simple choice

$$D(y_1, y_2) = (y_1 - a_1)(y_1 - a_1')(y_2 - a_2)(y_2 - a_2'), \tag{2.85}$$

with $a_1 \neq a_1' \neq a_2 \neq a_2'$, and may be described by

saying that the singularities *overlap*. An important case where they do not overlap is that of a function

$$D(y_1, y_2) = [y_1 - g_1(y_2)][y_1 - g_2(y_2)], \quad (2.86)$$

for which the equation

$$g_1(y) = g_2(y),$$

has no solution. This is closely related to the denominator function which arises in the ladder approximation to the Bethe–Salpeter equation, and motivates us to consider the nonoverlapping case separately. The purpose of this section is to show that the nonoverlapping case can be manipulated algebraically into a form containing denominator functions with only one singularity. In order to strike a reasonable balance between clarity and generality, we will do this in some detail for Eq. (2.82), and will then sketch a procedure for more general equations with nonoverlapping singularities.

The possible classes of equations with overlapping singularities seem so ramified that it does not seem worthwhile to treat them at this stage.

We may handle Eq. (2.82) by picking a constant a such that $a_1 < a < a_2$ and using the Heaviside θ-function θ_a:

$$\theta_a(x) = 0 \quad \text{for} \quad x < a,$$
$$= 1 \quad \text{for} \quad x > a,$$

to decompose the functions f, g, K by the following scheme:

$$\begin{aligned} f_1(x) &= \theta_a(x) f(x), \\ f_2(x) &= (1 - \theta_a(x)) f(x), \\ g_1(x) &= \theta_a(x) g(x), \\ g_2(x) &= (1 - \theta_a(x)) g(x), \\ K_{11}(x, y) &= \frac{\theta_a(x)\theta_a(y) K(x, y)}{y - a_1}, \\ K_{12}(x, y) &= \frac{\theta_a(x)(1 - \theta_a(y)) K(x, y)}{y - a_2}, \\ K_{21}(x, y) &= \frac{(1 - \theta_a(x))\theta_a(y) K(x, y)}{y - a_1}, \\ K_{22}(x, y) &= \frac{(1 - \theta_a(x))(1 - \theta_a(y)) K(x, y)}{y - a_2}, \end{aligned} \quad (2.87)$$

Then Eq. (2.82) reduces to the system

$$\begin{aligned} f_1(x) &= g_1(x) + \int \frac{K_{11}(x, y) f_1(y)\, dy}{y - a_2} + \int \frac{K_{12}(x, y) f_2(y)\, dy}{y - a_1}, \\ f_2(x) &= g_2(x) + \int \frac{K_{21}(x, y) f_1(y)\, dy}{y - a_2} + \int \frac{K_{22}(x, y) f_2(y)\, dy}{y - a_1}, \end{aligned} \quad (2.88)$$

in which the kernels K_{ij} are nonsingular. This solves the first problem.

The remaining singularities may now be removed by the general methods of Sec. 2.1. The appropriate conditions, generalizing (2.14) and subsequent equations, are easily written down for any particular case. Similarly, if we wish to handle the equation

$$f(x, y) = g(x, y) + \int \frac{K(x, z) f(z, y)\, dz}{(z - a_1)(z - a_2)},$$

by generalizing the methods of Sec. 2.2, the decomposition (2.87) is easily generalized by breaking all three functions up in the way K was broken up into K_{ij}, and again the generalization of Eqs. (2.39) and so on are simple enough.

The next stage, then, is to deal with the equations

$$\begin{aligned} f_1' &= g_1' + K_{11}' f_1' + K_{12}' f_2', \\ f_2' &= g_2' + K_{21}' f_1' + K_{22}' f_2', \end{aligned} \quad (2.89)$$

arising from (2.88) after removal of singularities. Here f_1' and g_1' will be certain functions in $H_1 = L^2(a, \infty)$, and f_2', g_2' will be certain functions in $H_2 = L^2(-\infty, a)$; the K_{ij}' will be certain completely continuous operators:

$$K_{ij}' : H_j \to H_i \quad (i, j = 1, 2).$$

Hence, on the product Hilbert space $H_1 \times H_2$, the equations take the standard Fredholm form,

$$\mathbf{f}' = \mathbf{g}' + \mathbf{K}'\mathbf{f}', \quad (2.90)$$

and may now be dealt with by standard techniques.

The idea of this method for nonoverlapping singularities is thus very simple: one isolates the singularities by decomposition with θ functions or other functions having appropriate support properties, and obtains a system of vector equations, n of them, where n is the number of singularities. It is evident why this method will not work for overlapping singularities: they cannot be "separated" in this way.

2.5. Further Generalizations

a. Equations with Other Singularities and Other Singular Functions

In order to cope with say $(x - a)^{-n}$ in (2.1), one simply replaces $(x - a)^{\frac{1}{2}}$ in (2.8) with $(x - a)^{\frac{1}{2}n}$, etc.

Similarly, for any otherwise smooth function with a singularity at $x = a$, we do the same.

If the singularities are too severe, one may have to impose conditions $f(a) = 0$, etc., with consequent modification of the subsidiary conditions (2.14), etc.

This tells us how to deal with the full field-theoretic Bethe–Salpeter equation (1.3) with complete propagators, for the mass-shell singularity is of the same order as for the bare propagator.

We have already stated the possibility of damping the behavior in the integral by using a function with the same singularity at $x = a$ as the given function, but falling off more rapidly at infinity.

b. Change of Measure etc.

We have never specified the space in which x, y, a are points [Eq. (2.1)], or the measure dy. In fact, we have never "evaluated" any integral. Hence, provided the singularity is expressed in a suitable functional form, it is clear that the space in which x, y vary can be *any* locally compact space and dy *any* measure on it.

This modification takes care of the case where the integration in (2.1) is of the form

$$\int \frac{K(x, y)f(y)P(y)\,dy}{y - a}, \tag{2.91}$$

where $P(y)$ is a given function. All we have to do is to replace dy throughout by $d\mu = P(y)\,dy$.

Note that the measure may be a function of the "external" variables, $\mu_x(y)$ say. The algebra still works for this situation, except that the symbol ——— [Eq. (2.11)] should then rather be written $\overset{x}{\text{———}}$. The only modification which occurs is that (2.14) becomes a functional relationship:

$$K_2(\overset{x}{y}\overline{f(y)} = K_2(\overset{x}{y}\overline{F(y)}f(a), \quad \text{etc.} \tag{2.92}$$

This situation arises when the Bethe–Salpeter equation is written in terms of momenta p_i; the measure $\mu_x(y)$ is the momentum-conserving Dirac measure $\delta^4(p_1 + p_2 - p_3 - p_4)$. Then (2.92) becomes pointwise in the external variable appearing in the delta function, and retains its form (2.14) in all the other variables of integration. Explicit use is made of this phenomenon below.

c. A Further Special Case

A further special case occurring in realistic Bethe–Salpeter equations is integration over "extra" variables without singularities, e.g.,

$$\int \frac{K_1(x, z_1, z_2, z_3)K_2(z_1, z_2, z_3, y)\,dz_1\,dz_2\,dz_3}{(z_1 - a)(z_2 - a)}. \tag{2.93}$$

This goes exactly as in Secs. 2.1 and 2.2, except that the transformation corresponding to (2.8) has, of course, *no* factor $(z_3 - a)^{\frac{1}{2}}$, etc. Such a situation is typical when one writes Bethe–Salpeter equations in invariants; the integration is taken over two variables s_3, s_4 of the form p_k^2 and having the usual propagator singularities, together with one or more cross-variables $s_{ij} = p_i p_j$ in which there is no singularity (at least in the direct channel). [There is then also a multiplicative function in the integrand, namely, the Jacobian of the transformation $\{p_i\} \to \{s_i, s_{ij}\}$.]

In the remainder of this paper, which will deal with more detailed applications, we will frequently take for granted the simple modifications mentioned in this section.

3. DIRECT SINGULARITIES IN THE BETHE–SALPETER EQUATION

We have already remarked that in field theory, the BS equation arises as an expression of unitarity. In terms of momenta, the field-theoretic form (1.3) reads

$$T(1, 2, 3, 4) - V(1, 2, 3, 4) = -\frac{i}{2(2\pi)^4} \times \int_S \frac{d^4(p_5, p_6)V(1, 2, 5, 6)T(5, 6, 3, 4)}{(p_5^2 - m^2 + i\epsilon)(p_6^2 - m^2 + i\epsilon)}, \tag{3.1}$$

where S denotes the manifold

$$p_1 + p_2 = p_5 + p_6.$$

We use the sign conventions of Ref. 6. Thus the variable $p_1 + p_2$ plays the role of the variable s in Eq. (1.13) (and, of course, we could transform to this form, but we prefer not to).

Thus we are effectively integrating over one four-vector variable $p_5 - p_6$. With these sign conventions, T has the symmetry

$$T(1, 2, 3, 4) = T(-3, -4, -1, -2).$$

The simplest thing for us to do is to transform to invariants $s_i = p_i^2$, $s_{ij} = (p_i + p_j)^2$, maintaining the p_i's in the measure (so as to avoid complications connected with the Jacobian, as these are known to be very awkward[15]). Thus we write

$$T = T(s_1, s_2, s_3, s_4, s_{12}, s_{13}, s_{14}), \quad \text{etc.}$$

Then looking at the explicit form of multiplication, we can divide the invariant variables in $T(s_{ij})$ into four groups:

(a): variables integrated over, and appearing in the singular denominator: s_3, s_4;

(b): variables not integrated over, but should be treated along same lines as group (*a*), for reasons of symmetry: s_1, s_2;

(*c*): variables integrated over, but not appearing in the singular denominators: s_{13}, s_{14};

(*d*): variables not integrated over, and not affected by symmetry considerations: s_{12} $(= s_{34})$.

We first look at an asymmetric treatment along the lines of equation (2.73). Thus we will write

$$(s_1, s_2, s_{12}, s_{13}, s_{14}) = S \text{ (say)},$$

and the first of Eqs. (2.73) will take the form

$$T(S, s_3, s_4) = F_1(S, s_3)F_2(S, s_4)T(S, m^2, m^2) - F_1(S, s_3)T(S, m^2, s_4) - F_2(S, s_4)T(S, s_3, m^2) + (s_3 - m^2)^{\frac{1}{2}}(s_4 - m^2)^{\frac{1}{2}}T'(S, s_3, s_4). \quad (3.2)$$

V will be transformed twice, differently each time. This corresponds exactly to the remark in the second paragraph following Eq. (1.12). The $K(x, y)f(y)$ notation must be modified to include integration over s_{13} and s_{14} as well as s_3 and s_4. Then the cancellations in Eqs. (2.74–76) go through without substantial modification.

The symmetry property of T in momenta results in a symmetry in invariants: T(invariants) is left unchanged by exchanging the (1, 2) with the (3, 4) set. Of course this property is not maintained by the transformation (3.2), and so if we wish to preserve it, we must introduce three transformations (one for T, two for V), analogous to (2.79). The form of these transformations, with the modifications connected with the above classification of the invariant variables, is so similar to that given in Sec. 2.3 that we will not write it out again. We merely note that the symmetry property of T is preserved if we make only one restriction on the arbitrary functions K^s appearing in the analog of (2.80) for T, namely, that each K_s should be equal to the corresponding K^s.

Thus we conclude that the removal of singularities from the field-theoretic Bethe–Salpeter equation (1.3), with simultaneous preservation of the symmetry property of T, presents no particular difficulties.

The next step concerns the application of Fredholm theory. As we discussed in the Introduction, this must depend on the given form of V; and according to our choice of transform, we can easily check in any particular case whether the standard Fredholm theory conditions apply or not.

In the abstract construction (which one of us has discussed elsewhere[6]) to establish nonexistence theorems for certain systems of equations containing the BS equation together with another to determine V, we require the existence of a suitable involution on the algebra of operators generated by T. This arises from the symmetry, as can be shown explicitly.[25] The construction of the present section shows that this property can be preserved during the process of removing the direct singularities. We are then in a position to show explicitly how the general construction may be carried through, avoiding all difficulties connected with propagator singularities. Since this is a rather technical question, and one to be dealt with by methods different from those of this paper, we will go into it elsewhere.

[25] M. M. Broido, J. Math. Phys. 8, 1 (1967).

4. GENERALIZED WICK ROTATIONS

We now turn to discuss the case where the potential V in the BS equation (1.1) is of the form (1.2), corresponding to single-particle exchange. This poses the new problem of crossed-channel singularities. A general potential will be expected to be the sum of a finite number of single-particle exchange terms together with a potential which is finite in momentum transfer t (or u) for all values of t (or u), and will be reasonably smooth in these variables (at least Hölder-continuous $H(\mu)$, $\mu \geq \frac{1}{2}$, at all real values of the variables). Our earlier discussion in Sec. 2 allows us to remove all the singularities in the BS equation arising from the nonsingular part of the potential. Thus if we can remove the singularities due to single-particle exchange we will be able to discuss a very wide class of potentials.

The new singularity introduced by the exchange term is also a propagator singularity. The basic difference is that it is now a moving singularity, depending on the values of the external variables, as distinct from the fixed singularities contained in the kernel G. In particular, with the notation of Fig. 1, the ladder approximation to the BS equation (1.1) is

$$M(p, q, r) = \frac{g^2}{(q - r)^2 - M^2} + \frac{ig^2}{(2\pi)^4}\int d^4k M(p, k, r)[(p + k)^2 - m^2]^{-1} \times [(p - k)^2 - m^2]^{-1}[(q - k)^2 - M^2]^{-1}. \quad (4.1)$$

This equation has as a one-dimensional analog

$$f(x) = f_0(x) + \int K(x, y)f(y)\,dy, \quad (4.2)$$

where the kernel $K(x, y)$ is of the form

$$K(x, y) = K_0(x, y)/[g_1(x) - g_2(y)], \quad (4.3)$$

with K_0 continuous, and g_1 and g_2 are polynomials in their variables. In the kernel $K(x, y)$ of Eq. (4.3), the singularity in the variable y is thus dependent on the "external" variable x; hence the appellation "moving singularity." Similarly, in (4.1) the moving singularity is at $(q - k)^2 = M^2$. This singularity is a simple pole, and integration over it is determined by the usual $i\epsilon$ prescription of Feynman. Owing to the pole nature of this singularity, we cannot reduce (4.1) or (4.3) to a

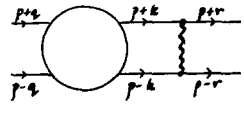

FIG. 1. Notational conventions for the interaction term in the Bethe–Salpeter equation (one-particle-exchange approximation).

Fredholm-type equation by the methods of Sec. 2, even though these do remove the fixed pole singularities in the integration variable k at $(p \pm k)^2 = m^2$. It is possible to perform a partial-wave reduction of Eq. (4.1); the exchange singularity in this case reduces to a logarithmic singularity, while the direct singularities at $(p \pm k)^2 = m^2$ remain unchanged. The methods developed in Sec. 2 may then be used to remove these direct singularities, thus reducing the equation for each partial wave to one of Fredholm type. However, it is then necessary to show that, for the solution to each partial-wave equation, the partial-wave expansion is convergent; this is a difficult problem. Moreover, the method of partial-wave expansion and resumming is not consistent with crossing symmetry. Nor is it useful for the removal of crossed-channel singularities in the more general nonlinear systems which arise when the potential V is an unknown determined by further equations, say field equations[3] or bootstrap conditions.[4]

Thus it is more appropriate to develop a crossing-symmetric method which will remove, or at least make amenable, the single-particle exchange singularity. Such a method has already been proposed[26] and applied to local field equations[17] and to the ladder approximation of the BS equation in partial waves.[7,18] We wish to discuss this method here for the BS equation outside partial-wave analysis. In order to do this, we will discuss the general basis of the method in the remainder of this section, and will turn to its detailed application to the ladder approximation to the BS equation, Eq. (4.1), in Sec. 5.

The method we will consider is an extension of the method of Wick rotations which work for (1.1) below the two-particle threshold, and may be extended directly up to the first inelastic threshold when working in coordinate space[11] or up to the second inelastic threshold in momentum space.[12,27]

The basic idea is to exploit the analyticity of the scattering amplitude in the energy variables of the various particles. In order to do this, it is necessary to determine this region of analyticity.

Such analyticity is not given *a priori*; for an equation such as (1.1), we may choose the analyticity so that the equation may be suitably transformed into one which is well-defined in the sense of Fredholm theory or of the theory of singular integral equations of Cauchy type.[19] In this sense we are extending the essentially real-variable notion of correctness class (implied in the work of Sec. 2) to a notion associated with suitably analytic functions of certain complex variables. As a first attempt to find a correctness class for (1.1), we note that the iterative solution has every term analytic in the product of cut planes of the energy variables q_0, r_0, $q_0 + r_0$. Indeed, such a cut plane analyticity is valid for the perturbation expansion of any Green's function with any local interaction.[16] For if the Green's function depends on n 4-vector momenta $p_1 \cdots p_n$ with $\sum_i p_i = 0$, then a typical internal line in a typical perturbation expansion term for it is $(p_I + k)^2 - m^2$, where k is an internal variable of integration and $p_I = \sum_{i \in I} p_i$, I being a suitable interval of integers in $[1, n]$. Then if $p_{I0} = x + iy$, with x and y real, a singularity in p_{I0} can arise only if

$$(x + k_0)^2 + 2iy(x + k_0) - y^2 - (\mathbf{p}_I + \mathbf{k})^2 - m^2 = 0. \tag{4.4}$$

Thus if $y \neq 0$, then $x + k_0 = 0$, and Eq. (4.4) can never be satisfied.

In order to find where the singularities are on the real p_{I0} axes, we may resort to a pinch analysis. Alternatively, we may use a consistency argument: assume a certain set of singularities in the variables p_{I0}, and show that the defining equations for the Green's functions preserve this set of singularities. Such a method may be used with (1.1) or the Green's function equations arising from any local field equation; they lead to pole singularities for

$$|p_{I0}| = (\mathbf{p}_I^2 + m_I^2)^{\frac{1}{2}},$$

and branch point singularities for

$$|p_{I0}| \geq (\mathbf{p}_I^2 + M_I^2)^{\frac{1}{2}}, \tag{4.5}$$

where m_I, M_I are the masses of the single-particle and threshold states in the I channel (that channel with particles with momenta $p_{i_1}, \cdots, p_{i_r}$, with $[i_1 \cdots i_r] \equiv I$).

Thus we may take as a preliminary condition on our correctness class for Eq. (4.1), or its generalization to bootstrap or local field equations, the set of Green's functions with the above cut-plane analyticity.

In order to use this analyticity to the full, we may write down an integral representation embodying it, following the methods of Bergmann, Oka, and Weil (BOW).[28] The BOW representation will be

$$\mathfrak{G}(p_1 \cdots p_n) = \int \frac{ds_1 \cdots ds_{n-1} W(s_1 \cdots s_{n-1}, \mathbf{p}_1 \cdots \mathbf{p}_{n-1})}{\prod_{i=1}^{n-1} (s_i - p_{I_i 0})}, \tag{4.6}$$

where

$$|s_i| \geq (\mathbf{p}_{I_i}^2 + m_{I_i}^2)^{\frac{1}{2}}$$

[26] J. G. Taylor, Bull. Am. Phys. Soc. **11**, 133 (1965).

[27] G. Tiktopoulos, Phys. Rev. **136**, B275 (1964). This has been extended to three-particle equations also in a limited energy range by J. Nuttall [Phys. Rev. **160**, 1459 (1967)]; see also R. M. Saegner, Ref. 12.

[28] B. A. Fuks, *Introduction to the Theory of Analytic Functions of Several Complex Variables* (American Mathematical Society Translations No. 8, 1963).

and the summation is over all possible choices of $(n-1)$ independent sets $I_1 \cdots I_{n-1}$ of integers from $1 \cdots n$ (where linear independence corresponds to linear independence of the vectors $\mathbf{I}_1 \cdots \mathbf{I}_n$, which may be used to represent the sets $I_1 \cdots I_{n-1}$ in R^n with basis $1 \cdots n$).

The representation (4.6) does not have the requirement of positive energy built into it. In order to see how to restrict it so that it does, we will derive a restricted form of (4.6) from a field-theoretic basis for the Green's functions.[29]

We have

$$\delta^4\left(\sum_{i=1}^{n+1} p_i\right)\mathcal{G}(p_1 \cdots p_{n+1}) = \int \prod_{j=1}^{n+1} dx_j \exp\left(-i \sum_{j=1}^{n+1} p_j x_j\right) \times \langle 0|\, T(\phi(x_1) \cdots \phi(x_{n+1}))\, |0\rangle, \quad (4.7)$$

where we take one scalar field ϕ for simplicity. Then we have

$$\langle 0|\, T(\phi(x_1) \cdots \phi(x_{n+1}))\, |0\rangle = \sum_P \theta(x_{P(1)0} - x_{P(2)0}) \cdots \theta(x_{P(n)0} - x_{P(n+1)0}) x \times \langle 0|\, \phi(x_{P(1)0}) \cdots \phi(x_{P(n+1)0})\, |0\rangle, \quad (4.8)$$

where the summation in (4.8) is over all permutations P of $1, \cdots, n+1$. We introduce the variables

$$y_r = x_{P(r)} - x_{P(r+1)} \quad (1 \leq r \leq n),$$

so that if

$$q_r = \sum_{j=1}^{r} p_{P(j)},$$

then

$$\sum_{j=1}^{n+1} p_j x_j = \sum_{r=1}^{n} q_r y_r + x_{P(n+1)}\left(\sum_{i=1}^{n+1} p_i\right),$$

under which circumstances

$$\langle 0|\, \phi(x_{P(1)}) \cdots \phi(x_{P(n+1)})\, |0\rangle$$

is a function of $y_1 \cdots y_n$ only. Performing the Fourier transformation in the variables $y_1 \cdots y_n$ as a convolution product in (4.8), we find

$$\mathcal{G}(p_1 \cdots p_{n+1}) = \sum_P \int \frac{ds_1 \cdots ds_n \rho(s_1 \cdots s_n, \mathbf{q}_1 \cdots \mathbf{q}_n)}{\prod(s_i - q_{i0})}, \quad (4.9)$$

where

$$\rho(s_1 \cdots s_n, \mathbf{q}_1 \cdots \mathbf{q}_n) = \int \prod_{i=1}^{n} dy_i \exp\left[i \sum_{j=1}^{n} q'_j y_j\right] \times \langle 0|\, \phi(x_{P(1)}) \cdots \phi(x_{P(n+1)})\, |0\rangle \quad (4.10)$$

and $q'_{j0} = s_j$, $\mathbf{q}'_j = \mathbf{q}_j$. We remark that the difference between (4.9) and (4.6) is a "nesting" property in the factors in the denominator of (4.9) as compared with (4.6). We may expand the integrand in (4.10) by inserting complete sets of intermediate states between the various field operators and, using the spectral conditions, derive the conditions met before:

$$s_i = (\mathbf{q}_i^2 + m_i^2)^{\frac{1}{2}}, \quad s_i \geq (\mathbf{q}_i^2 + M_i^2)^{\frac{1}{2}}, \quad (4.11)$$

though now with only *positive* values of s_i.

Elsewhere[26] we denote the representation (4.9), the *energy-analytic representation*, or EAR. It may have to be altered by a suitable number of subtractions, if the weight function ρ is of polynomial growth in its variables. This representation contains explicitly the energy-analyticity. In the following section, we use it to simplify and make more accessible the moving singularities in the ladder approximation to the BS equation.

A more ambitious program is to use (4.9) in the complete set of Green's function equations arising from a particular field equation.[17] We may regard a satisfactory treatment of the Bethe–Salpeter equation as the first step towards a more complete understanding of these field equations. We will return to the further problems posed by such field equations elsewhere.

We must obtain a prescription for obtaining the physical amplitude from (4.9). This is the $i\epsilon$ prescription: $s_j \to s_j - i\epsilon$, as follows from the derivation of Eq. (4.9)

Finally, we must justify using (4.9) in place of (4.6) in (4.1) or other Green's function equations. One of us has shown[17] that (4.9) is consistent with the principle of complete unitarity.[3] All Green's function equations of the form (1.3) or its many-body generalizations[6] may be derived from this principle,[17,30] and this is the justification.[31]

5. THE SINGLE-PARTICLE EXCHANGE POTENTIAL OR "LADDER APPROXIMATION"

5.1. Reduced Energy-Analytic Representation

We now apply the energy-analytic representation (EAR) of the scattering amplitude, Eq. (4.9), to the Bethe–Salpeter equation in the ladder approximation, Eq. (4.1). We do not need the full power of the EAR to do this, because it is sufficient to continue the two energy variables q_0, k_0, [in the notation of Eq. (4.1)] into the complex plane. Thus we study the reduced EAR[15] for the two-body scattering amplitude, which

[29] H. Araki, J. Math. Phys. **2**, 163 (1961).

[30] J. G. Taylor, *Lectures at the Winter School in Theoretical Physics at Karpacz, 1967* (University of Wroclaw, Wroclaw, 1967).

[31] Thus, although people have used other integral representations in the BS equation [N. Nakanishi, J. Math. Phys. **4**, 1229 (1963); J. W. Greenman, M.I.T. preprint], there is no reason to believe that they have any applicability to more general problems. Analyticity ideas have also been applied to the computational problem; see Ref. 14a.

takes the form

$$M(p, q, r) = \int_{\alpha_+(p,\mathbf{q},r)}^{\infty} \frac{\rho_+(p, \mathbf{q}, t, r)\, dt}{t - q_0} + \int_{-\infty}^{\alpha_-(p,\mathbf{q},r)} \frac{\rho_-(p, \mathbf{q}, t, r)\, dt}{t - q_0}. \quad (5.1)$$

In Eq. (5.1) we wish to determine the limits $\alpha_\pm$ by self-consistency arguments, as sketched in Sec. 4. The physical amplitude is then obtained by putting $t \to t - i\epsilon$ in the first integral, and $t \to t + i\epsilon$ in the second, and letting $\epsilon \to 0$. This prescription is obtained immediately from the complete EAR for $M(p, q, r)$, Eq. (4.9), by concentrating attention on those terms where q_0 appears.

Now we wish to insert the representation (5.1) into the BS equation (4.1). Equation (4.1) may be written

$$M = M_B + F[M], \quad (5.2)$$

where $M(B)$ is the Born term (single-particle exchange potential) and $F[M]$ is its iteration. In order to pick out the terms of $F[M]$ corresponding to the decomposition (5.1), we write

$$F[M] = F_+[M] + F_-[M], \quad (5.3)$$

where

$$F_\pm[M(p, q, r)] = \pm \frac{ig^2}{(2\pi)^4} \int \frac{d^4k M(p, k, r)}{[(p + k)^2 - m^2][(p - k)^2 - m^2][q_0 - k_0 \mp ((\mathbf{q} - \mathbf{k})^2 + M^2)^{\frac{1}{2}}]((\mathbf{q} - \mathbf{k})^2 + M^2)^{\frac{1}{2}}} \quad (5.4)$$

Using the usual $+i\epsilon$ prescriptions in the propagators in (5.4), we see that $F_\pm[M]$ have analytic continuations in q_0 into the upper and lower half-planes, respectively. If we decompose M in a similar way, $M = M_+ + M_-$, corresponding to the right-hand side of Eq. (5.1), with a similar decomposition for M_B, we have

$$M_\pm(p, q, r) = M_{B\pm}(p, q, r) + F_\pm[M(p, q, r)]. \quad (5.5)$$

We will evaluate $F_\pm[M]$, with M given by (5.1), by performing the k_0 integration explicitly:

$$F_+[M(p, q, r)] = \frac{ig^2}{(2\pi)^4} \int d^3\mathbf{k} \int dk_0 \{\text{propagators}\}^{-1} \times \left\{ \int_{\alpha_+(\mathbf{k})}^{\infty} \frac{\rho_+(\mathbf{k}, t)\, dt}{t - k_0 - i\epsilon} + \int_{-\infty}^{\alpha_-(\mathbf{k})} \frac{\rho_-(k, t)\, dt}{t - k_0 + i\epsilon} \right\}. \quad (5.6)$$

In Eq. (5.6), we have suppressed the dependence of $\rho_\pm(p, \mathbf{k}, t, r)$ on p, r; similarly for $\alpha_\pm$. The dependence on k_0 is trivial. We close the contour of integration in the lower half of the k_0 plane, and by taking account of the k_0 poles lying there, evaluate the integral by the method of residues. It is convenient for this purpose to restrict ourselves to the C.M. system ($\mathbf{p} = 0$).

5.2. Evaluation of the $F_\pm$ Integrals in the Center-of-Mass System

For the expression (5.6) we obtain the explicit expression

$$\begin{aligned} F_+[M(p, q, r)] = g' \int \frac{d^3k}{b} \Big\{ &- \int dt[\rho_+(\mathbf{k}, t) + \rho_-(\mathbf{k}, t)] \\ &\times [8ap_0a_-(t + a_-)(b_+ + a_-)]^{-1} \\ &+ \int dt[\rho_+(\mathbf{k}, t) + \rho_-(\mathbf{k}, t)] \\ &\times [8ap_0a_-(b_+ - a_-)(t - a_+)]^{-1} \\ &+ \int dt[\rho_+(\mathbf{k}, t)][(t + a_+)(t + a_-)(t - a_+) \\ &\times (t - a_-)(t - b_+)]^{-1}, \end{aligned} \quad (5.7)$$

where

$$a_\pm = p_0 \pm a, \quad a^2 = \mathbf{k}^2 + m^2,$$
$$b_\pm = q_0 \mp b, \quad b^2 = (\mathbf{q} - \mathbf{k})^2 + M^2,$$
$$g' = g^2/16\pi^3.$$

Notice that no residues from moving poles have to be evaluated, since (by the $i\epsilon$ prescription) the choice of contours always excludes these poles. Similarly, we evaluate $F_-[M]$ by closing the contour in the upper half k_0-plane to give

$$\begin{aligned} F_-[M(p, q, r)] = g' \int \frac{d^3k}{b} \Big\{ &- \int dt[\rho_+(\mathbf{k}, t) + \rho_-(\mathbf{k}, t)] \\ &\times [8ap_0a_+(a_+ + t)(a_+ + b_-)]^{-1} \\ &- \int dt[\rho_+(\mathbf{k}, t) + \rho_-(\mathbf{k}, t)][8ap_0a_-(t - a_-) \\ &\times (b_- - a_-)]^{-1} + \int dt\rho_-(\mathbf{k}, t) \\ &\times [(t + a_+)(t - a_+)(t + a_-)(t - a_-)(t - b_-)]^{-1}. \end{aligned} \quad (5.8)$$

Next, we take the discontinuities across the real q_0 axis of the quantities appearing in Eq. (5.5), which gives

$$2\pi i\rho_\pm = \text{disc } M_{B\pm} + \text{disc } F_\pm[M], \quad (5.9)$$

where, using (5.7–8),

$$\begin{aligned} \text{disc } F_+[M(p, q, r)] = (2\pi i) \cdot g' \\ &\times \int \frac{d^3k}{b} \Big\{ - \int dt[\rho_+(\mathbf{k}, t) + \rho_-(\mathbf{k}, t)] \\ &\times [8ap_0a_-(t + a_-)]^{-1}\delta(b_+ + a_-) \\ &+ \int dt[\rho_+(\mathbf{k}, t) + \rho_-(\mathbf{k}, t)][8ap_0a_+(t - a_+)]^{-1} \\ &\times \delta(b_+ - a_+) - \int dt[\rho_+(k, t)] \\ &\times [(t + a_+)(t + a_-)(t - a_+)(t - a_-)]^{-1}\delta(b_+ - t), \end{aligned} \quad (5.10)$$

$$\text{disc } F_-[M(p,q,r)] = (2\pi i)\cdot -g'$$
$$\times \int \frac{d^3k}{b}\Big\{\int dt[\rho_+(\mathbf{k},t)+\rho_-(\mathbf{k},t)][8ap_0a_+(a_++t)]^{-1}$$
$$\times \delta(a_++b_-)+\int dt[\rho_+(\mathbf{k},t)+\rho_-(k,t)]$$
$$\times [8ap_0a_-(t-a_-)]^{-1}\delta(b_--a_-)$$
$$+ dt\rho_-(\mathbf{k},t)[(t+a_+)(t+a_-)(t-a_+)(t-a_-)]^{-1}$$
$$\times \delta(b_--t). \tag{5.11}$$

Similarly,

$$\text{disc } M_{B\pm}(p,q,r) = (2\pi i)\cdot \frac{\pm g^2}{[2(\mathbf{q}-\mathbf{r})^2+M^2]^{\frac{1}{2}}}$$
$$\times \delta(q_0-r_0\mp((q-r)^2+M^2)^{\frac{1}{2}}). \tag{5.12}$$

In all these equations, the variable t appearing in Eq. (5.1), where free, has been replaced by q_0. Now we write Eqs. (5.9)–(5.12) as a pair of coupled linear integral equations, with

$$\mathbf{m} = \begin{pmatrix}\rho_+\\ \rho_-\end{pmatrix}, \quad \mathbf{m}_B = \frac{1}{2\pi i}\,\text{disc}\begin{pmatrix}M_{B+}\\ M_{B-}\end{pmatrix}.$$

We obtain

$$\mathbf{m}(p,q,r) = \mathbf{m}_B(p,q,r) + \int \mathbf{K}(p,q,\mathbf{k},t)\mathbf{m}(p,\mathbf{k},t,r)d^3k\,dt, \tag{5.13}$$

in which, introducing the new notation

$$\left.\begin{aligned}\Delta_1 &= [8ap_0a_-(t+a_-)]^{-1}\delta(b_++a_-),\\ \Delta_2 &= [8ap_0a_+(t-a_+)]^{-1}\delta(b_+-a_+),\\ \Delta_3 &= [8ap_0a_+(t+a_+)]^{-1}\delta(b_-+a_+),\\ \Delta_4 &= [8ap_0a_-(t-a_-)]^{-1}\delta(b_--a_-),\end{aligned}\right\} \tag{5.14}$$

$$\left.\begin{aligned}\Gamma_1 &= [(t^2-a_+^2)(t^2-a_-^2)]^{-1}\delta(b_+-t),\\ \Gamma_2 &= [(t^2-a_+^2)(t^2-a_-^2)]^{-1}\delta(b_--t),\end{aligned}\right\} \tag{5.15}$$

the elements of the 2×2 matrix $\mathbf{K}$ can be written

$$\left.\begin{aligned}K_{++} &= g'b^{-1}(-\Delta_1+\Delta_2-\Gamma_1),\\ K_{+-} &= g'b^{-1}(-\Delta_1+\Delta_2),\\ K_{-+} &= -g'b^{-1}(\Delta_3+\Delta_4),\\ K_{--} &= -g'b^{-1}(\Delta_3+\Delta_4+\Gamma_2).\end{aligned}\right\} \tag{5.16}$$

Before discussing the singularities of the matrix elements of K, we compute the limits $\alpha_\pm$ of the t integration in (5.1). In fact, we have

$$\left.\begin{aligned}\alpha_+(p_0,\mathbf{q},r) &= \min\{-p_0+[\mathbf{q}^2+(M+m)^2]^{\frac{1}{2}},\\ &\qquad r_0+[(\mathbf{q}-\mathbf{r})^2+4M^2]^{\frac{1}{2}}\},\\ \alpha_-(p_0,\mathbf{q},r) &= \max\{+p_0-[\mathbf{q}^2+(M+m)^2]^{\frac{1}{2}},\\ &\qquad +r_0-[(\mathbf{q}-\mathbf{r})^2+4M^2]^{\frac{1}{2}}\},\end{aligned}\right\} \tag{5.17}$$

provided that the Born term is explicitly subtracted. We perform this subtraction by writing

$$\mathbf{m} = \mathbf{m}_B + \mathbf{n}, \tag{5.18}$$

so that $\mathbf{n}$ satisfies the integral equation

$$\mathbf{n}(p,q,r) = \mathbf{n}_B(p,q,r) + \int \mathbf{K}(p,q,\mathbf{k},t)\mathbf{n}(p,\mathbf{k},t,r)\,d^3k\,dt, \tag{5.19}$$

where $\mathbf{n}_B$ is the weight function in the EAR arising from the fourth-order box diagram. Explicitly

$$\mathbf{n}_B(p,q,r) = \int \mathbf{K}(p,q,\mathbf{k},t)\mathbf{m}_B(p,\mathbf{k},t,r)d^3k\,dt,$$

so that

$$n_{B+} = g^2\int \frac{d^3\mathbf{k}}{[2(\mathbf{k}-\mathbf{r})^2+M^2]^{\frac{1}{2}}} \times [K_{++}(p,q,\mathbf{k},r_0+((\mathbf{k}-\mathbf{r})^2+M^2)^{\frac{1}{2}}) - K_{+-}(p,q,\mathbf{k},r_0-((\mathbf{k}-\mathbf{r})^2+M^2)^{\frac{1}{2}})],$$
$$n_{B-} = g^2\int \frac{d^3\mathbf{k}}{[2(\mathbf{k}-\mathbf{r})^2+M^2]^{\frac{1}{2}}} \times [K_{-+}(p,q,\mathbf{k},r_0+((\mathbf{k}-\mathbf{r})^2+M^2)^{\frac{1}{2}}) - K_{--}(p,q,\mathbf{k},r_0-((\mathbf{k}-\mathbf{r})^2+M^2)^{\frac{1}{2}})]. \tag{5.20}$$

We see that the integration over the variable $\mathbf{k}$ removes the δ functions which appear in the matrix elements of $\mathbf{K}$ as well as the δ functions and principal value singularities arising from the poles in the terms Δ_i, Γ_i, so that $\mathbf{n}_B$ is a continuous function of its variables.

We now claim that (5.17) determines the correct range of t integration in (5.19). We could have read off (5.17) immediately from the discussion of the EAR in the previous section—in particular, from Eq. (4.11). However, we cannot immediately use such a result in our present discussion, since (5.13) has not been derived on a field-theoretic basis. We will show this by a self-consistent argument: we assume that the range of integration over t in (5.19) is correctly given by (5.17) and then show that the integral in (5.19) has support in the variable q_0 satisfying

$$q_0 > \alpha_+(p_0,\mathbf{q},r) \quad [q_0 < \alpha_-(p_0,\mathbf{q},r)],$$

for the integral contribution to $n_+(n_-)$, with $\alpha_\pm$ again given by Eq. (5.17). We will also show from (5.20) that $\mathbf{n}_B$ satisfies these support conditions. Thus it is possible to search for solutions to (5.19) with (5.17), for example, by iteration.

To discuss the integral in (5.19), we have that $K_{+\pm}(p,q,\mathbf{k},t)$ are nonzero only provided q_0 takes one of the values $[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}+[\mathbf{k}^2+m^2]^{\frac{1}{2}}\pm p_0$

or $[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}+t$, where

$$t \geq \min\{-p_0+[\mathbf{k}^2+(M+m)^2]^{\frac{1}{2}}, \quad r_0+[(\mathbf{k}-\mathbf{r})^2+4M^2]^{\frac{1}{2}}.\}$$

The minimum of these values as $\mathbf{k}$ or t vary over their allowed ranges is

$$\min\{-p_0+[\mathbf{q}^2+(M+m)^2]^{\frac{1}{2}}, \quad r_0+[(\mathbf{q}-\mathbf{r})^2+9M^2]^{\frac{1}{2}}\},$$

which is greater than (5.17).

Similarly, $K_{-\pm}(p,q,\mathbf{k},t)$ are nonzero only provided q_0 takes one of the values $-[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}-[\mathbf{k}^2+m^2]^{\frac{1}{2}}\pm p_0$ or $-[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}+t$, where

$$t \leq \max\{p_0-[\mathbf{k}^2+(M+m)^2]^{\frac{1}{2}}, \quad r_0-[(\mathbf{q}-\mathbf{r})^2+M^2]^{\frac{1}{2}}\}.$$

The maximum of these values as $\mathbf{k}$ or t vary over their allowed ranges is $\max\{p_0-[\mathbf{q}^2+(M+m)^2]^{\frac{1}{2}}, r_0-[(\mathbf{q}-\mathbf{r})^2+9M^2]^{\frac{1}{2}}\}$, which is again less than $\alpha_-(p_0,\mathbf{q},r)$ given by (5.17).

Finally, we note that the supports of the integrands of (5.20) are restricted to the following manifolds:

n_{B+}:

$$\begin{cases} q_0=[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}+[\mathbf{k}^2+m^2]^{\frac{1}{2}}\pm p_0, \\ q_0=r_0+[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}+[(\mathbf{k}-\mathbf{r})^2+M^2]^{\frac{1}{2}}, \end{cases}$$

n_{B-}:

$$\begin{cases} q_0=-[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}-[\mathbf{k}^2+m^2]^{\frac{1}{2}}\pm p_0, \\ q_0=-[(\mathbf{q}-\mathbf{k})^2+M^2]^{\frac{1}{2}}-[(\mathbf{k}-\mathbf{r})^2+M^2]^{\frac{1}{2}}+r_0. \end{cases}$$

As before, the minimum value of q_0 for which the integrand of n_{B+} does not vanish will be $\alpha_+(p_0,\mathbf{q},r)$ of (5.17), while the maximum value of q_0 for which that of n_{B-} does not vanish. will be $\alpha_-(p_0,\mathbf{q},r)$ of (5.17).

Now we can list the singularities in the matrix elements of $\mathbf{K}$. In K_{++} the apparent singularities at $t=a_+$, $t=-a_-$ have zero residue because of cancellations between the three terms; similarly for the singularities in K_{--} at $t=a_-$, $t=-a_+$. This leaves us with the following singularities: in

$$\begin{aligned} K_{++} &\text{ at } t=-a_+,\ t=a_- \text{ due to } \Gamma_1, \\ K_{+-} &\text{ at } t=-a_- \text{ due to } \Delta_1, \\ &\text{ at } t=a_+ \text{ due to } \Delta_2, \\ K_{-+} &\text{ at } t=a_- \text{ due to } \Delta_3, \\ &\text{ at } t=-a_+ \text{ due to } \Delta_4, \\ K_{--} &\text{ at } t=a_+,\ t=-a_- \text{ due to } \Gamma_2. \end{aligned}$$

The support conditions on $\mathbf{n}$ allow us to remove all the a_+ singularities, provided certain conditions hold on p_0, r_0. For instance, in K_{++}, if the outgoing particles with momenta $p\pm r$ are near their mass shells, we have $r_0\sim 0$; so if $p_0>0$, the $t=-a_+$ singularities cannot occur, as this would require $-p_0-[\mathbf{k}^2-m^2]^{\frac{1}{2}} \geq r_0+[(\mathbf{k}-\mathbf{r})^2+4M^2]^{\frac{1}{2}}$. One easily verifies that this works for all other $t\pm a_+$ singularities.

With p_0 and r_0 in these ranges, then, we are left with the following singularities:

$$\begin{aligned} &\text{in } K_{++} \text{ at } t=a_- \text{ due to } \Gamma_1, \\ &\text{in } K_{+-} \text{ at } t=-a_- \text{ due to } \Delta_1, \\ &\text{in } K_{-+} \text{ at } t=a_- \text{ due to } \Delta_4, \\ &\text{in } K_{--} \text{ at } t=-a_- \text{ due to } \Gamma_2. \end{aligned} \tag{5.21}$$

[If necessary, we can recover the entire p_0, r_0 behavior by using the full EAR, Eq. (4.9). But we will not need this.]

Let us consider the general nature of these singularities. They will occur at values of t given by the singular denominators alone, i.e., respectively,

$$t=\mp[p_0\pm(\mathbf{k}^2+m^2)^{\frac{1}{2}}], \tag{5.22}$$

and only when the space components k satisfy the support condition.

Let us see what remains to be done before the fixed singularities can be removed by the methods of Sec. 2. The following additional complications have arisen:

(a) The surfaces of singularity corresponding to the various factors in (5.14) and (5.15) appear to intersect. But in fact this problem will only arise for $p_0=0$ if we relax our earlier restrictions on p_0 and r_0 and so allow a_+ singularities as well; for we cannot have $a_+=\pm a_-$ except if $p_0=0$. We know that the singular nature of $p_0=0$ is due to the equality of the two direct propagators; such a difficulty has been considered recently in relation to representations of the Lorentz group.[32] We will not discuss this problem further here.

(b) Four different surfaces of singularity are involved, namely, $t=\pm a_\pm$. These are dealt with by the methods of Sec. 2.4.

(c) The equations contain delta functions. These will not give any problems of principle, provided that the supports of delta functions do not coincide with surfaces of singularity (though they may intersect them, of course). We can immediately see that this does not happen in our case. In more general situations it will happen, but may then be dealt with by

[32] R. Delbourgo, A. Salam, and J. Strathdee, IAEA preprint IC/67/9.

using the theory of products of distributions (developed by one of us elsewhere).[33]

A further general difficulty with kernels containing complicated delta functions is that, when these are evaluated, the resulting equations are no longer integral equations in the conventional sense; the unknown function appearing under the integral sign has the "wrong arguments." This phenomenon, which has nothing to do with singular kernels as such, is discussed in detail in the Appendix. However, it will cause us difficulties when we wish to expand functions about surfaces of singularity, for this requires some continuity properties. These continuity properties for the kernels can be assured by the Fourier transform methods introduced in the Appendix, but then we are no longer, in general, able to use the delta functions to perform part of the integrations in the integral equation. Since it is extremely desirable to reduce the number of variables under the integral sign in an integral equation, both from the point of view of general discussion and for computation, we will consider how the formalism introduced in the Appendix is to be applied to our equation. It will, in fact, turn out that this difficulty about the "wrong arguments" can be avoided, in our case, by judicious selection of the variables to be integrated by the delta functions and by some tricks.

Let us see in detail how this will come about. We see from the form of (5.14) and (5.15) that all our delta functions involve $b_{\pm}$, hence implicitly all space parts of q and k. The effect of using the delta functions to perform the $|\mathbf{k}|$ integrations (in any terms) or the t integrations (in the Γ terms) would be to introduce artificial moving (q-dependent) singularities. On the other hand, if we regard $b_{\pm}$ as independent variables and use the delta functions to perform the $b_{\pm}$ integrations, we no longer have integral equations (another form of the "wrong arguments" problem). The origin of this difficulty is demonstrated in detail for some simple kernels containing delta functions in the Appendix. Thus to justify the expansion processes of Sec. 2, we will remove the delta functions altogether, by the methods of the Appendix. This effectively means [compare the treatment of the simple cases (A8), (A11)] *solving* the equation, for example in the Γ_2-term, which expresses the restriction given by the delta function:

$$t = b_{-}(q_0, \mathbf{q}, \mathbf{k}),$$

for some variable z having the following properties:

(z_1) z is not a function of q_0 or of $\mathbf{q}$,

(z_2) z is not a function of t or of $|\mathbf{k}|$.

[33] J. G. Taylor, Nuovo Cimento **17**, 695 (1960).

The first of these conditions is necessary in order to ensure that evaluation (or the use of Fourier transform on z) preserves the essential integral equation structure; the second, to ensure that no moving singularities are introduced (by evaluation) or that the singularities are not *masked* and made inaccessible (by Fourier transform). We have

$$(t - q_0)^2 - M^2 - |\mathbf{q}|^2 - |\mathbf{k}|^2 + 2|q|\,|k| \cos\psi = 0, \tag{5.23}$$

where ψ is the angle between the 3-vectors $\mathbf{q}$ and $\mathbf{k}$. Condition (z_2) tells us that we must exploit the presence of $\cos\psi$, and condition (z_1) that it must be broken down so that its dependence on the angular parts of $\mathbf{q}$ and $\mathbf{k}$ becomes explicit. This *could* be done by using the invariance of the equation under the little group (the rotation group in the C.M. frame we are using) to choose $\mathbf{q} = (q_1, 0, 0)$ say, so that ψ would depend on k only. However, this would destroy the symmetry between the "external" variables $(q_0, \mathbf{q})$ and the "internal" variables $(t, \mathbf{k})$ so that again we would not have an integral equation. We prefer to introduce a fixed reference frame with $\mathbf{q}$ (respectively, $\mathbf{k}$) having polar and azimuthal angles θ_q and ϕ_q (or θ_k and ϕ_k). Then we have

$$\cos\psi = \cos\theta_q \cos\theta_k + \sin\theta_q \sin\theta_k \cos(\phi_q - \phi_k). \tag{5.24}$$

We will attempt to use the delta functions to perform the ϕ_k integration. According to the Appendix, we will have to justify this by performing the Fourier transformation on ϕ_q, so as to obtain an integral equation. Neither of these operations will involve the singular denominators, since these depend only on t and $\mathbf{k}$. We can solve for $\phi_q - \phi_k$ in the form

$$\phi_k - \phi_q = \cos^{-1}\left(\frac{\cos\psi - \cos\theta_q \cos\theta_k}{\sin\theta_q \sin\theta_k}\right). \tag{5.25}$$

(We can ignore the multivaluedness of the solution; this is taken into account by a trivial summation as described in full generality in the Appendix.) Thus we replace $\delta(t - b_{-})$ by

$$\delta\left(\phi_k - \phi_q - \cos^{-1}\left\{\frac{[(t - q_0)^2 - M^2 - |q|^2 - |k|^2]/2|q|\,|k| - \cos\theta_q \cos\theta_k}{\sin\theta_q \sin\theta_k}\right\}\right)$$
$$\equiv \delta[\phi_k - \phi_q - G(q_0, |q|, \theta_q, t, |k|, \theta_k) \text{ say}. \tag{5.26}$$

Then the Γ_2 terms, for instance, are of the form

$$\int \mathcal{K}(\phi_k - \phi_q; \mathbf{q}, \mathbf{t})\delta[\phi_k - \phi_q - G(\mathbf{q}, \mathbf{t})] \times n(\phi_k, \mathbf{t})\, d\phi_k\, d\mathbf{t}, \quad (5.27)$$

where $\mathbf{q}$ stands for $(q_0, |q|, \theta_q)$ and $\mathbf{t}$ for $(t, |k|, \theta_k)$. Here we have made use of the fact that the kernel

$$\mathcal{K} = -g' b^{-1}(t^2 - a_+^2)^{-1}(t^2 - a_-^2)^{-1}, \quad (5.28)$$

involves ϕ_k and ϕ_q only through b, hence in the form $(\phi_k - \phi_q)$. Thus the integral equation reads

$$\mathbf{n}(\phi_q, \mathbf{q}) = \mathbf{n}_B(\phi_q, \mathbf{q}) + \iint \mathcal{K}(\phi_k - \phi_q; \mathbf{q}, \mathbf{t})\mathbf{n}(\phi_k, \mathbf{t}) \times \delta[\phi_k - \phi_q - G(\mathbf{q}, \mathbf{t})]\, d\phi_k\, d\mathbf{t} + \text{other terms}, \quad (5.29)$$

so that we are dealing with a special case of Eq. (A10), with $F(x, y, y') = x - F'(y, y')$, say. Now, however, using the delta function to perform the ϕ_k integration gives

$$\mathbf{n}(\phi_q, \mathbf{q}) = \mathbf{n}_B(\phi_q, \mathbf{q}) + \int \mathcal{K}[G(\mathbf{q}, \mathbf{t}), \mathbf{q}, \mathbf{t}]\mathbf{n}[\phi_q - G(\mathbf{q}, \mathbf{t}), \mathbf{t}]\, d\mathbf{t} + \text{other terms}. \quad (5.30)$$

This is no longer an integral equation for $\mathbf{n}$ because of the appearance of q dependence under the integral sign in $\mathbf{n}$. We deal with this (see the Appendix) by taking the Fourier transform in ϕ_q. But since ϕ_q does not appear in the kernel of (5.30), this transformation can be carried out by inspection [in the Appendix, the x integration in (A7) and the q integration in (A6) are now trivial] to yield

$$\mathbf{n}'(\xi_q, \mathbf{q}) = \mathbf{n}'_B(\xi_q, \mathbf{q}) + \int \mathcal{K}[G(\mathbf{q}, \mathbf{t}), \mathbf{q}, \mathbf{t}]e^{i\xi_q G(\mathbf{q}, \mathbf{t})}\mathbf{n}'(\xi_q, \mathbf{t})\, d\mathbf{t} + \text{terms of similar structure}, \quad (5.31)$$

where the prime on $\mathbf{n}'$ denotes Fourier transform with respect to ϕ_q, and ξ_q denotes the transformed variable corresponding to ϕ_q. Thus, by a careful selection of the variable in which to perform the evaluation of the delta functions, together with an observation on the way in which this variable appears in the kernel, we have managed to avoid all the difficulties usually (Appendix) associated with evaluation of complicated delta functions. The object ξ_q is now [in 5.31] simply a parameter (like p_0); the $(t \pm a_\pm)^{-1}$ singularities of $\mathcal{K}$ are still explicitly present and are fixed, and there are no more delta functions. No complications now prevent us from applying the methods of Sec. 2 and removing the fixed singularities. This we do by expanding about the surfaces $\pm q_0 = p_0 \pm (q^2 + m^2)^{\frac{1}{2}}$ in the $\mathbf{q}$ variables and $\pm t = p_0 \pm (\mathbf{k}^2 + m^2)^{\frac{1}{2}}$ in the $\mathbf{t}$ variables. Thus we have demonstrated explicitly what we claimed in the abstract—that the equation can be written as a conventional set of singular integral equations without moving singularities or delta functions, in which the unitarity cuts are explicitly exhibited so that it is valid at all energies, and from which the fixed singularities may be removed by our methods. As an additional bonus, there are only three variables of integration. This is what we set out to do in the present paper. Elsewhere we will present a more detailed computation, treating in a precise fashion the connection between the values of the coupling constant, the exchanged mass, and the appearance of bound states in the direct channel.

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APPENDIX: KERNELS CONTAINING DELTA FUNCTIONS

This appendix discusses a problem which arises already, in connection with kernels having no non-integrable singularities and which has hardly any connection with the problem of singular kernels discussed in the present paper. Nevertheless, delta functions do arise—for instance, in the ladder approximation to the Bethe–Salpeter equation as discussed in Sec. 5. We now give a brief general discussion of them. In the physical literature there is a tendency to avoid kernels containing delta functions because such kernels cannot represent completely continuous operators and so the Fredholm theory of integral equations cannot be directly applied to them.[34] To be a little more concrete without much loss of generality, consider the integral equation

$$f = g + \lambda K f, \quad (A1)$$

with $g \in L^2(\infty, -\infty)$. If the kernel K is the delta function

$$K(x, y) = \delta(x - y), \quad (A2)$$

so that the equation reads

$$f(x) = g(x) + \lambda \int \delta(x - y)f(y)\, dy, \quad (A3)$$

then K is the *identity operator*. [K is initially defined and is clearly continuous on the continuous functions, and reproduces them, and so can be extended by continuity to the whole of $L^2(\infty, -\infty)$.] Clearly, then,

[34] The problem of delta functions in the kernels arises already in multiparticle Lippmann–Schwinger equations; see for instance S. Weinberg, Phys. Rev. 133, B232 (1964), especially Appendix A.

more complex kernels containing delta functions will also not give rise to completely continuous operators, and Fredholm theory will not be directly applicable.

In particular, we cannot *assume* that the Fredholm alternative is available; that is, we will not automatically have either a unique solution of (A1) or a solution of the corresponding homogeneous equation

$$f = \lambda K f. \tag{A4}$$

But the Fredholm alternative is quite a general property of continuous operators with discrete spectrum, and not only of Fredholm operators. The tendency of the delta function to have a discrete spectrum is obvious; hence also the tendency of the Fredholm alternative to remain valid for kernels containing delta functions, if the rest of the kernel is square summable in all variables simultaneously.

A second valuable feature of the Fredholm theory is the possibility of solving the equation by iteration. But here again the presence of delta functions will not normally make this impossible. The Neumann series for Eq. (A1),

$$f = \sum_{r=0}^{\infty} \lambda^r K^r g,$$

will converge to a solution of (A1) in the norm topology of Hilbert space, provided, for example, that $|\lambda|\,\|K\| < 1$, and that λ is not in the spectrum of K. (Where the Fredholm alternative *is* available, this last condition says essentially that, for the given value of E, the center-of-mass energy, the coupling constant λ must not be just such as to produce a bound state of mass E.)

The text of this paper is largely concerned with expansions of kernels and unknown functions about surfaces of singularity. We assumed in Sec. 2 that our kernels were continuous functions of their variables, apart from certain explicitly exhibited singularities. However, in Sec. 5 where we examined the full Bethe–Salpeter equation with one-particle exchange, the process of getting rid of the moving singularities left us with a kernel which contained a delta function in addition to fixed singularities due to the direct-channel propagators. We manipulated as though these expansions can be carried out even in the presence of delta functions. Such manipulations require justification; let us see how to justify them.

Where functions of one variable are concerned, the issue is trivial; we can always use the delta function to perform the integration, for instance,

$$\begin{aligned} f(x) &= g(x) + \int K(x, y)\delta(y - a) f(y)\, dy \\ &= g(x) + K(x, a) f(a). \end{aligned}$$

Put $x = a$: $f(a) = (1 - K(a, a))^{-1} g(a)$, and, substituting back, we get the solution

$$f(x) = g(x) + \frac{g(a)}{1 - K(a, a)}.$$

This example is completely trivial, but the process of solving at one particular value and then computing the general solution from the equation itself is quite a general one, as we will see. Similarly, the solution of

$$f(x) = g(x) + \int K(x, y)\delta(x - y) f(y)\, dy,$$

is

$$f(x) = \frac{g(x)}{1 - K(x, x)}.$$

The simpler cases with functions of two variables follow the same general lines:

$$\begin{aligned} f(x, y) &= g(x, y) + \iint K(x, y, x', y') \\ &\qquad \times \delta(x' - y') f(x', y')\, dx'\, dy' \\ &= g(x, y) + \int K(x, y, x', x') f(x', x')\, dx', \end{aligned}$$

so that at $y = x$ we have an ordinary one-dimensional integral equation, from whose solution we can compute $f(x, y)$ from the equation itself. We deal similarly with the slightly more complicated equation

$$\begin{aligned} f(x, y) = g(x, y) + \iint & K(x, y, x', y') \\ & \times \delta[F(x', y')] f(x', y')\, dx'\, dy'. \end{aligned}$$

The case of a "moving delta function" is dealt with similarly:

$$\begin{aligned} f(x, y) &= g(x, y) + \iint K(x, y, x', y') \\ &\qquad \times \delta(x - x') f(x', y')\, dx'\, dy' \\ &= g(x, y) + \int K(x, y, x, y') f(x, y')\, dy', \end{aligned}$$

and we have a straightforward one-dimensional integral equation.

However, we run into trouble with the apparently only slightly more complicated integral equation

$$\begin{aligned} f(x, y) = g(x, y) + \iint & K(x, y, x', y') \\ & \delta[x' - F(x)]\, f(x', y')\, dx' dy', \end{aligned}$$

which, when the delta function is used to perform one integration, yields

$$\begin{aligned} f(x, y) &= g(x, y) \\ &\quad + \int K(x, y, F(x), y') f[F(x), y']\, dy'. \end{aligned} \tag{A5}$$

This is not an integral equation in the normal sense at all, because of the "wrong" argument appearing in the f under the integral sign. The best thing we can do in order to get a true integral equation, albeit a two-dimensional one, is to carry out a Fourier transformation on the variable x, yielding the integral equation

$$\tilde{f}(\tilde{x}, y) = \tilde{g}(\tilde{x}, y) + \iint L(\tilde{x}, y, q, y')\tilde{f}(q, y')\,dy'\,dq, \quad \text{(A6)}$$

where

$$L(\tilde{x}, y, q, y') = \int K(x, y, F(x), y')e^{i\tilde{x}x - iqF(x)}\,dx. \quad \text{(A7)}$$

The kernel $L(\tilde{x}, y, q, y')$ is not, of course, square summable in all four variables at once, but is square summable in $(\tilde{x}, y)$ and in (q, y), and will inherit appropriate continuity properties from K. This gives us the clue to the equation

$$\begin{aligned} f(x, y) &= g(x, y) + \iint K(x, y, x', y')\delta[F(x, x')] \times f(x', y')\,dx'\,dy' \\ &= g(x, y) + \sum_i \int K(x, y, F_i'(x), y') \times f[F_i'(x), y']\,dy', \quad \text{(A8)} \end{aligned}$$

where $x' = F_i'(x)$ are the various solutions of $F(x, x') = 0$. The transformation, analogous to (A7),

$$L'(\tilde{x}, y, q, y') = \sum_i \int K(x, y, F_i'(x), y')e^{i\tilde{x}x - iqF_i'(x)}dx, \quad \text{(A9)}$$

yields an equation exactly analogous to (A6). Similarly, we may consider the generalization of (A8), where the delta function involves y and y' as well as x and x':

$$\begin{aligned} f(x, y) &= g(x, y) + \iint K(x, y, x', y') \times \delta[x' - F(x, y, y')]f(x', y')\,dx'\,dy' \\ &= g(x, y) + \int K[x, y, F(x, y, y'), y'] \times f[F(x, y, y'), y']\,dy', \quad \text{(A10)} \end{aligned}$$

where we transform the kernel by

$$L''(\tilde{x}, y, q, y') = \int K[x, y, F(x, y, y'), y'] \times e^{i\tilde{x}x - iqF(x, y, y')}\,dx,$$

again obtaining an equation of the structure of (A6). Finally, we can combine the last two cases to deal with the most general possible delta function multiplying the kernel of a two-variable integral equation:

$$f(x, y) = g(x, y) + \iint K(x, y, x', y') \times \delta[F(x, y, x', y')]f(x', y')\,dx'\,dy', \quad \text{(A11)}$$

where we must solve the equation $F(x, y, x', y') = 0$ (say) for x', with solutions (say) $x' = F_i'(x, y, y')$. Then the transformed kernel leading to the form (A6) will be

$$L'''(\tilde{x}, y, q, y') = \sum_i \int K[x, y, F_i'(x, y, y'), y'] \times e^{i\tilde{x}x - iqF_i'(x, y, y')}dx. \quad \text{(A12)}$$

The generalization to integral equations involving higher numbers of variables presents no new difficulties and, hence, no new interest.

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Kinetic Description of an Inhomogeneous Plasma*

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The general description of a strongly inhomogeneous one-component plasma in the so-called "ring" approximation is derived. Using the general theory of inhomogeneous systems, the closed system of two equations in one-particle phase space is obtained. The additional equation for some function, which appears in the collisions term, has the form of a Vlasov equation linearized around the inhomogeneous one-particle distribution function. The meaning of the parameters which appear in this equation is discussed. This equation is solved in the hydrodynamic approximation. The collision operator in the Markoffian limit reduces to the well-known form. The velocity distribution function for the inhomogeneous state is discussed and some additional terms to the usual Balescu–Guernsey–Lenard equation, in the case of no square-integrable inhomogeneity factors, are obtained. The influence of initial correlation is discussed.

1. INTRODUCTION

In recent years, the problem of the kinetic description of fully ionized plasmas has been studied intensively. In 1960, the kinetic equation for a stable homogeneous plasma was derived independently by Balescu,[1] who used the Prigogine perturbation technique, and by Guernsey[2] and Lenard,[3] starting from the BBGKY hierarchy. This equation has been rederived by Frieman[4] and Résibois[5] in non-Markoffian form and generalized by Balescu[6] to the case of unstable plasmas. The first successful attempt to describe the inhomogeneous system has been made by Guernsey[7] for slightly inhomogeneous (linear in inhomogeneity factor) plasma in a state close to equilibrium. The generalization of this equation for the case of a plasma far from equilibrium has been done by Balescu and the author.[8,9]

From another side the work on the general theory of inhomogeneous systems has recently made great progress. The general master equation for an inhomogeneous system has been derived by Severne[10] and by Balescu,[11] who discussed, in a very compact and elegant way, the problem of the master equation as well as the asymptotic kinetic equation for very general statistical systems. The aim of the present paper is to obtain a closed system of equations describing an inhomogeneous plasma far from equilibrium in the so-called ring approximation. We will use here the perturbation technique introduced by Prigogine *et al.*[12,13] and will follow the general line of the theory as presented by Balescu.[10] We will here only sketch the main points of the theory in order to clarify the notation; for more detail, see Refs. 10–13.

For the sake of simplicity we will consider here a system consisting of the electron gas imbedded in a homogeneous continuous neutralizing background. The generalization of most of the present results to the case of a many-component plasma is straightforward. We will indicate the points which are somewhat more complicated in the multicomponent plasma case.

Our system is described by the Liouville equation which can be written in the following form:

$$Lf_N = (\partial_t - \mathfrak{L}^0 - e^2\mathfrak{L}^1)f_N, \tag{1.1}$$

where

$$\begin{aligned} &\mathfrak{L}^0 = -\sum \mathbf{v}_j \cdot \boldsymbol{\nabla}_j, \\ &\mathfrak{L}^1 = m^{-1}\sum_{j\neq n} (\boldsymbol{\nabla}_j V_{jn}) \cdot \boldsymbol{\partial}_{jn}; \\ &\partial_t = \frac{\partial}{\partial t}, \qquad \boldsymbol{\nabla}_j = \frac{\partial}{\partial \mathbf{x}_j}, \\ &\boldsymbol{\partial}_j = \frac{\partial}{\partial \mathbf{v}_j}, \quad \boldsymbol{\partial}_{jn} = \boldsymbol{\partial}_j - \boldsymbol{\partial}_n, \end{aligned} \tag{1.2}$$

and the following obvious notation is used: m, e, $\mathbf{v}_j$, and $\mathbf{x}_j$ denote the mass, electric charge, velocity, and position of particle j, respectively, and f_N is the N-particle distribution function.

The Coulomb interaction potential can be written in the following form of Fourier transform:

$$V_{jn} = \frac{1}{|\mathbf{x}_j - \mathbf{x}_n|} = (2\pi^2)^{-1}\int k^{-2}\, d\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{x}_j - \mathbf{x}_n)}. \tag{1.3}$$

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We introduce here the reduced one-particle distribution function

$$f_1(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t) = c\left[\varphi(\mathbf{v}_\alpha; t) + \int d\mathbf{k}\, \rho_{\mathbf{k}}(\mathbf{v}_\alpha; t) e^{i\mathbf{k}\cdot\mathbf{x}_\alpha}\right], \quad (1.4)$$

where $\varphi(\mathbf{v}_\alpha; t)$ is the velocity-distribution function and $\rho_{\mathbf{k}}(\mathbf{v}_\alpha; t)$ is the inhomogeneity factor.

According to Balescu,[11] the space of distribution functions can be divided into the correlated and uncorrelated "subspaces." Let us denote the "projection" operator on the uncorrelated subspace (vacuum of correlations) by V and the "projection" on the "orthogonal" correlation subspace by C. These operators have the following properties:

$$\begin{aligned} V + C &= I, \\ V^2 &= V, \\ C^2 &= C, \\ VC &= CV = 0. \end{aligned} \quad (1.5)$$

The general master equation (which is completely equivalent to the Liouville equation) can be written in the following form:

$$\begin{aligned} \partial_t f_N(t) = \mathfrak{L}^0 f_N(t) &+ e^2 \mathfrak{L}' V f_N(t) + \int_0^t d\tau\, G(\tau) f_N(t-\tau) \\ &+ e^2 \mathfrak{L}' U^0(t) C f_N(0) \\ &+ \int_0^t d\tau\, G(\tau) U^0(t-\tau) C f_N(0), \end{aligned} \quad (1.6)$$

where

$$\begin{aligned} G(t) &= \frac{1}{2\pi} \int_C dz\, e^{-izt} \sum_{n=1}^{\infty} \mathfrak{L}'(R^0(z) C \mathfrak{L}')^n \\ &= \frac{1}{2\pi} \int dz\, e^{-izt} \psi(z) \end{aligned} \quad (1.7)$$

is the "irreducible evolution operator" such that its V–V component is the diagonal fragment; its V–C component together with the V–C component of the fourth term on the left-hand side of Eq. (1.6) is the destruction fragment,

$$R^0(z) = (-\mathfrak{L}^0 - iz)^{-1} \quad (1.8)$$

is the unperturbed resolvent operator, and

$$U^0(t) = \exp \tau \mathfrak{L}^0,$$

is, for $t > 0$, the inverse Laplace transform of $R^0(z)$. The master equation for the uncorrelated N-particle distribution function may be immediately obtained by acting with the projection operator on Eq. (1.6):

$$\begin{aligned} \partial_t V f_N(t) = \mathfrak{L}^0 V f_N(t) &+ V \mathfrak{L}' V f_N(t) \\ &+ \int_0^t d\tau\, V G(\tau) V f_N(t-\tau), \end{aligned} \quad (1.9)$$

where, at the moment, all terms coming from the initial correlation have been neglected. The contribution of initial correlation will be discussed in Sec. 6. The problem now reduces to finding operator $G(t)$ in closed form. It is evident that it is impossible to perform the summation on all possible irreducible diagonal diagrams. We will use here the so-called ring approximation. We will take into account only the terms which are of the order $e^2(e^2 c)$. For a more detailed discussion of this approximation, see Refs. 1 and 13. Here c denotes the mean density

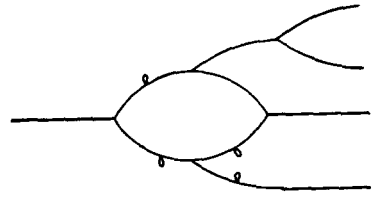


FIG. 1. Typical pseudo-diagonal ring.

$$c = N\Omega^{-1}, \quad (1.10)$$

where Ω is the volume of system.

The general contribution to collision-operator in this approximation is shown in Fig. 1.

We would like to stress here that our considerations are valid for a general inhomogeneous case. Up to now no assumption of wide separation between the molecular and hydrodynamical scale has been introduced.

2. SUMMATION OF RING DIAGRAMS

The collision term in Eq. (1.9) may be rewritten in a somewhat more convenient form:

$$\begin{aligned} \int_0^t d\tau V G(\tau) V f_N(t-\tau) &= \frac{1}{2\pi} \int e^{-izt}\, dz V \psi(z) V f_N(z) \\ &= \frac{1}{2\pi} \int dz \int_0^t e^{-iz(t-\tau)}\, d\tau V \psi(z) V f_N(\tau). \end{aligned} \quad (2.1)$$

We are interested only in the contribution to the reduced one-particle distribution function. We can perform the integration over positions and velocities of all particles except particles with subscript α. After this integration, we may omit the operator V acting on the left:

$$\begin{aligned} \Omega^{-(N-1)} \int d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1} \int d\mathbf{v}_1 \cdots d\mathbf{v}_{N-1} & \\ \times \int_0^t d\tau V G(\tau) V f_N(t-\tau) & \\ = \frac{1}{2\pi} \int dz \int_0^t e^{-iz(t-\tau)} \Omega^{-(N-1)} & \\ \times \int d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1}\, d\mathbf{v}_1 \cdots d\mathbf{v}_{N-1} \psi(z) V f_N(\tau)\, d\tau & \\ \equiv \frac{1}{2\pi} \int dz \int_0^t e^{-iz(t-\tau)} Q(z, \tau)\, d\tau. & \end{aligned} \quad (2.2)$$

Let us perform now the Fourier transform of Eq. (2.2) with respect to the position $\mathbf{x}_\alpha$:

$$Q_{\mathbf{k}}(\mathbf{v}_\alpha, z, \tau) = \frac{1}{(2\pi)^3}\int d\mathbf{x}_\alpha e^{-i\mathbf{k}\cdot\mathbf{x}_\alpha} Q(z, \tau). \quad (2.3)$$

The typical contribution to $Q_{\mathbf{k}}(\mathbf{v}_\alpha, z, \tau)$ has been shown in Fig. 1. Now the problem is reduced to the summation of all inhomogeneous ring diagrams.

In order to evaluate this contribution we will use here the procedure of summation developed in Ref. 9 and based on the Résibois factorization theorem.[5]

Let us consider the disconnected diagram which consists of two subdiagrams. A diagram in which all vertices of one subdiagram are placed to the left of all the vertices of the second subdiagram will be called a primitive diagram. The set of diagrams which is obtained by permutation of the relative position of the vertices of one subdiagram with respect to the vertices of the second one (the order of vertices of each subdiagram separately remaining unchanged) is called the permutation class of diagrams generated by the primitive one. According to Résibois's theorem,[5,13] the contribution to the whole permutation class is equal to the convolution of the contributions of the two subdiagrams.

In our case, we may simply use the Résibois theorem by separating out a common factor in all diagrams. The contribution $Q_{\mathbf{k}}(\alpha, z, \tau)$ may indeed be written in the following way:

$$\begin{aligned} &Q_{\mathbf{k}}(\alpha, z, \tau) \\ &= i\omega_p^2 \int l^{-2}\, d\mathbf{l}\, \mathbf{l}\cdot\partial_\alpha \int d\mathbf{v} \\ &\quad \times \int (dz'/2\pi) P_{\mathbf{k}+\mathbf{l}}(\mathbf{q}, \mathbf{v}_\alpha, z') P_{-\mathbf{l}}(\mathbf{p}, \mathbf{v}, z - z') \psi_{\mathbf{pq}}(\tau), \end{aligned} \quad (2.4)$$

where the operator $P_{\mathbf{k}}(\mathbf{p}, \alpha, \tau)$ acting on some function of $\mathbf{p}$, $\mathbf{v}_\alpha$ and τ, say $\chi_{\mathbf{p}}(\tau)$, is determined by a series of diagrams shown in Fig. 2. The function $\psi_{\mathbf{pq}}(\tau)$ is represented diagrammatically in Fig. 3. In this figure we use the notation that brackets denote that only the respective vertex is taken into account. We may express $\psi_{\mathbf{pq}}(n, m, \tau)$ analytically in the following form:

$$\begin{aligned} &\psi_{\mathbf{pq}}(n, m, \tau) \\ &= \frac{e^2}{m}\Big\{ -V_p i\mathbf{p}\cdot\partial_{nm}\varphi(n;\tau)\varphi(m;\tau)\delta_{\mathbf{p}+\mathbf{q}} \\ &\quad + V_q i\mathbf{q}\cdot\partial_{nm}\rho_{\mathbf{p}+\mathbf{q}}(n;\tau)\varphi(m;\tau) \\ &\quad - V_p i\mathbf{q}\cdot\partial_{nm}\rho_{\mathbf{p}+\mathbf{q}}(m;\tau)\varphi(n;\tau) \\ &\quad + \int d\mathbf{l}' V_{l'} i\,\mathbf{l}\cdot\partial_{nm}\rho_{\mathbf{p}+\mathbf{l}'}(n;\tau)\rho_{\mathbf{p}-\mathbf{l}'}(m;\tau)\Big\}, \end{aligned} \quad (2.5)$$

$$V_l = (2\pi^2)^{-1} l^{-2}.$$

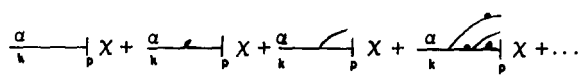


FIG. 2. Series of contributions to $P_{\mathbf{k}}(\rho, \alpha, z)$.

We have to notice here that one must carefully handle Eq. (2.4) because in the case $\mathbf{k} = 0$ the homogeneous ring will be taken into account.

One may immediately recognize that the term

$$\begin{aligned} &P_{\mathbf{k}+\mathbf{l}}(\mathbf{k}+\mathbf{l}, n, z') P_{-\mathbf{l}}(-\mathbf{l}, m, z - z') \\ &\quad \times \{(-e^2/m) V_{\mathbf{k}} i\mathbf{k}\cdot\partial_{nm}\varphi(n;\tau)\varphi(m;\tau)\}\delta\mathbf{k} \end{aligned} \quad (2.6)$$

gives us exactly the homogeneous collision operator multiplied by $\delta_{\mathbf{k}}$.

The series of diagrams shown in Fig. (2) may be summed, and as a result we obtain the following integral equation for $P_{\mathbf{k}}(\mathbf{m}, \alpha, z)x(\alpha, \tau)$, $x(\alpha)$ being an arbitrary function of $\mathbf{m}$, $\mathbf{v}_\alpha$, and τ:

$$\begin{aligned} &P_{\mathbf{k}}(\mathbf{m}, \alpha, z)x(\alpha) \\ &= \frac{x(\alpha)}{i[\mathbf{k}\cdot\mathbf{v}_\alpha - z]} + \frac{\omega_p^2}{k^l}\frac{\mathbf{k}\cdot\partial_\alpha\varphi(\alpha;\tau)}{\mathbf{k}\cdot\mathbf{v}_\alpha - z}\int d\mathbf{v}_1 P_{\mathbf{k}}(\mathbf{m}, 1, z)x(1) \\ &\quad - \frac{1}{i[\mathbf{k}\cdot\mathbf{v}_\alpha - z]}\frac{1}{2\pi}\int dz'\int d\mathbf{l} \\ &\quad \times \int d\mathbf{v}_1 \Big\{ l^{-2}\omega_p^2(-i\mathbf{l})\cdot\partial_\alpha R_{\mathbf{k}-\mathbf{l}}(\alpha, z - z') P_{\mathbf{l}}(\mathbf{m}, 1, z')x(1) \\ &\quad + \frac{\omega_p^2}{|\mathbf{l} - \mathbf{k}|^{-2}} i(\mathbf{l} - \mathbf{k})\cdot\partial_\alpha R_{\mathbf{k}-\mathbf{l}}(1, z - z') \\ &\quad \times P_{\mathbf{l}}(\mathbf{m}, \alpha, z')x(\alpha)\Big\}, \end{aligned} \quad (2.7)$$

where $R_{\mathbf{k}}(\alpha, z)$ is the solution to the nonlinear Vlasov equation with the following initial condition:

$$\mathcal{R}_{\mathbf{k}}(\alpha, \theta)|_{\theta=0} = \rho_{\mathbf{k}}(\alpha;\tau), \quad (2.8)$$

where by $\mathcal{R}_{\mathbf{k}}(\alpha, \theta)$ we have denoted the inverse Laplace transform of $R_{\mathbf{k}}(\alpha, z)$. Equation (2.7) has the form of Vlasov equation linearized around the function $R_{\mathbf{k}}(\alpha, z)$, with the initial condition

$$\mathcal{S}_{\mathbf{k}}(\mathbf{m}, \alpha, \theta)x(\alpha)|_{\theta=0} = x(\alpha). \quad (2.9)$$

[Obviously $\mathcal{S}_{\mathbf{k}}(\mathbf{m}, \boldsymbol{\alpha}, \theta)x(\alpha)$ is the inverse Laplace transform of $P_{\mathbf{k}}(\mathbf{m}, \alpha, z)x(\alpha)$.]

The description of the inhomogeneous plasma is

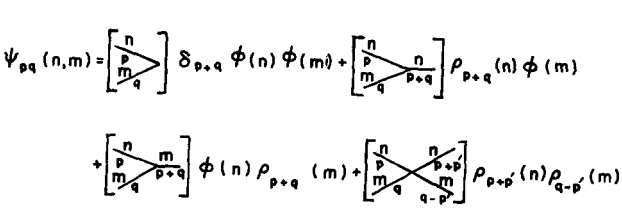


FIG. 3. Diagrammatic representation of function $\psi_{\mathbf{pq}}(n, m)$.

now completed by this system of equations: the kinetic equation (1.9), the nonlinear Vlasov equation for the function $R_{\mathbf{k}}(\alpha, z)$, and Eq. (2.7). Because the nonlinear Vlasov equation, as well as the one linearized around the inhomogeneous distribution function, can not be solved analytically, we have to look for some approximations. Let us consider first the nonlinear Vlasov equation. We note here that the function $\rho_{\mathbf{k}}(\alpha; \theta + \tau)$ is a short-time solution of the kinetic equation with the initial condition $\rho_{\mathbf{k}}(\alpha; \tau)$. This is exactly the initial condition (2.8). From this fact we can conclude that $\mathcal{R}_{\mathbf{k}}(\alpha, \theta)$ differs from $\rho_{\mathbf{k}}(\alpha; \tau + \theta)$ only by terms of order e^2 (because $\theta + \tau$ is short). As far as the ring approximation is concerned, we need only terms of order up to e^2 in the kinetic equation. Adding a term of order e^2 to $\mathcal{R}_{\mathbf{k}}(\alpha, \theta)$ in the collision term produces a change of the latter only in the order $\geq e^4$ and so is beyond our order of accuracy.

In concluding, we may write

$$\mathcal{R}_{\mathbf{k}}(\alpha; \theta) = \rho_{\mathbf{k}}(\alpha; \theta + \tau). \tag{2.10}$$

In order to eliminate the difficulties coming from the distinct treatment of the different component of the one-particle distribution function, we will take into account $\varphi(\alpha; \theta + \tau)$ instead of $\varphi(\alpha; \tau)$. The difference in the collision term is also at least of fourth order in e. Using this approximation, we are left with only two equations; the kinetic equation (1.9) and the equation for $\mathcal{F}_{\mathbf{k}}(\mathbf{m}, \alpha, \theta)x(\alpha)$ in the following form:

$$\begin{aligned}
&(\partial_\theta + i\mathbf{k}\cdot\mathbf{v}_\alpha)\mathcal{F}_{\mathbf{k}}(\mathbf{m}, \alpha; \theta)x(\alpha) \\
&= i\omega_p^2 \int l^{-2}\, d\mathbf{l}\, \mathbf{l}\cdot\partial_\alpha\{\varphi(\alpha; \theta + \tau)\delta_{\mathbf{k}-\mathbf{l}} + \rho_{\mathbf{k}-\mathbf{l}}(\alpha; \theta + \tau)\} \\
&\quad \times \int d\mathbf{v}_1 \mathcal{F}_{\mathbf{l}}(\mathbf{m}, 1; \theta)x(1) \\
&\quad - i\omega_p^2 \int \frac{d\mathbf{l}}{|\mathbf{l} - \mathbf{k}|^2}(\mathbf{l} - \mathbf{k})\cdot\partial_\alpha \mathcal{F}_{\mathbf{l}}(\mathbf{m}, \alpha; \theta)x(\alpha) \\
&\quad \times \int d\mathbf{v}_1 \rho_{\mathbf{k}-\mathbf{l}}(1; \theta + \tau),
\end{aligned} \tag{2.11}$$

with the initial condition (2.9).

The physical meaning of this equation and the possible way of its approximate solution will be discussed in the next section.

3. DISCUSSION OF LINEARIZED VLASOV EQUATION

Equation (2.11) may be rewritten in the position representation as follows:

$$\begin{aligned}
&(\partial_\theta + \mathbf{v}_\alpha\cdot\nabla_\alpha)\mathcal{F}(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \theta)x(\alpha) \\
&\quad - (e/m)\mathbf{E}^{(1)}(\mathbf{x}_\alpha, \theta)\partial_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; \theta) \\
&\quad - (e/m)\mathbf{E}(\mathbf{x}_\alpha, \theta)\partial\mathcal{F}(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \theta)x(\alpha) = 0,
\end{aligned} \tag{3.1}$$

where f is connected with φ and $\rho_{\mathbf{k}}$ by relation (1.4). The two electric fields appearing in (3.1) are determined by the following equations:

$$\begin{aligned}
&\nabla_\alpha\cdot\mathbf{E}(\mathbf{x}_\alpha, \theta) \\
&\quad = 4\pi e\int [f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; \theta + \tau) - c\varphi(\mathbf{v}_\alpha; \theta + \tau)]\, d\mathbf{v}_\alpha
\end{aligned} \tag{3.2}$$

and

$$\nabla_\alpha\cdot\mathbf{E}^{(1)}(\mathbf{x}_\alpha, \theta) = 4\pi e\int \mathcal{F}(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \theta)x(\alpha)\, d\mathbf{v}_\alpha. \tag{3.3}$$

For Eq. (3.1) the field $\mathbf{E}$ [which is the Vlasov self-consistent field generated by the distribution $f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t)$] may be considered as the external field and $\mathbf{E}^{(1)}$ plays the role of the self-consistent field generated by the function $\mathcal{F}_\chi$.

This field describes the collective effects which appear during the collision. The nature of these two fields seems to be quite different and it will be interesting to investigate in more detail their physical role. For Eq. (3.1) we have still to find the appropriate initial condition. This is done by the inverse Fourier transform of $\psi_{\mathbf{pq}}$ defined by Eq. (2.5):

$$\begin{aligned}
&\psi(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{x}_\beta, \mathbf{v}_\beta, \tau) \\
&\quad = (-1/mc^2)\nabla_\alpha V(|\mathbf{x}_\alpha - \mathbf{x}_\beta|)\partial_{\alpha\beta} f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t) f(\mathbf{x}_\beta, \mathbf{v}_\beta; t) \\
&\quad \equiv \psi(\alpha, \beta; \tau).
\end{aligned} \tag{3.4}$$

In order to better understand the meaning of the operator $\mathcal{F}(\mathbf{x}_\alpha, \mathbf{v}_\alpha; \theta)$, as well as the form of the initial condition (3.4) and of the collision operator, the explicit calculation of the contributions of certain simple diagrams in the position representation has been done in the Appendix.

The collision operator, as well as the two-particle correlation function,[13] may be constructed from this operator. From the other side, the kernel in the collision term vanishes for times greater than the collision time t_{coll}. But we have also another characteristic time in our system: the hydrodynamical time. This time is supposed to be the natural time scale of change of the function $f(x, \theta; t)$. In many physical situations we may assume that

$$t_n \gg t_{\text{coll}}. \tag{3.5}$$

As we have already mentioned, $\mathcal{F}\psi(\alpha, \beta, \tau)$ is a component of the correlation function. It means that the natural scale of its x dependence is the range of correlations L_c. This fact may be easily deduced from the collision operator in the form given by (2.4). Following the arguments of Balescu,[13] we may deduce that

$$\mathbf{l} \sim (L_h/L_c)\mathbf{k} \tag{3.6}$$

and this in nothing else but the introduction of the two natural scales in x dependence. There exist many physical situations where we may assume that

$$\lambda = L_c/L_h \ll 1. \tag{3.7}$$

The natural way of solving Eq. (3.1) is the separation of the x dependence in fast and slow dependence as it has been used by Klimontovitch.[14] We will adopt here the multiscale perturbation introduced by Bogoliubov and used by Frieman[4] for the solution of BBGKY hierarchy. It occurs, however, that the most suitable starting point of that technique is not Eq. (3.1) but Eq. (2.7) with $R_k(v)$ determined by the nonlinear Vlasov equation. In the $(\mathbf{x}, \mathbf{v})$ space the system of equations to be solved is

$$\partial_\theta \bar{f} + \mathbf{v} \cdot \nabla \bar{f} - (e/m)\bar{\mathbf{E}} \cdot \partial \bar{f} = 0 \tag{3.8}$$

and

$$\partial_\theta (Px + \mathbf{v} \cdot \nabla Px - (e/m)\bar{\mathbf{E}} \cdot \partial Px - (e/m)\mathbf{E}^{(1)} \cdot \partial \bar{f} = 0, \tag{3.9}$$

where we use the notation

$$\bar{f} = c\left[\varphi(v; \theta) + \int d\mathbf{k} R_{\mathbf{k}}(\mathbf{v}; \theta) e^{i\mathbf{k}\cdot\mathbf{x}}\right] \tag{3.10}$$

and $\mathbf{E}$ is Vlasov field induced by $\bar{f}$.

We may regard the field $\bar{\mathbf{E}}$ in Eqs. (3.8) and (3.9) as an external field, and, according to the discussion of the previous paragraph, we may substitute $\bar{\mathbf{E}}$ for $\mathbf{E}$.

We assume now that all functions have their $\mathbf{x}$ dependence separated in different scales $A(\mathbf{x}_0, \lambda\mathbf{x}_1, \cdots \lambda^n \mathbf{x}_n)$, where, after the whole calculation is finished, we are going to put

$$\begin{aligned} \partial \mathbf{x}_n/\partial \mathbf{x} &= 1, \\ \mathbf{x}_n(0) &= 0. \end{aligned} \qquad n = 0, 1, 2 \cdots, \tag{3.11}$$

From our discussion it is clear that the one-particle distribution function depends only on slow variables, so we may assume their perturbation expansion in the following form:

$$\bar{f}(\mathbf{x}, \mathbf{v}, \theta) = \sum_{n=0}^{\infty} \lambda^n f^{(n)}(\lambda\mathbf{x}_1, \lambda^s \mathbf{x}_s, \mathbf{v}; \theta). \tag{3.12}$$

The expansion for $(\partial/\partial \mathbf{x})\bar{f}$ may be written in the form (see Ref. 4)

$$\frac{\partial}{\partial \mathbf{x}} \bar{f} = \sum_{n=1}^{\infty} \lambda^n \sum_{s=1}^{n} \frac{\partial}{\partial(\lambda^s \mathbf{x}_s)} f^{(n-s)}(\lambda^p x_p, \mathbf{v}; \theta). \tag{3.13}$$

The analogous expansion of $\mathfrak{F}\psi$ has the following form:

$$\mathfrak{F}x = \sum_{n=0}^{\infty} \lambda^n \mathfrak{F}^{(n)}(\mathbf{x}_0, \cdots, \lambda^p \mathbf{x}_p, \cdots, \mathbf{v}; \theta)x \tag{3.14}$$

and for the field

$$\mathbf{E}^{(1)} = \sum_{n=0}^{\infty} \lambda^n \mathbf{E}_n^{(1)}(\mathbf{x}_0, \cdots, \lambda^p \mathbf{x}_p, \cdots, \mathbf{v}; \theta), \tag{3.15}$$

where the relations between the $\mathbf{E}_n^{(1)}$ and $\mathfrak{F}^{(n)}x$ are of the type (3.3). The respective expansion for gradients may be written as follows:

$$\frac{\partial \mathfrak{F}x}{\partial \mathbf{x}} = \sum_{n=0}^{\infty} \lambda^n \sum_{s=0}^{n} \frac{\partial}{\partial(\lambda^s \mathbf{x}_s)} \mathfrak{F}^{(n-s)}x. \tag{3.16}$$

Substituting the above expansion into Eqs. (3.8) and (3.9) and ordering with respect to λ, we obtain an infinite set of equations. Because Eqs. (3.8) and (3.9) have nonconstant coefficients, we cannot split the equation in each order by equating to zero the contribution of each function with subscript l separately as is usually done. In our case, we consider, rather, in the equation of order l, the contribution coming from a function of order $<l$ as an inhomogeneous term in the equation. In the lowest order the equations have the following form:

$$\partial f^0/\partial t - (e/m)\mathbf{E} \cdot \partial f^0(\lambda \mathbf{x}_1, \mathbf{v}; t) = \theta \tag{3.17}$$

and

$$\partial \mathfrak{F}^0 \psi/\partial t + \mathbf{v} \cdot \nabla_0 \mathfrak{F}^0 \psi - (e/m)\mathbf{E}\partial \mathfrak{F}^0 \psi - (e/m)\mathbf{E}_0^{(1)} \partial f^0 = 0, \tag{3.18}$$

where

$$\nabla_0 = \frac{\partial}{\partial \mathbf{x}_0}. \tag{3.19}$$

Because the operators in the above equations are diagonal in $\mathbf{x}_l$ for $l \geq 1$, we can consider these variables as parameters.

The field $\mathbf{E}$ induced by the function f may be assumed to depend only on the variables $\lambda\mathbf{x}_1$. This system of equations describes the plasma oscillation in the presence of a uniform external field and, in the case of a one-component plasma, it may be solved analytically.[15] At this point, our approximation can not be applied to a many-component plasma. In that case the system of equations, analogous to (3.17) and (3.18), cannot be solved analytically and some approximation has to be applied.[16]

The solution of Eq. (3.15) may be found immediately:

$$f^0(\alpha, \theta) = f(\mathbf{x}_1, \mathbf{v}_\alpha - \boldsymbol{\eta}; \tau), \tag{3.20}$$

where we have denoted

$$\boldsymbol{\eta}(\theta) = \frac{e}{m} \int_0^\theta \mathbf{E}(t')\, dt'. \tag{3.21}$$

Substituting this result into Eq. (3.18) and performing

[14] Yu. L. Klimontovitch, *Statistichiskaya Teoriya Niravnavisnich Protsisav Plasmi* (Moskovskova Gasudarstinnova Universiteta, Moskva, 1964).

[15] B. P. Fried, H. Gell-Mann, J. D. Jacson, and H. W. Wyld, J. Nucl. Energy **C1**, 190 (1960).

[16] A. Kuszell and A. Senatorski, Institute of Nuclear Research, Report P. No. 829, Warsaw, 1967.

the change of variables

$$\mathbf{u} = \mathbf{v}_\alpha - \boldsymbol{\eta}, \qquad \theta' = \theta, \tag{3.22}$$

we get Eq. (3.18) in the following form:

$$\partial_\theta \mathfrak{T}^0 x + (\mathbf{u} + \boldsymbol{\eta}) \cdot \mathbf{k} \mathfrak{T}^0 x - (e/m)\mathbf{E}_0^{(1)}(\mathbf{k}) \cdot \partial f(\mathbf{x}_1, \mathbf{u}, \tau) = 0, \tag{3.23}$$

where we have performed a Fourier transform with respect to $\mathbf{x}$.

By a simple substitution

$$\mathfrak{T}^0 x = \exp -i\mathbf{k} \cdot \int_0^\theta \boldsymbol{\eta}(\theta')\, d\theta' \phi(\alpha, \theta), \tag{3.24}$$

we get immediately the equation for ϕ in the very familiar form

$$\partial_\theta \phi + i\mathbf{u} \cdot \mathbf{k}\phi - (e/m)\mathcal{E} \cdot \partial f(\mathbf{x}_1, \mathbf{u}, \tau) = 0, \tag{3.25}$$

where

$$i\mathbf{k} \cdot \mathcal{E} = 4\pi e \int \phi\, du. \tag{3.26}$$

We may immediately write the solution of this equation (see, for example, Ref. 13) in the following form:

$$\phi = \frac{1}{2\pi} \int dz\, e^{-iz\theta} \left(\frac{x(u)}{i[\mathbf{k} \cdot \mathbf{u} - z]} + \frac{\omega_p^2}{ck^2} \frac{\mathbf{k} \cdot \partial f(\mathbf{x}_1, u, \tau)}{\mathbf{k} \cdot \mathbf{u} - z} \times \left\{ \int \frac{d\mathbf{v}_1 x(\mathbf{v}_1, \mathbf{x}_1)}{i[\mathbf{k} \cdot \mathbf{v}_1 - z]} \right\} \Big/ \epsilon_k(\mathbf{x}_1, z) \right), \tag{3.27}$$

where the dielectric constant is defined as follows:

$$\epsilon_k(\mathbf{x}_1, z) = 1 - \frac{\omega_p^2}{ck^2} \int \frac{\mathbf{k} \cdot \partial f(\mathbf{x}_1, \mathbf{u}, \tau)^{du}}{(\mathbf{k} \cdot \mathbf{u} - z)}. \tag{3.28}$$

Finally, we obtain the following formula for $\mathfrak{T}x$, where we have put $x_1 = x_0 = x_\alpha$:

$$\mathfrak{T}_k^0 x(\alpha) = \exp\left(-i\mathbf{k} \cdot \int_0^\theta \boldsymbol{\eta}(t')\, dt' \right) \frac{1}{2\pi} \times \int dz\, e^{-iz\theta} \left\{ \frac{x(\mathbf{v}_\alpha - \boldsymbol{\eta})}{i[\mathbf{k} \cdot (\mathbf{v}_\alpha - \boldsymbol{\eta}) - z]} + \frac{\omega_p^2}{ck^2} \frac{\mathbf{k} \cdot \partial_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha - \boldsymbol{\eta}; \tau)}{\mathbf{k} \cdot (\mathbf{v}_\alpha - \boldsymbol{\eta}) - z} \frac{1}{\epsilon_k(\mathbf{x}_\alpha, z)} \int \frac{x(\mathbf{v})\, d\mathbf{v}}{i[\mathbf{k} \cdot \mathbf{v} - z]} \right\}. \tag{3.29}$$

The solution (3.29) yields a very complicated collision operator in non-Markoffian form. It seems, however, that there may exist cases of some physical importance in which one cannot neglect the contributions coming from the field $\mathbf{E}$ (the $\boldsymbol{\eta}$ terms) in (3.27). Even within the hydrodynamic approximation in some cases the change of the distribution function due to the Vlasov field $\mathbf{E}$ during the collision cannot be neglected. In such case (separation of electric charge) the proper description is given by the collision terms of the type produced by (3.29). But in the cases where the separation of charges does not appear, we may neglect $\boldsymbol{\eta}$ in (3.29) and we got a much simpler expression for $\mathfrak{T}x$:

$$\mathfrak{T}^0 x(\mathbf{v}_\alpha, z) = \frac{x(\mathbf{v}_\alpha)}{i[\mathbf{k} \cdot \mathbf{v}_\alpha - z]} + \frac{\omega_p^2}{ck^2} \frac{\mathbf{k} \cdot \partial_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; \tau)}{\mathbf{k} \cdot \mathbf{v}_\alpha - z} \left\{ \int \frac{x(\mathbf{v})\, d\mathbf{v}}{i(\mathbf{k} \cdot \mathbf{v} - z)} \right\} \Big/ \epsilon_k(\mathbf{x}_\alpha, z). \tag{3.30}$$

We must mention here that, in order to be consistent with our expansion in $\lambda^{(n)}$, we have to neglect the x_0 dependence in the one-particle distribution function in the initial condition $\psi(\alpha, \beta)$.

There is in principle no difficulty in calculating $\mathfrak{T}\psi$ to higher order of λ.

4. THE KINETIC EQUATION

By integrating Eq. (1.9) over positions and velocities of all particles except the one denoted by subscript α, we immediately obtain the kinetic equation in the following form:

$$\partial_t f(\alpha) + \mathbf{v}_\alpha \cdot \nabla_\alpha f(\alpha) - \frac{e}{m} \mathbf{E} \cdot \partial_\alpha f(\alpha) = \frac{1}{2\pi} \int dz \int_0^t d\tau\, e^{-iz(t-\tau)} Q(z, \tau), \tag{4.1}$$

where $Q(z, \tau)$ is determined by (2.4). For a more detailed discussion of the identity

$$-\frac{e}{m} \mathbf{E} \cdot \partial_\alpha f(\alpha) = \Omega^{-(N-1)} \int d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1} \times \int d\mathbf{v}_1 \cdots d\mathbf{v}_{N-1} V e^{2\mathfrak{L}'} V f_N \tag{4.2}$$

see Ref. 11.

We may now express the collision operator in the term of $\mathfrak{T}(x, \theta, z)$ operators (see Appendix). The kinetic equation may be written in the following form:

$$\partial_t f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t) + \mathbf{v}_\alpha \cdot \nabla_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t) - \frac{e^2}{m} \partial_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t) \cdot \nabla_\alpha \int d\mathbf{x}\, d\mathbf{v} V(|\mathbf{x}_\alpha - \mathbf{x}|) \times [f(\mathbf{x}, \mathbf{v}; t) - c\varphi(\mathbf{v}_\alpha, t)] = -\frac{e^2 c}{m} \int d\mathbf{l}\, V(l) i\mathbf{l} \cdot \partial_\alpha \int \frac{d\mathbf{y}}{(2\pi)^3} e^{i\mathbf{l} \cdot (\mathbf{y} - \mathbf{x}_\alpha)} \times \int d\mathbf{v} \int \frac{dz}{2\pi} \int \frac{dz'}{2\pi} \int_0^t d\tau\, e^{-iz(t-\tau)} \times P(\mathbf{x}_\alpha, \mathbf{v}_\alpha, z'; \tau) P(\mathbf{y}, \mathbf{v}, z - z'; \tau) \psi(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{y}, \mathbf{v}; \tau), \tag{4.3}$$

where we have written the Vlasov term explicitly.

Equation (4.3), together with Eq. (3.1), form the complete general kinetic description of the inhomogeneous plasma in the ring approximation. Up to now the only assumption we have made is that we can neglect the influence of initial correlations. The physical picture described by these equations is the interaction of plasma waves described by Eq. (3.1) which forms the collision operator in Eq. (4.3). These are rather complicated, non-Markoffian equations but they are the proper starting point for all approximations. We will show here how these equations in the Markoffian hydrodynamic approximation reduce to the well-known results.

The very first step is the change of variable in Eq. (4.3)

$$\tau' = t - \tau \tag{4.4}$$

and the neglect of the τ dependence in the one-particle function.

Because the only dependence of τ is through the one-particle distribution function, after neglecting this dependence, we are left with the term e^{izt} alone, and we are able to perform the τ-integration explicity. The collision term can be written in the following form:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{e^2 c}{m}\int d\mathbf{l}\, V(l) i\,\mathbf{l}\cdot\partial_\alpha \int \frac{d\mathbf{y}}{(2\pi)^3}\, e^{i\mathbf{l}\cdot(\mathbf{y}-\mathbf{x}_\alpha)} \times \int d\mathbf{v} \int \frac{dz}{2\pi}\frac{e^{-izt}}{iz}\int \frac{dz'}{2\pi} P(\mathbf{x}_\alpha, \mathbf{v}_\alpha, z', t) \times P(\mathbf{y}, \mathbf{v}, z - z', t)\psi(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{y}, \mathbf{v}, t). \tag{4.5}$$

In this collision term all transient effects, which are inconsistent with the asymptotic form of kinetic equations, are still taken into account. For the sake of simplicity we assume here that the plasma is stable. In the unstable (or weakly stable) case we have to take into account additional contributions, similarly as in the homogeneous case.[6]

Our assumption that the plasma is stable means that all the poles of $P(\mathbf{x}, \mathbf{v}, z)\psi$ are located in the lower half plane z and that

$$|\operatorname{Im} z_\nu| \gg \omega_p, \tag{4.6}$$

where z_ν denotes the pole of $P\psi$ closest to the real axis. In this case, for large t we may neglect the contribution coming from these poles and take into account only the pole $z = 0$:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{e^2 c}{m}\int d\mathbf{l}\, V(l) i\,\mathbf{l}\cdot\partial_\alpha \int \frac{d\mathbf{y}}{(2\pi)^3}\, e^{i\mathbf{l}\cdot(\mathbf{y}-\mathbf{x}_\alpha)} \times \int d\mathbf{v} \int \frac{dz'}{2\pi} P(\mathbf{x}_\alpha, \mathbf{v}_\alpha, z', t) \times P(\mathbf{y}, \mathbf{v}, -z', t)\psi(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{y}, \mathbf{v}; t). \tag{4.7}$$

To be consistent with Eq. (4.7), we have to perform the same approximation for Eq. (3.1). As it has been discussed in the preceding paragraph, the neglect of the change of the function f during the collision is possible only for a weak self-consistent field. In such cases we neglect the time dependence of f in (3.1) and drop the term with $\mathbf{E}$.

The simplified equation for Px has now the form

$$(\partial_\theta + \mathbf{v}_\alpha\cdot\nabla_\alpha)\mathfrak{P}(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \theta)x - (e/m)\mathbf{E}^{(1)}(\mathbf{x}_\alpha, \theta)\cdot\partial_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha, t) = 0, \tag{4.8}$$

where θ denotes the Laplace variable conjugate to z. This system of equations is much simpler than previous one, but again Eq. (4.8) has no known analytical solution.

We would like to mention here that the discussion of the present paragraph is in some sense complementary to the previous one. Applying both approximations (Markoffian and hydrodynamical) together yields the solution of Eq. (4.8) in the hydrodynamic approximation which has already been obtained in Eq. (3.28).

Using this solution, we obtain the collision operator in the following form:

$$\left(\frac{\partial f}{\partial t}\right)_{\substack{\text{coll}\\ \text{hyd}}} = -\frac{8\pi^3}{c} i\frac{e^4}{m^2}\int d\mathbf{l}\, V^2(l)\,\mathbf{l}\cdot\partial_\alpha \int d\mathbf{v}_1 \int d\mathbf{v}_2 \times \left\{\frac{\delta(\mathbf{v}_1 - \mathbf{v}_\alpha)}{i\mathbf{l}\cdot(\mathbf{v}_1 - \mathbf{v}_2)\epsilon_l(\mathbf{x}_\alpha, -\mathbf{l}\cdot\mathbf{v}_1, t)} - \frac{\omega_p^2}{cl^2}\int \frac{dz'}{2\pi}\frac{\mathbf{l}\cdot\partial_\alpha f(\mathbf{x}_\alpha, \mathbf{v}_\alpha, t)}{|\epsilon_l(\mathbf{x}, z', t)|^2} \times [(\mathbf{l}\cdot\mathbf{v}_\alpha - z')(\mathbf{l}\cdot\mathbf{v}_1 - z')]^{-1}\right\} \times i\mathbf{l}\cdot\partial_{12} f(\mathbf{x}_\alpha, \mathbf{v}_1; t) f(\mathbf{x}_\alpha, \mathbf{v}_2; t), \tag{4.9}$$

where we have taken into account the following property of the dielectric constant:

$$\epsilon_{-l}(\mathbf{x}, -z; t) = \epsilon_l^*(\mathbf{x}, z, t), \tag{4.10}$$

where the asterisk denotes the complex conjugate.

This solution has the form obtained by Résibois[5,13] in the case of a homogeneous plasma with the only difference that $f(\mathbf{x}, \mathbf{v}, t)$ replaces $\varphi(v, t)$. This contribution may be written in much simpler form, because only the real part of the collision operator gives a nonvanishing contribution (for a detailed discussion see Balescu.[13] We will not repeat here this calculation, but give only the final result:

$$\left(\frac{\partial f}{\partial t}\right)_{\substack{\text{coll}\\ \text{hyd}}} = 8\pi^4 e^4 m^{-2}\int d\mathbf{l}\int d\mathbf{v}_1 \mathbf{l}\cdot\partial_\alpha\left\{\frac{\dot{V}(l)}{|\epsilon_l(\mathbf{x}, \mathbf{l}\cdot\mathbf{v}_\alpha, t)|}\right\}^2 \times \delta(\mathbf{l}\cdot[\mathbf{v}_\alpha - \mathbf{v}_1])\mathbf{l}\cdot\partial_{\alpha_1} f(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t) f(\mathbf{x}_\alpha, \mathbf{v}_1; t) \tag{4.11}$$

and one can immediately recognize that this is exactly the form of the kinetic equation in hydrodynamic approximation given by Balescu[13]).

We would like to stress here that, in the general physical situation, the correct kinetic description is given by Eqs. (3.1) and (4.3). In some cases, it may be simplified either by a hydrodynamical or by a Markoffian type of approximation. In both limits together the known result is rederived.

It seems to be very important to clarify the role of the field **E** in Eq. (3.1). This field may play an important role in the case of large charge separation and in instabilities connected with this separation. It seems that this problem may be even discussed in the hydrodynamic approximation.

5. THE VELOCITY DISTRIBUTION FUNCTION

The velocity distribution function in the inhomogeneous system does not always behave as the distribution function in the homogeneous state. The behavior of the velocity distribution function depends on the inhomogeneity factor. For inhomogeneity factors, whose Fourier transforms are the ordinary functions, there is no difference between these two functions. But if we take into account the more general case, where the Fourier transform of an inhomogeneity factor is a distribution (for example, of the type of Heaviside step function), the time evolution of the velocity distribution function is no longer determined by this function alone, but also by the inhomogeneity factor.

In some cases of physical interest (for example, two adjacent half spaces, each in equilibrium with different temperatures) the inhomogeneity factor is of general type. This problem in the frame of Vlasov approximation has been discussed by Grecos.[17]

The main point is that, for such inhomogeneity, factor $\rho_{\mathbf{k}}$ is no longer a function but a distribution in the Schwartz sense and because of the property

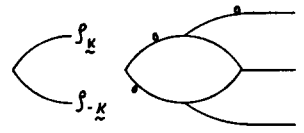
$$\rho_{\mathbf{k}}(\alpha) = \rho^{*}_{-\mathbf{k}}(\alpha), \tag{5.1}$$

their product is illdefined and proportional to Ω This is the reason why the usual Ω dependence analysis fails and one has to take into account additional diagrams of the type shown in Fig. 4.

As can be easily seen, however, inclusion of those diagrams does not change either the summation technique for an inhomogeneous plasma or the result of this summation. This is because these diagrams complete the respective inhomogeneous contribution.[17]

[17] A. P. Grecos, Ph.D. thesis, Université Libre de Bruxelles, 1968.

FIG. 4. Contributions to $\varphi(\alpha)$ for general inhomogeneity factor.



Our Eqs. (3.1) and (4.3) are valid as well as in this more general case. In order to obtain the proper evolution equation for the velocity distribution function, we have to integrate Eq. (4.3). From the definition we have

$$\varphi(\mathbf{v}; t) = c\Omega^{-1}\int d\mathbf{x} f(\mathbf{x}, \mathbf{v}; t). \tag{5.2}$$

The equation for $\varphi(\mathbf{v}; t)$ has the following form:

$$\begin{aligned}\partial_t\varphi(\mathbf{v}_\alpha; t) - \frac{e}{m}\Omega^{-1}\int d\mathbf{x}_\alpha\, \mathbf{E}(\mathbf{x}_\alpha; t)\partial_\alpha H(\mathbf{x}_\alpha, \mathbf{v}_\alpha; t)\\ = \frac{e^2c^2}{m}\Omega^{-1}\int d\mathbf{l}\, V(l) i\,\mathbf{l}\cdot\partial_\alpha \int\frac{d\mathbf{y}}{(2\pi)^3}\int d\mathbf{x}_\alpha\, e^{i\mathbf{l}\cdot(\mathbf{y}-\mathbf{x}_\alpha)}\\ \times\int d\mathbf{v}\int\frac{dz}{2\pi}\int\frac{dz'}{2\pi}\int_0^t d\tau\, e^{iz(t-\tau)}P(\mathbf{x}_\alpha, \mathbf{v}_\alpha, z', \tau)\\ \times P(\mathbf{y}, \mathbf{v}, z - z', \tau)\psi(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{y}, \mathbf{v}; \tau),\end{aligned} \tag{5.3}$$

where by $H(\mathbf{x}, \mathbf{v}; t)$ we denote the inhomogeneity factor.

The most important point in our discussion is that in the case of non-square-integrable inhomogeneity factors, the evolution of the velocity distribution function cannot be regarded as independent of inhomogeneity factor. In other words the Balescu–Guernsey–Lenard equation is valid only for square-integrable inhomogeneity factors. The physical meaning of this limitation is clear, because square integrability means that, in some sense, the inhomogeneity is localized, and its influence on the infinite homogeneous background is negligible. We would like to mention here that the second term of (5.3) is exactly the starting point of the quasilinear theory derived by Vedenov, Velikov, and Sagdeev[18] and by Drumond and Pines.[19]

6. EFFECT OF INITIAL CORRELATIONS

In order to make our consideration more complete, we discuss now the effect of initial correlations. The contribution of the initial correlation in the general case has been discussed recently by Balescu.[20] Following this discussion, we can take into account only the

[18] A. A. Vedenov, E. P. Velikov, and R. Z. Sagdeev, Proc. Conf. Plasma Phys. Cont. Nucl. Fusion, Salzbourg, 1961, paper CN-10/199.

[19] W. E. Drumond and O. Pines, Proc. Conf. Plasma Phys. Contr. Nucl. Fusion, Salzbourg, 1961, paper CN-10/134.

[20] R. Balescu, Physica **36**, 433 (1967).

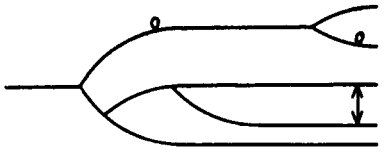


FIG. 5. Ring contribution to destruction fragment.

systems in which the correlations are due to interactions, and in that case their contribution disappears after a collision time. The contribution due to the initial correlation is described by the two left terms in Eq. (1.6) and is called the destruction fragment. This contribution in ring approximation (and additional assumption of very short collision time) consists of diagrams of the type shown in Fig. 5, where the arrow denotes the lines acting on irreducible two-particle correlation.

A similar approximation has been studied in the homogeneous state by Nishikava and Osaka[21] and they find that this description is inadequate in the case of unstable plasmas, because the destruction term is exponentionally growing in time with constant-growing ratio. This difficulty may be solved by taking into account the diagrams of the type shown in Fig. 6.[22] This means, however, that one can no longer consider the time of the influence of initial correlation as short. In fact, this time is of the order of the stabilizing time. A similar argument may be used for the collision term; this case will be discussed in the next section.

The contributions to destruction fragment, which has the ring placed on the lines acting on two-particle correlation functions, are not taken into account, because their contribution is due to irreducible ternary correlation approximation. It will be interesting to examine the contribution of a ternary correlation function in the case of unstable plasmas, but in our paper we shall limit ourselves only to the ring approximation.

The summation procedure used in Sec. 2 may be used successfully in the present case and the result is

$$Q_D = \frac{1}{\Omega^{N-1}} \int d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1} \int d\mathbf{v}_1 \cdots d\mathbf{v}_{N-1} \times V\left\{e^2 \mathfrak{L}' U^0(t) + \int_0^t d\tau\, G(\tau) U(t-c)\right\} C f_N(0)$$
$$= \int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}_\alpha} \int \frac{dz}{2\pi} e^{-izt} \frac{\omega_p^2}{i[\mathbf{k}\cdot\mathbf{v}_\alpha - z]} \int d\mathbf{l}\, l^{-2}\mathbf{l}\cdot\partial_\alpha \times \int d\mathbf{v}_1 \int \frac{dz'}{2\pi} T_{\mathbf{k}+\mathbf{l}}(\mathbf{p}, \alpha, z') T_{-\mathbf{l}}(\mathbf{q}, 1, z - z') \times \rho_{\mathbf{p},\mathbf{q}}(\alpha, 1; 0), \quad (6.1)$$

where $\rho_{\mathbf{p},\mathbf{q}}(\alpha, 1; 0)$ denote the Fourier transform of the irreducible two-particle correlation function and the operator T is defined similarly as P in Eq. (2.4).

Letting the operator $\partial_t + \mathbf{v}_\alpha \nabla_\alpha$, act on both sides of (6.1), we can write the contribution to kinetic equation in the following form:

$$\left(\frac{\partial f}{\partial t}\right)_D = \int d\mathbf{k}\, \omega_p^2 \int l^{-2} e^{i\mathbf{v}\cdot\mathbf{x}} \mathcal{C}_{\mathbf{k}+\mathbf{l}}(\mathbf{p}, \alpha; t) \times \mathcal{C}_{\mathbf{l}}(\mathbf{q}, d; t) \rho_{\mathbf{p},\mathbf{q}}(\alpha, l; 0), \quad (6.2)$$

where $\mathcal{C}_{\mathbf{k}}(\mathbf{q}, 1; t)$ is the Laplace transform of the operator $T_{\mathbf{k}}(\mathbf{q}, 1, z)$ and is the solution of the integral equation

$$(\partial_t + i\mathbf{k}\cdot\mathbf{v}\alpha)\mathcal{C}_k(\mathbf{p}, \alpha; t)x(\alpha) = i\omega_p^2 \int l^{-2}\mathbf{l}\cdot\partial_\alpha \{\varphi(\alpha; t)\delta_{\mathbf{k}-\mathbf{l}} + \rho_{\mathbf{k}-\mathbf{l}}(\alpha; t)\} \times \int d\mathbf{v}_1 \mathcal{C}_{\mathbf{l}}(\mathbf{p}, 1; t)x(1) + i\omega_p^2 \times \int \frac{d\mathbf{l}}{(|\mathbf{l} - \mathbf{k}|)^2} (\mathbf{l} - \mathbf{k})\cdot\partial_\alpha \mathcal{C}_l(\mathbf{p}, \alpha, t)x(\alpha) \times \int d\mathbf{v}_1 \rho_{\mathbf{k}-\mathbf{l}}(1; t), \quad (6.3)$$

with the following initial condition

$$\mathcal{C}_{\mathbf{k}}(\mathbf{p}, \alpha; t)x(\alpha)\big|_{t=0} = x(\alpha), \quad (6.4)$$

and where $x(\alpha)$ is an arbitrary function. Equation (6.3) is very similar to (2.11) with the difference of the coefficient. In (2.11) the function φ and ρ_u has been taken in the point $\theta + \tau$.

In the stable case we can use again the argument that the time is short and we may neglect the terms of the order e^2 in (6.3). As has been already mentioned in previous paragraphs, this is equivalent to replacing the functions φ and $\rho_{\mathbf{k}}$, the solution of kinetic equation, by the solution of nonlinear Vlasov equation with the appropriate initial condition.

In our case

$$f(\mathbf{x}, \mathbf{v}; t)\big|_{t=0} = f(\mathbf{x}, \mathbf{v}; 0), \quad (6.5)$$

where we use here the notation of Sec. 3.

Again, in this situation the hydrodynamic approximation may be used and we may obtain the solution to Eq. (6.3) in closed form. The solution should be

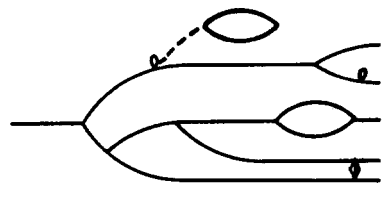


FIG. 6. Long-term contribution to destruction fragment.

[21] K. Nishikava and Y. Osaka, Progr. Theor. Phys. (Kyoto) 33, 402 (1965).

[22] R. Balescu (private communication).

exactly of the form (3.29), where we replace operator $\mathcal{T}$ by $\mathcal{C}$, $f(\mathbf{x}, \mathbf{v} - \boldsymbol{\eta}; \tau)$ by $f(\mathbf{x}, \mathbf{v} - \boldsymbol{\eta}, 0)$, and $\mathbf{E}$ in Eq. (3.21) by the solution of the following equation:

$$\nabla \cdot \mathbf{E} = -y\pi e \int d\mathbf{v}[f(\mathbf{x}, \mathbf{v}; t) - c\varphi(\mathbf{v}; t)]. \quad (6.6)$$

The above solution permits us to write the contribution to kinetic equation Q_ρ in the stable hydrodynamic case. In the unstable case, we can no longer use the Vlasov equation for function f instead of kinetic equation and Eq. (6.3) has to be solved.

7. THE UNSTABLE PLASMAS

In the previous paragraph we have discussed the contribution of initial correlations to the evolution of one-particle distribution functions. It occurs that in the unstable case one cannot neglect this contribution and one has to regard the lifetime of initial correlations as long time. This leads to the inclusion of the diagram of the type shown in Fig. 6 into the destruction fragment. Similar analysis shows that in the unstable case we have to consider the collision time as a long one (of the order of stabilization time) and, by a similar argument, the new contributions to the collision operator (of the form shown in Fig. 7) have to be included. One immediately recognizes, however, that inclusion of this diagram is nothing else than the exchange for function $R_{\mathbf{k}}(z)$ by $\rho_{\mathbf{k}}(z)$ and $\varphi(\tau)$ by $\varphi(z, \tau)$ in formula (2.4).

In other words, the collision term for unstable plasmas is described by Eq. (3.11). But in this case we no longer have freedom to exchange the function $\rho_{\mathbf{k}}$ by R_n.

This means that the approximation proposed in Sec. 3 is not valid and the system has to be described by two couple equations. Also, in the unstable case the destruction fragments have to be taken into account.

ACKNOWLEDGMENTS

We wish to express our gratitude to Professor I. Prigogine for his kind hospitality and for the interest he took in this work. We would like to thank Professor R. Balescu, Dr. A. Grecos, Dr. S. Kulinski, Dr. A. Senatorski, and Dr. G. Severne for numerous helpful discussions.

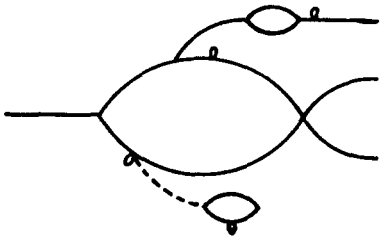


FIG. 7. The contribution to collision operator in the unstable case.

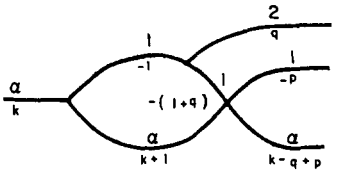


FIG. 8. Diagram evaluated in the Appendix.

APPENDIX

In order to illustrate the meaning of the operator $P(\mathbf{x}, \mathbf{v}_\alpha, z)$ and of the function $\psi(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{x}_\beta \mathbf{x}_\beta, \tau)$ we shall calculate the explicit contribution of some simple diagram represented in Fig. 8. We may write this contribution in the following form:

$$\begin{aligned}\Theta = \frac{e^2c^2}{m} &\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}_\alpha} \int d\mathbf{l}\, l^{-2} i\,\mathbf{l}\cdot\partial_\alpha \int d\mathbf{v}_1 \\ &\times \int \frac{dz}{2\pi}\, i[-\mathbf{l}\cdot\mathbf{v}_1 - z + z'] \int \frac{dz''}{2\pi} \int d\mathbf{v}_2 \\ &\times \int d\mathbf{q}\, m^{-1} V(q) i\,\mathbf{q}\cdot\partial_1 \frac{1}{i(\mathbf{q}\cdot\mathbf{v}_2 - z + z' + z'')} \\ &\times \frac{1}{i([\mathbf{l}+\mathbf{q}]\cdot\mathbf{v}_1 - z + z')} \frac{1}{i([\mathbf{k}+\mathbf{l}]\cdot\mathbf{v}_\alpha - z)} \\ &\times \int d\mathbf{p}\, m^{-1} V(|\mathbf{p} - \mathbf{q} - \mathbf{l}|) i(\mathbf{p} - \mathbf{q} - \mathbf{l}) \\ &\cdot \partial_{\alpha_1} \rho_{\mathbf{k}+\mathbf{p}-\mathbf{q}}(\alpha) \rho^{(1)}_{-\mathbf{p}} \rho^{(2)}_{\mathbf{q}}. \end{aligned} \quad (A1)$$

We may transform the expression (A1), introducing the unit operators $\int d\mathbf{k}'\delta(\mathbf{k} + \mathbf{l} - \mathbf{k}')$ and $\int d\mathbf{l}'\delta(\mathbf{l} + \rho - \mathbf{l}')$ and taking an appropriate Fourier representation of the δ function, to the following form:

$$\begin{aligned}\Theta = \frac{e^2c^2}{m} &\int d\mathbf{l}\, l^{-2} i\,\mathbf{l}\cdot\partial_\alpha \int d\mathbf{v}_1 \int \frac{dz'}{2\pi} \int \frac{dz''}{2\pi} \\ &\times \int d\mathbf{v}_2 \int d\mathbf{q} \frac{1}{\mathbf{l}\cdot\mathbf{v}_1 - z + z'} m^{-1} V(q) \\ &\times \frac{1}{(2\pi)^3} \int d\mathbf{x} \int d\mathbf{y}\, \delta(\mathbf{x}_\alpha - \mathbf{x}) e^{i\mathbf{l}\cdot(\mathbf{y}-\mathbf{x})} \\ &\times e^{i\mathbf{q}\cdot\mathbf{x}\cdot\mathbf{y}} \frac{1}{i[\mathbf{q}\cdot\mathbf{v}_2 - z + z' + z'']} \rho_{\mathbf{q}}(\mathbf{v}_2) \end{aligned} \quad (A2)$$

$$\mathbf{q}\cdot\partial_1 \Xi_\alpha(\mathbf{x}; z') \Xi_1(\mathbf{y}; z'') \psi_1(\mathbf{x}, \mathbf{v}_\alpha, \mathbf{y}, \mathbf{v}_1),$$

where we denote by ψ_1 the contribution to $\psi(\alpha, \beta)$ due to our diagram (Fig. 8):

$$\begin{aligned}&\psi_1(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{x}_\beta, \mathbf{v}_\beta) \\ &\quad = -\frac{e^2}{mc^2} \nabla_\alpha V(|\mathbf{x}_\alpha - \mathbf{x}_\beta|) \cdot \partial_{\alpha\beta} H(\alpha) H(\beta), \end{aligned} \quad (A3)$$

where $H(\alpha)$ is the inhomogeneity factor.

The operator Ξ is defined by its acting in the Fourier space in the following way:

$$\Xi_\alpha(\mathbf{x}, z)\phi(x) = \int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}} \frac{1}{i[\mathbf{k}\cdot\mathbf{v}_\alpha - z]} \phi_{\mathbf{k}}(\alpha), \quad \text{(A4)}$$

where $\phi_{\mathbf{k}}(\alpha)$ denote the Fourier transform of an arbitrary $\phi(x)$.

It may be easily seen that the function determined by the relation

$$\mathbf{E}(\mathbf{x}, z) = \int d\mathbf{q}\, V(q) i\mathbf{q} e^{ix\cdot q} \int d\mathbf{v}_2 \frac{\rho_{\mathbf{q}}(\mathbf{v}_2)}{i[\mathbf{q}\cdot\mathbf{v}_2 - z]} \quad \text{(A5)}$$

represents the contribution to the electric field $\mathbf{E}(x, z)$ due to our diagram.

FIG. 9. Contribution to $P\psi_1$ coming from diagram shown in Fig. 5.

Finally, Θ may be written in the following form:

$$\Theta = \frac{e^2c^2}{m} \int d\mathbf{l}\, V(l) i\, \mathbf{l}\cdot\partial_\alpha \int \frac{dz'}{2\pi} \int \frac{d\mathbf{y}}{(2\pi)^3} \int d\mathbf{v}_1\, e^{i\mathbf{l}\cdot(\mathbf{y}-\mathbf{x}_\alpha)}$$
$$\Xi_\alpha(\mathbf{x}_\alpha; z') \frac{e}{m} \int \frac{dz''}{2\pi} \Xi_1(\mathbf{y}, z - z')\partial_1 \mathbf{E}(\mathbf{y}, z - z' - z'')$$
$$\times \Xi_1(\mathbf{y}, z'')\psi_1(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \mathbf{y}, \mathbf{v}_1). \quad \text{(A6)}$$

From this form one can easily deduce the meaning of all quantities introduced in the paper. One recognizes that $\Xi_\alpha(\mathbf{x}_\alpha, z')$ is the contribution to the operator $P(\mathbf{x}_\alpha, \mathbf{v}_\alpha, z')$ due to the simple propagator alone and that

$$\Xi_1(\mathbf{y}, z - z') \frac{e}{m} \int \frac{dz''}{2\pi} \partial_1 \cdot \mathbf{E}(\mathbf{y}, z - z' - z'')\Xi_1(\mathbf{y}, z'') \quad \text{(A7)}$$

is the contribution to $P(\mathbf{y}, \mathbf{v}_1, z - z')$ due to the diagram shown in Fig. 9.

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Combinatorial Structure of State Vectors in U_n.*† I. Hook Patterns for Maximal and Semimaximal States in U_n

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It is shown that, in the boson-operator realization, the state vectors of the unitary groups U_n—in the canonical chain $U_n \supset U_{n-1} \supset \cdots \supset U_1$—can be obtained *ab initio* by a combinatorial probabilistic method. From the Weyl branching law, a general state vector in U_n is uniquely specified in the canonical chain; the algebraic determination of such a general state vector is in principle known (Cartan–Main theorem) from the state vector of highest weight; the explicit procedure is a generalization of the $SU(2)$ lowering-operator technique. The present combinatorial method gives the normalization of these state vectors in terms of a new generalization of the combinatorial entity, the Nakayama hook, which generalization arises *ab initio* from a probabilistic argument in a natural way in the lowering procedure. It is the advantage of our general hook concept that it recasts those known algebraic results into a most economical algorithm which clarifies the structure of the boson-operator realization of the U_n representations.

In the past few years there has been strong research interest centering about the general problem of the structural properties of the unitary groups—a more familiar rubric for this research is that it aims at the generalization of the angular-momentum calculus to all $SU(n)$. The research problems that arise in this generalization are more or less familiar: the explicit construction of state vectors (in particular, the boson-operator realization) the determination of the matrices of the generators, construction of general representation matrices, the classification and construction for tensor operators, etc. It is evident that such research is relevant to particular problems (and associated symmetry groups) in physics, such as "the eight-fold way" $SU(3)/Z(3)$, $SU(6), \cdots$; it is less evident that the structural properties for arbitrarily large $U(n)$ can be relevant to physics as models for separable Hilbert spaces. It is this latter view which underlies the present paper for we have in mind results not only for special values ($n = 2, 3, 6, \cdots$) but also insist that the structural properties of the general case be clearly in evidence.

The present paper is concerned with a detailed discussion of the boson-operator realization of the state vectors of all $U(n)$. In an earlier[1] paper we found for the *semimaximal* states of $U(n)$—those states for which the $U(n-1)$ subgroup is maximal—that there existed a remarkably simple, yet comprehensive, technique: that of the *generalized hook* and the *hook measure*. This result was merely asserted in our earlier work; the present paper contains, first of all, a careful proof of these earlier results.

Since we are primarily concerned with structural properties, our proof is designed to show a close relationship to the classical result of Young and Robinson in the theory of the symmetric group. (It is not commonly realized how many of the results in the recent literature are classical in content.[2])

It is a second purpose of this article to show existence of a combinatorial rationale for the structure upon which the states of $U(n)$ are built. A few calculations in $U(2)$ and $U(3)$ suffice to make clear that the complexity of the computations increases extremely rapidly from $U(2)$ to $U(3)$ and beyond. The combinatorial method greatly simplifies the process of determination of the explicit algebraic expressions of $U(n)$ states including their normalization constants.

We take as our point of departure the results in Robinson's book,[3] which emphasize the method of hooks in the representation theory of the symmetric group and the general linear group. However, the hook in its original form—the Nakayama hook—is not sufficient for the boson-operator realization of $U(n)$ states; therefore we introduce a particular generalization of the Nakayama-hook concept. It will be seen that the hook is a remarkable combinatorial entity, and in its present generalized form it reveals the underlying structural content of the boson-operator realization of the representations of $U(n)$.

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† Excerpted in part from the Ph.D. thesis presented by M. Ciftan to Duke University, Durham, North Carolina, 1967.

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[1] G. E. Baird and L. C. Biedenharn, J. Math. Phys. **4**, 1449 (1963).

[2] Refer, for example, to: H. Weyl, *Classical Groups* (Princeton University Press, 1946); D. E. Littlewood, *The Theory of Group Characters* (Oxford University, Clarendon Press London, 1958); Major P. A. MacMahon, *Combinatory Analysis* (Chelsea Publishing Co., New York, 1960).

[3] G. de B. Robinson, *Representation Theory of the Symmetric Group* (University of Toronto Press, Toronto, Canada, 1961).

We first present (in Sec. I) the hook method which provides an algorithm for the construction of semimaximal $U(n)$ states; only afterwards do we give the proof of the validity of this algorithm by explicitly constructing the corresponding $U(n)$ states using the familiar lowering-operator technique of $SU(2)$ angular-momentum theory extended to $SU(n)$. It must be borne in mind that by using the classical results of Cartan, *all* the states can be obtained from the highest-weight vector (the state of highest weight) by means of the generators. Therefore the use of lowering operators as such does not constitute a novelty and we avail ourselves of the existing results—particularly one set of lowering operators—to achieve a most economical proof of the hook algorithm; however, we use the lowering operators in a novel *combinatorial* context which clarifies the meaning of the hook and the *combinatorial structure* of these $U(n)$ states. This last aspect is particularly interesting in view of modern developments[4] in combinatorial analysis which have freed combinatorics from being merely a tool of enumeration by establishing close connection to group structure and geometry. Apart from shedding light on the structure, this combinatorial point of view is shown to give also the normalization constant of all lowering operators of all $U(n)$ in a conceptually very simple and economical way.

The content of Paper I is as follows. After a few preliminaries in Sec. I we define the concept of a generalized hook. In Sec. II we show the existence of a hook algorithm for maximal states, i.e., states whose labels have their maximum values. We do not give a proof of this algorithm since the proof already exists in the works of Robinson.[3] Using the concept of a generalized hook, in Sec. III we obtain an algorithmic procedure to construct the explicit algebraic expressions of those $U(n)$ states whose $U(n-1)$ state labels have their maximum values, i.e., states called *semimaximal*. The normalization constants of these semimaximal states are given in terms of a chain of products of determinants, a decomposition rule, built upon the underlying representation structure of the permutation group of $U(n)$. The results are shown to admit of an interpretation in terms of the ordering relations of the invariants of $U(n)$ and $U(n-1)$, the invariants that are tabulated in the triangular "Gel'fand pattern." Finally, in Sec. IV we give the constructive algebraic proof of the validity of the hook algorithm for the semimaximal states using the lowering-operator technique. At the same time we demonstrate the existence of a combinatorial rationale upon which the hook algorithm and the lowering technique rests.

It may be useful here to summarize the contents of the second part of this investigation. In Paper II we show the manner in which the state vectors of $U(n)$ expressed in terms of boson operators (rather than in abstract operator form) embody a generalization of ordinary hypergeometric functions. We demonstrate that these state vectors—i.e., orthonormal functions together with their normalization constants—can be expressed in terms of a calculus of tableaux; conversely, the explicit algebraic expressions of these $U(n)$ states may be written down directly from the tableaux calculus. The general $SU(4)$ state vectors are derived as an example of the method for $SU(n)$; it is shown that these general states are built upon products of the constituents of hypergeometric functions of many variables, each such function being a Radon transform of linear forms; the totality of the expression of $SU(4)$ states is then a "contracted" or "folded" form over the constituents of such transforms.

I. THE YOUNG FRAME AND THE MAXIMAL STATE

We refer the reader to the review of the *invariant operator basis* (the Gel'fand basis upon which the boson-operator realization of state vectors is constructed below) contained in the article by Louck.[5] The present article is an outgrowth of the concepts presented previously[1] in an article in which it was stated that the hook-calculus approach would be discussed separately later.

The second reference, which we use extensively, is Chap. II of the book by Robinson[3]; in particular, we make frequent use of the results in Sec. 2.3, Theorem 2.33, and Eq. (2.37). For brevity we do not repeat nor summarize these results here.

To reveal the *combinatorial* content of state vectors of the unitary groups $U(n)$, we need to understand precisely in what manner each irreducible representation[6] $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$[7] of $U(n)$ is associated with a *Young frame* (or diagram) of boxes (or nodes) and with the *Gel'fand pattern* of the invariants of $U(n)$. Figure 1 reproduces this association discussed previously[1] in detail. We now restudy this association.

[4] E. F. Beckenbach, *Applied Combinatorial Mathematics* (John Wiley & Sons, Inc., New York, 1964).

[5] J. D. Louck, J. Math. Phys. **6**, 1786 (1965).

[6] For a modern approach to representation theory, see C. W. Curtis and I. Reiner, *Representation Theory of Finite Groups and Associative Algebras* (Interscience Publishers, Inc., John Wiley & Sons, Inc., New York, 1962).

[7] We reserve the symbol [ ] for the representations of the symmetric (permutation) group S_k on k objects. We use the symbol { } for the representations of $U(n)$ rather than $\langle\ \rangle$ used in Robinson for the general linear group and reserve the $\langle\ \rangle$ symbols for *operators* on $U(n)$ following the Dirac bra-ket notation.

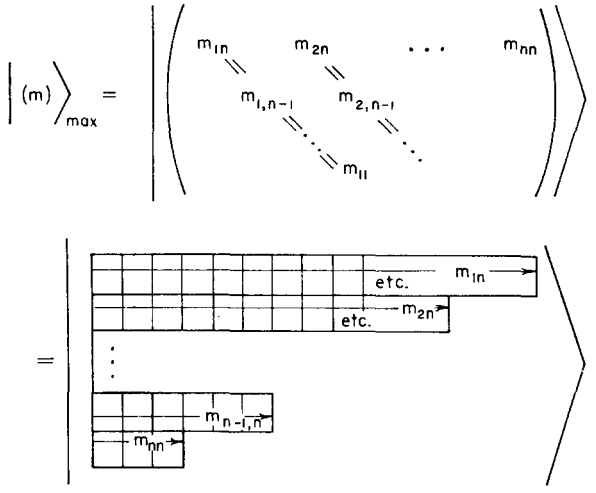


FIG. 1. The maximal state vector for the irreducible representation $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ of $U(n)$ expressed in terms of the Gel'fand pattern and the Young frame of the associated representation $[\lambda_1, \cdots, \lambda_n]$ of the permutation group S_N where $\lambda_i \equiv m_{in}$. This Young frame is to be filled with bosons, an $a_i^\dagger$ boson in each box of the ith row, to represent the state vector of Eq. 2.

Recall that the values m_{kj} of the invariants[5] I_k^j satisfy the *betweenness conditions*[8]

$$m_{k,j+1} \geq m_{k,j} \geq m_{k+1,j+1}, \tag{1}$$

and therefore the Gel'fand pattern is a lattice in the sense of partial ordering.[9] Thus the maximal state indicated in Fig. 1 is unique. Furthermore, by Cartan's theorem, each irreducible representation is "composed" of elementary irreducible representations. It is known[2,10] that associated with each of the n elementary[11] irreducible representation of $U(n)$ is a Young frame of a single vertical column of boxes, k boxes in all, for the kth representation. The Young frame of a general irreducible representation is composed of these vertical columns of boxes, with possible repetitions, such that there are λ_i boxes in the ith row, the λ_i being called the representation labels satisfying $\lambda_i \geq \lambda_{i-1}$ and being the values m_{in} of the invariants $I_i^{(n)}$ at the $U(n)$ "level" of the canonical subgroup decomposition $U(n) \supset U(n-1) \supset \cdots \supset U(1)$.

Now in the representations of the permutation group S_N, where N is the total number $\lambda_1 + \lambda_2 + \cdots + \lambda_n = N$ of boxes of the Young frame, one considers the symmetrizer and the antisymmetrizer of the group algebra[3,8,10]; through this arises the association of a completely antisymmetric form[12]

$$a_{12\cdots k} = \sum \epsilon(i_1 i_2 \cdots i_n) a_{i_1}^1 a_{i_2}^2 \cdots a_{i_k}^k,$$

with each column of k boxes in the Young frame. One can now specify further that the objects a_j^i be boson operators having the commutation relations that define them. It is therefore clear that associated with the maximal state of an irreducible representation is the *vector*

$$|(m)\rangle_{\max} = \frac{1}{\mathbf{M}^{\frac{1}{2}}} (a_{12\cdots n})^{\lambda_n} (a_{12\cdots(n-1)})^{\lambda_{n-1}-\lambda_n} \cdots \times (a_{12})^{\lambda_2-\lambda_3} (a_1^1)^{\lambda_1-\lambda_2} |0\rangle. \tag{2}$$

The nonnegative integers m_{in} denote the number of boxes in the ith row of the Young frame. The diagrammatic meaning of other m_{ik}'s with $k \neq n$ is given in the sequel. The ith row of boxes is to be filled with $a_i^\dagger$'s.

The $\mathbf{M}^{-\frac{1}{2}}$ factor in Eq. 2 is the normalization constant that will be given below. A *tableau* is a diagram of boxes filled with special symbols. A *Young tableau* is a Young diagram filled in with integers, which increase from left to right and top to bottom; an *extended* Young diagram is one which allows multiple occurrences—of one or more integers in each row—in the row. Observe that each column contains the boson operators that appear in the expansion of the associated antisymmetric form; we may symbolize this by using the leading term (diagonal element) of the form. [Writing the (numerical) subscripts only, then, yields an extended Young tableau or what we also call a *Weyl basis tableau.*] To evaluate the normalization constants of $U(n)$ state vectors below, we shall need the concept of *entanglement* that follows.

Recall the indistinguishability of bosons of a given type a_j^i among themselves. Thus one cannot say, for example, *which* boson of the first row is associated with a given boson of the second row. However, by fixing our attention on a given *box*, we can always qualify it by the *type* of boson it carries. Therefore, in what follows, we may consider the *box* rather than the boson which characterizes the box.

Entanglement.[13] In any vertically and/or horizontally connected portion of a diagram, a box is said to be *entangled* to all other boxes to its right in the same row and below in the same column which carry any

[8] H. Weyl, *The Theory of Groups and Quantum Mechanics*, translated by H. P. Robertson (Methuen and Co., Ltd., London, 1931). The proof of the betweenness condition is given on page 391.

[9] G. Birkhoff and S. MacLane, *A Survey of Modern Algebra* (The Macmillan Company, New York, 1953).

[10] M. Hammermesh, *Group Theory and Its Applications to Physical Problems* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1962).

[11] Also called "fundamental."

[12] The sum is over all permutations and $\epsilon(i_1 i_2 \cdots i_n)$ is $+1$ or -1 according to whether the permutation is odd or even. We will use the phrase "antisymmetric form" even for $a_i \equiv a_i^\dagger$.

[13] Even though in a somewhat different context, the concept of disentanglement as a concept of re-ordering of operators appears in a paper by R. P. Feynman, Phys. Rev. **84**, 108 (1951).

boson operator that appears in the antisymmetric form[14] to which the box belongs.

In this context of entanglement, we define a generalization[1] of the Nakayama hook.[3]

Generalized hook. The *hook* of a box is the number of *connected* boxes to its right in the same row and vertically below it, plus 1 for itself, the type of boxes considered being those which are entangled to the given box.

In the following sections we show how these two concepts are instrumental in the determination of $U(n)$ state vectors.

II. NORMALIZATION CONSTANT FOR MAXIMAL STATES OF $U(n)$

We now obtain the normalization constant, the $\mathbf{M}^{-\frac{1}{2}}$, of maximal states given by Eq. 2. $\mathbf{M}^{-1}$ will be shown to be the "degree" f—the dimensionality of the representation $[\lambda_1, \cdots, \lambda_n]$ of the underlying S_N, *not*[15] the dimensionality of the irreducible representations $\{\lambda_1, \cdots, \lambda_n\}$ of $U(n)$. Equivalently, f is the number of *standard* tableaux[15] divided by $N!$, in other words, the square of the normalization constant is the *probability* P of obtaining standard tableaux out of all $N!$ possible tableaux, a standard tableau[3] being formed when the boxes are filled with the integers $1, 2, \cdots, N$ which increase from left to right in any row and from top to bottom in any column.

Upon establishing the one-to-one correspondence of the maximal states of a given irreducible representation of $U(n)$ with the representative Young tableau, the results found in Robinson's book[3] on the representations of S_N can then be taken over verbatim for these maximal states. One needs to obtain the representation $[\lambda_1, \lambda_2, \cdots, \lambda_n]$ which has a Young frame constructed from the constituents of skew diagrams, since probability calculations are very simply carried out if the diagrams are skew. It has been shown by Robinson that any representation $[\lambda_1, \cdots, \lambda_n] \equiv [\lambda]$ may be associated with a determinant

$$[\lambda_1, \lambda_2, \cdots, \lambda_n] = |[\lambda_i - i + j]|, \tag{3}$$

and the degree $f^{[\lambda_1, \lambda_2, \cdots, \lambda_n]}$ of the representation $[\lambda]$ is then given by

$$\frac{f^{[\lambda_1, \cdots, \lambda_n]}}{N!} = \left| \frac{1}{(\lambda_i - i + j)!} \right|, \tag{4}$$

which is the number of standard Young tableaux out of all $N!$ possible tableaux; we now note that this last determinant is the $1/\mathbf{M}$ that we set out to calculate, as direct calculation of the norm using

$$\langle (m) \,|\, (m') \rangle = \delta_m^{m'} \tag{5}$$

shows. (Compare Secs. 7–8 to 7–11 of Ref. 8.) The square of the normalization constant is also[3] the inverse of the total hook product $H([\lambda])$ (cf. Ref. 3):

$$\frac{f^{[\lambda]}}{N!} = \frac{1}{H([\lambda])}, \tag{6}$$

where f and H now refer to those of the Young diagram (frame).

III. SEMIMAXIMAL STATES OF $U(n)$

The states of $U(n)$ whose $U(n-1)$ substates are maximal are called *semimaximal* states. We first give the hook method of evaluating the normalization constant of these states, and then in Sec. IV we give the justification of this procedure by evaluating the normalization constant, using a direct algebraic method. First consider the $U(2)$ states. The most general $U(2)$ state is necessarily semimaximal. The associated representative tableau and the betweenness lattice (we call this the Gel'fand pattern) are shown in Fig. 2.

The operator part of the explicit algebraic expression of the state,

$$\mathbf{M}^{-\frac{1}{2}}(a_{12})^{m_{22}}(a_1)^{m_{11}-m_{22}}(a_2)^{m_{12}-m_{11}}\,|0\rangle, \tag{7}$$

which, for the example in Fig. 2, becomes

$$\mathbf{M}^{-\frac{1}{2}}(a_{12})^3(a_1)^2(a_2)^4\,|0\rangle, \tag{8}$$

can be read from the tableau.

We note that the m_{11} value is required to be between the m_{12} and m_{22} values (or equal to either one) by the betweenness condition, Eq. 1, depicted by the corresponding Gel'fand pattern in Fig. 2. Thus the m_{11} boundary in the diagram of boxes indicated in Fig. 2 is positioned between the m_{22} and m_{12} boundaries indicated by arrows and heavily drawn lines. It must be noted that this tableau already represents a

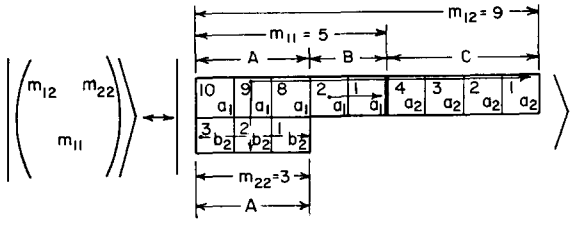


FIG. 2. The general U_2 state vector expressed in terms of the Gel'fand pattern and a generalization of the Young diagram.

[14] Of the elementary (fundamental) irreducible representation denoted by the column of boxes.

[15] In the sense given in Ref. 3; this number is also the number of lattice permutations.

generalization of the familiar concept of a Young tableau.

To calculate the normalization constant $\mathbf{M}^{-\frac{1}{2}}$ of this $U(2)$ state we use the concept of entanglement and generalized hooks as follows.

We dissect the tableau of Fig. 2 into three parts, A, B, and C, such that each part carries one type of antisymmetric form; the parts carry the antisymmetric forms a_{12}, a_1, and a_2, respectively.

Observe that, in section A, each vertical pair of boxes shows a type of entanglement in which not only a_1 and b_2 are involved, but also a_2, since this a_2 appears in the expression $a_{12} \equiv (a_1 b_2 - a_2 b_1)$ where for simplicity, we let $a_i^2 \equiv b_i$; thus, as the numbers in Fig. 2 which are the hook values of the boxes indicate, the hook of a box in the *first* row in section A extends over all the a_2's as well, up to the rightmost m_{12} boundary. The hook value of each box in Fig. 2 is given; a few of the hooks are also drawn. To take the product of all such hooks from the first row in section A, one uses the following computational aid.

Take the product of all hooks, $(m_{12}+1)!$, as if the m_{22} extended all the way to the m_{12} boundary—thus overestimating the hook contribution from the first row of section A; divide the expression by $(m_{12}+1-m_{22})!$, another hook product, thereby cancelling out the overcounted (and nonexistent) hooks. This completes the contribution[16] of the first row of section A. The second row of section A contributes $m_{22}!$.

In section B, the a_1 bosons are not entangled with any other type; therefore a hook of a box in this section extends up to the m_{11} boundary. Likewise for section C. The product of all these contributions gives $\mathbf{M}$, the square of the normalization constant, inverted:

$$\mathbf{M} = \left(\frac{(m_{12}+1)!}{(m_{12}+1-m_{22})!} \cdot m_{22}!\right) \times (m_{11}-m_{22})! \times (m_{12}-m_{11})!, \quad (9)$$

which, for the example, is

$$\mathbf{M} = \left(\frac{(9+1)!}{(9+1-3)!} \cdot 3!\right) \times (5-3)! \times (9-5)!,$$

which is just the product H of all the hooks in the tableau

$$H = (10 \cdot 9 \cdot 8) \cdot (3 \cdot 2 \cdot 1) \cdot (2 \cdot 1) \cdot (4 \cdot 3 \cdot 2 \cdot 1).$$

The $\mathbf{M}^{-1}$ can be put in a form which will be shown to be more meaningful:

$$\frac{1}{\mathbf{M}} = \frac{(m_{12}+1-m_{22})!}{(m_{12}+1)!\, m_{22}!} \cdot \frac{1}{(m_{11}-m_{22})!} \cdot \frac{1}{(m_{12}-m_{11})!} = \frac{1}{H(A)} \cdot \frac{1}{H(B)} \cdot \frac{1}{H(C)}. \quad (10)$$

Rearranging, using Eqs. (3), (4), and (6),

$$\begin{aligned}\frac{1}{\mathbf{M}} &= \frac{(m_{12}+1-m_{22})!}{(m_{12}+1)!\, m_{22}!\,(m_{12}-m_{22})!} \cdot \frac{(m_{12}-m_{22})!}{1} \times \frac{1}{(m_{11}-m_{22})!} \cdot \frac{1}{(m_{12}-m_{11})!} \\ &= \frac{f^{[m_{12},m_{22}]}}{N_{[m_{12},m_{22}]}!} \cdot \frac{N_{[m_{12}-m_{22}]}!}{f^{[m_{12}-m_{22}]}} \cdot \frac{f^{[m_{11}-m_{22}]}}{N_{[m_{11}-m_{22}]}!} \cdot \frac{f^{[m_{12}-m_{11}]}}{N_{[m_{12}-m_{11}]}} \\ &= \begin{vmatrix} \frac{1}{m_{12}!} & \frac{1}{(m_{12}+1)!} \\ \frac{1}{(m_{22}-1)!} & \frac{1}{m_{22}!} \end{vmatrix} \cdot \left|\frac{1}{(m_{12}-m_{22})!}\right| \times \left|\frac{1}{(m_{11}-m_{22})!}\right| \cdot \left|\frac{1}{(m_{12}-m_{11})!}\right|,\end{aligned}$$

where superscript $[\cdots]$ to f and subscript $[\cdots]$ to N indicate the part of the diagram to which f and N belong. This can then be put in symbolic "representation" form[3] as in Fig. 3 and Eq. (11):

$$\begin{bmatrix} m_{12} & m_{22} \\ & m_{11} \end{bmatrix} = \begin{vmatrix} [m_{12}] & [m_{12}+1] \\ [m_{22}-1] & [m_{22}] \end{vmatrix} \times [m_{12}-m_{22}]^{-1} \times [m_{11}-m_{22}] \times [m_{12}-m_{11}]. \quad (11)$$

We emphasize that Eq. (11) is a direct outcome of our generalization of the hook idea, in conjunction with the present combinatorial use of Robinson's formula given by Eq. (6) above. The result may be verified by direct computation of the normalization constant.[1] To illustrate the workings of the generalized hook, we now take up $SU(3)$ and $U(4)$ examples. We first represent the hook method and give the

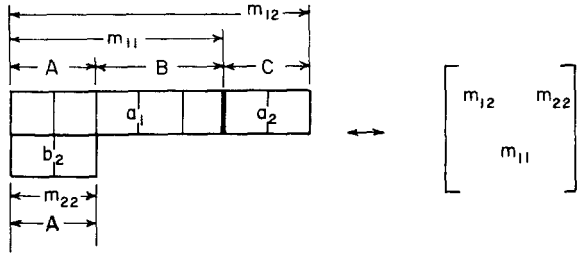


FIG. 3. The connection, given by Eq. (11), of the determinantal form of the U_2 state operator to the generalization of the Young diagram.

[16] This procedure of taking factorials and eliminating overcounted nonexistent hooks by a corresponding inverse factorial is an instance of the powerful combinatorial technique of inclusion–exclusion [see, e.g., J. Riordan, *An Introduction to Combinatorial Analysis* (John Wiley & Sons, Inc., New York, 1958)].

algebraic justification of this procedure for all the semimaximal states of all $U(n)$, in the next section.

In accord with the betweenness condition, the semimaximal states of $SU(3)$ are denoted by the representative tableau in Fig. 4. To find the contributions to the total hook product, and therefore to $\mathbf{M}^{-1}$, the following points are to be noted. The hook of a box in the first row of section A extends only up to the $m_{11} = m_{12}$ right boundary of section C, since the antisymmetric form a_{12} to which the box belongs does *not* contain a_3. However, in section B, the hook of a box in the first row extends *all the way* to the m_{13} boundary. Summarizing, we have the following.

Contributions to Total Hook Product

$$(a_{12})^{m_{22}}\colon \frac{(m_{12}+1)!\,m_{22}!}{(m_{12}-m_{22}+1)!},$$

$$(a_{13})^{m_{23}-m_{22}}\colon \frac{(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!}{(m_{13}-m_{23}+1)!},$$

$$(a_1)^{m_{12}-m_{23}}\cdot(a_3)^{m_{13}-m_{12}}\colon (m_{12}-m_{23})!\,(m_{13}-m_{12})!.$$

Upon rearrangement, these can be put into the concise symbolic form:

$$\begin{bmatrix} m_{13} & m_{23} & 0 \\ m_{12} & m_{22} & \\ m_{12} & & \end{bmatrix} = \begin{vmatrix} [m_{12}] & [m_{12}+1 \\ [m_{22}-1] & [m_{22}] \end{vmatrix} \times [m_{12}-m_{22}]^{-1} \times \begin{vmatrix} [m_{13}-m_{22}] & [m_{13}-m_{22}+1] \\ [m_{23}-m_{22}-1] & [m_{23}-m_{22}] \end{vmatrix} \times [m_{13}-m_{23}]^{-1} \times [m_{13}-m_{12}] \times [m_{12}-m_{23}]. \tag{12}$$

The full significance of the structure shown by this result is not quite apparent, due to the circumstance that $SU(3)$ is still a bit too special.

However, the Gel'fand pattern of $U(4)$ states has a large enough number of m_{ik}'s to reveal the generalization of the decomposition rules embodied by Eqs. (11) and (12). Figure 5 shows the representative tableau and the Gel'fand pattern of semimaximal $U(4)$ states. The decomposition rule is given by:

$$\begin{bmatrix} m_{14} & m_{24} & m_{34} & m_{44} \\ m_{13} & m_{23} & m_{33} & \\ m_{12} & m_{22} & & \\ m_{11} & & & \end{bmatrix} = \begin{vmatrix} [m_{14}] & & & \text{etc.} \\ & [m_{24}] & & \\ & & [m_{34}] & \\ \text{etc.} & & & [m_{44}] \end{vmatrix} \times \begin{vmatrix} [m_{14}-m_{44}] & & & \text{etc.} \\ & [m_{24}-m_{44}] & & \\ & & [m_{34}-m_{44}] & \\ \text{etc.} & & & \end{vmatrix}^{-1}$$
$$\times \begin{vmatrix} [m_{13}-m_{44}] & & \text{etc.} \\ & [m_{23}-m_{44}] & \\ \text{etc.} & & [m_{33}-m_{44}] \end{vmatrix} \times \begin{vmatrix} [m_{13}-m_{33}] & \text{etc.} \\ \text{etc.} & [m_{23}-m_{33}] \end{vmatrix}^{-1}$$
$$\times \begin{vmatrix} [m_{14}-m_{33}] & & \text{etc.} \\ & [m_{24}-m_{33}] & \\ \text{etc.} & & [m_{34}-m_{33}] \end{vmatrix} \times \begin{vmatrix} [m_{14}-m_{34}] & \text{etc.} \\ \text{etc.} & [m_{24}-m_{44}] \end{vmatrix}^{-1}$$
$$\times \begin{vmatrix} [m_{13}-m_{34}] & \text{etc.} \\ \text{etc.} & [m_{23}-m_{34}] \end{vmatrix} \times |\,[m_{13}-m_{23}]\,|^{-1} \times \begin{vmatrix} [m_{14}-m_{23}] & \text{etc.} \\ \text{etc.} & [m_{24}-m_{23}] \end{vmatrix}$$
$$\times |\,[m_{14}-m_{24}]\,|^{-1} \times |\,[m_{13}-m_{24}]\,| \times |\,[m_{14}-m_{13}]\,|. \tag{13}$$

As in Eqs. (11) and (12), this result is also in symbolic determinantal representation form from which the normalization constant can be evaluated by inverting the entries of the determinants and taking factorials in accordance with Eqs. (3) and (4).

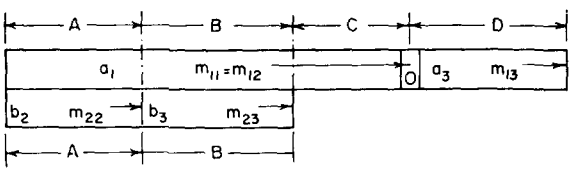
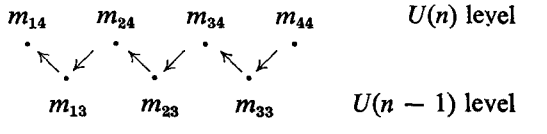


FIG. 4. The generalized diagram for the semimaximal states of $SU(3)$.

This seemingly complicated result actually embodies a very simple law of construction as follows.

First notice that each determinant is fully specified by enumerating the diagonal elements only. Hence our algorithm for $\mathbf{M}$ need specify only diagonal elements.

The algorithm begins by listing the two top rows of the Gel'fand pattern and the "path" as shown:



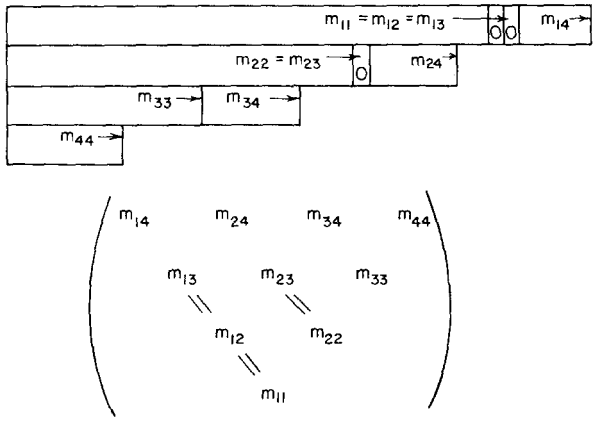


FIG. 5. The Gel'fand pattern and the generalized diagram for the semimaximal $U(4)$ states.

The m_{ij} are "stations" on the path. One follows the stations along the path. At each station two contributions are obtained, one a determinant in the numerator and the other a determinant in the denominator. For the diagonal elements of the determinant in the numerator, write the m_{ik}'s to the left of the station (in the row of the station), including the station and subtract from those m_{ik}'s the (same) m_{ik} that belongs to the previous station on the path. For the second contribution at the station, namely, the determinant in the denominator, instead of subtracting the m_{in} of the previous station, subtract the m_{ik} of the station itself.

Let us note that, instead of the above algorithm, one might have given an equivalent procedure using the algebraic expression of the generalized hook in terms of the m_{ik}'s of the diagram of boxes for the semimaximal case just short of passing to the determinantal form; this latter method is precisely what was done in Ref. (1) in their Eq. 52 which we do not reproduce here.

To summarize, let us note that two equivalent procedures have been given above for the determination of the normalization factor **M**, the measure of the semimaximal $U(n)$ states. Both use the concept of generalized hooks. These two equivalent procedures differ in that the determinantal form allows an interpretation in terms of the ordering relations of the betweenness lattice, and attains a logical simplicity at the price of redundant factors. (Let us note in passing that the various determinantal identities used above, which are classical results of Young and Robinson, frequently reappear in the literature under less than classical guise.)

IV. COMBINATORIAL CONTENT OF THE LOWERING OPERATOR

We now obtain the semimaximal states of all $U(n)$ by the familiar lowering-operator method of the theory of angular momentum; thereby we provide a constructive algebraic proof of the hook algorithm presented in the previous sections, and reveal the combinatorial structure of these $U(n)$ states. Again we obtain the $U(4)$ case in a form which is valid for all semimaximal states of $U(n)$. The operator part is shown to be given via Eq. (13), or its equivalent form given by Eq. (52) of Ref. (1).

To obtain the state vectors by an algebraic lowering operation, we need the following formulas involving the operators E_{ij}:

$$\begin{aligned}
&[E_{ij}, a_l] = a_i\delta(j, l),\\
&[E_{ij}, a_{lm}] = a_{im}\delta(j, l) + a_{li}\delta(j, m),\\
&[E_{ij}, a_{klm}] = a_{kim}\delta(j, l) + a_{kli}\delta(j, m) + a_{ilm}\delta(j, k),\\
&\quad\vdots\\
&(E_{ij})^n(a_{jl})^\alpha = \sum_{k=0}^{n}\binom{n}{k}\frac{\alpha!}{(\alpha-k)!}(a_{jl})^{(\alpha-k)}(a_{il})^k(E_{ij})^{(n-k)}.
\end{aligned} \tag{14, 15}$$

We apply Eqs. (14) and (15) to $U(2)$, $U(3)$, and $U(4)$ in that order. Furthermore, we obtain these normalization constants of states in two different ways which demonstrates the usefulness of the combinatorial approach, both in economy of labor and in elucidating the substructure upon which these states are built.

Consider the $U(2)$ maximal state

$$\frac{1}{\mathbf{M}_{\max}^{\frac{1}{2}}}(a_{12})^{m_{22}}(a_1)^{m_{12}-m_{22}}|0\rangle, \tag{16}$$

with the normalization constant

$$\frac{1}{\mathbf{M}_{\max}^{\frac{1}{2}}} = \left|\frac{(m_{12}-m_{22}+1)!}{(m_{12}+1)!\,m_{22}!\,(m_{12}-m_{22})!}\right|^{\frac{1}{2}}. \tag{17}$$

Operating with $(E_{21})^{m_{12}-m_{11}}$ on Eq. (16), using Eqs. (14) and (15), letting $n \equiv m_{12} - m_{11}$, $\alpha \equiv m_{12} - m_{22}$, $\beta \equiv m_{22}$ (cf. Fig. 6) we obtain

$$\begin{aligned}
&(E_{21})^n\frac{1}{\mathbf{M}_{\max}^{\frac{1}{2}}}(a_{12})^\beta(a_1)^\alpha|0\rangle\\
&\quad= \frac{1}{\mathbf{M}_{\max}^{\frac{1}{2}}}\frac{\alpha!}{(\alpha-n)!}(a_{12})^\beta(a_1)^{\alpha-n}(a_2)^n|0\rangle.
\end{aligned} \tag{18}$$

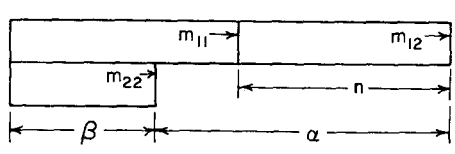


FIG. 6. The generalized diagram for $U(2)$ states redrawn in a simpler form.

At this point there are two alternative methods to find the correct normalization factor for the operators in the semimaximal states of $U(2)$ expressed by the right-hand side of Eq. (18). First, one may use the known normalization constant $\mathcal{N}^{-1}$ (e.g., Ref. 17) of the lowering operator $(E_{21})^m$ defined by

$$\mathcal{N}^{-1}(E_{21})^n \left|\begin{pmatrix} m_{12} & m_{22} \\ & m_{12} \end{pmatrix}\right\rangle = \left|\begin{pmatrix} m_{12} & m_{22} \\ & m_{11} \end{pmatrix}\right\rangle, \quad (19)$$

this constant being

$$\mathcal{N}^{-1} = \left[\frac{(m_{11} - m_{22})!}{(m_{12} - m_{11})!\,(m_{12} - m_{22})!}\right]^{\frac{1}{2}}. \quad (20)$$

Combining factors, we obtain (denoting "semimaximal" by s.m.):

$$\frac{1}{\mathbf{M}^{\frac{1}{2}}_{\text{s.m.}}} \equiv \frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max}} \frac{\alpha!}{(\alpha - n)!}\,\mathcal{N}^{-1} = \left[\frac{(m_{12} - m_{22} + 1)!}{(m_{11} + 1)!\,m_{22}!\,(m_{11} - m_{22})!\,(m_{12} - m_{11})}\right]^{\frac{1}{2}}, \quad (21)$$

which is precisely the expression given by Eq. (9) obtained by the method of generalized hooks. Second, and more importantly, we observe the combinatorial aspect of this lowering operation, the aspect embodied by the *incomplete* binomial coefficient

$$\frac{\alpha!}{(\alpha - n)!}.$$

Since the *completed* binomial coefficient $\binom{\alpha}{n}$ is necessarily appropriately "normalized" in the combinatorial sense, combining this with the probability coefficient

$$P^{\max}_{U_2} \equiv \frac{1}{\mathbf{M}^{\max}_{U_2}} = \frac{1}{H^{\max}_{U_2}}, \quad (22)$$

which, we noted,[3] also has a definite combinatorial meaning, we obtain the probability

$$P^{\text{s.m.}}_{U_2} = \frac{1}{\mathbf{M}^{\max}_{U_2}}\binom{\alpha}{n} = \frac{1}{\mathbf{M}^{\text{s.m.}}_{U_2}}, \quad (23)$$

which is the square of the normalization constant Eq. (21) of the semimaximal $U(2)$ states. This second method obviates the use of the normalization constant of the lowering operator, and in fact at the same time *determines the normalization constant of the lowering operator*. We show that this situation is quite general and applies to all semimaximal $U(n)$ states, and gives the normalization constant of all lowering operators of all $U(n)$.

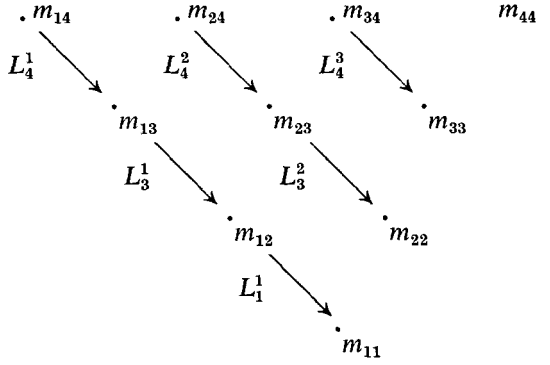
One form[1] of the unnormalized lowering operators of $U(n)$ is given[17] by

$$\begin{aligned}
U_2&: L^1_2 \equiv E_{21},\\
U_3&: L^1_3 \equiv \delta_{12}E_{31} + E_{32}E_{21},\\
&\quad L^2_3 \equiv E_{32},\\
U_4&: L^1_4 \equiv \delta_{12}E_{13}E_{41} + \delta_{13}E_{42}E_{21} + \delta_{12}E_{43}E_{31} + E_{43}E_{32}E_{21},\\
&\quad L^2_4 \equiv \delta_{23}E_{42} + E_{43}E_{32},\\
&\quad L^3_4 \equiv E_{43},
\end{aligned} \quad (24)$$

where

$$\delta_{ij} \equiv E_{ii} - E_{jj} + (j - i)\mathbb{1},$$

etc., which can be easily interpreted in terms of the Gel'fand pattern, the subscript of L^i_k referring to the U_kth level and the superscript the particular "link" of the m_{ik} to $m_{i,k-1}$, the L^i_k operator lowering the $m_{i,j}$ values *simultaneously for all* $j = k - 1, k - 2, \cdots$ by one:



The $U(3)$ Semimaximal States

Applying the operator L^1_3 on the maximal $U(3)$ state and using Eqs. (14) and (15), one finds

$$\begin{aligned}
L^1_3 \frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max}} (a_{123})^\alpha (a_{12})^\beta (a_1)^\gamma |0\rangle &= \frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max}} (a_{123})^\alpha L^1_3 (a_{12})^\beta (a_1)^\gamma |0\rangle\\
&= \frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max}} (a_{123})^\alpha \gamma(\gamma + \beta + 1)(a_{12})^\beta (a_1)^{\gamma-1} a_3 |0\rangle,
\end{aligned}$$

with

$$[L^1_3, a_{123}] = 0 \quad [L^1_3, a_3] = 0. \quad (25)$$

Whence (see Fig. 7):

$$(L^1_3)^{n_1}(a_{12})^\beta (a_1)^\gamma |0\rangle = \frac{\gamma!}{(\gamma - n_1)!}\frac{(\gamma + \beta + 1)!}{(\gamma + \beta + 1 - n_1)!} \times (a_{12})^\beta (a_1)^{\gamma - n_1}(a_3)^\gamma |0\rangle. \quad (26)$$

[17] J. G. Nagel and M. Moshinsky, J. Math. Phys. **6**, 682 (1965). See also references quoted in Ref. 5 above.

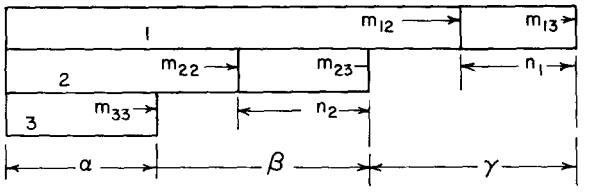


FIG. 7. The generalized diagram for $U(3)$ states redrawn in a simpler form.

Next we find, in a similar way, with $n_2 \equiv m_{23} - m_{22}$:

$$(E_{32})^{n_2}(L_3^1)^{n_1}\frac{1}{\mathbf{M}_{\max}^{\frac{1}{2}}}(a_{12})^{\beta}(a_1)^{\gamma}\,|0\rangle$$
$$= \frac{1}{\mathbf{M}_{\max}^{\frac{1}{2}}}\frac{\beta!}{(\beta-n_2)!}\frac{\gamma!}{(\gamma-n_1)!}\frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!}$$
$$\times (a_{12})^{\beta-n_2}(a_{13})^{n_2}(a_1)^{\gamma-n_1}(a_3)^{n_1}\,|0\rangle. \quad (27)$$

In order to complete the factorials of Eq. (26), one needs to observe that, since the m_{12} boundary is restricted to remain between the m_{13} and m_{23} boundaries, the factor $\gamma!/(\gamma - n_1)!$ is indicative of the repartitioning of the section γ and therefore the associated combinatorial factor is merely $\binom{\gamma}{n_1}$, involving hooks on *one* row of boxes. Similarly the hooks of the second row of the β section need to be readjusted when m_{22} is moved from $m_{22} = m_{23}$ into its general position and again the associated combinatorial factor is a binomial coefficient, $\binom{\beta}{n_2}$. On the other hand, we observe that the boxes of the first row in section $\beta - n_2$ involve hooks over *two* rows of boxes and the effect of moving the m_{12} boundary from its $m_{12} = m_{13}$ position involves a readjustment of these hooks. To complete the term

$$\frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!}$$

(where the integer 1 indicates that the hooks are over *two* rows) one needs the hypergeometric distribution coefficient

$$h_{\alpha;N}(k;n) \equiv \frac{\binom{\alpha}{k}\binom{N-\alpha}{n-k}}{\binom{N}{n}}, \quad (28)$$

which has a clearly defined combinatorial meaning[18]; it is the probability that given N objects, α of which say are black and the rest $N - \alpha$ white, when n of the N objects are drawn out at random *without replacement*, k of the n objects will be black and $n - k$ white. For the present case we need the $k = 0$ term of

$$h^{-1}_{\beta-n_2;\beta+\gamma+1}(k;n_1) \quad (29)$$

which is

$$\frac{(\gamma+\beta+1)}{(\gamma+\beta+1-n_1)!}\cdot\frac{(\gamma+1+n_2-n_1)!}{(\gamma+1+n_2)!}. \quad (30)$$

The missing part is

$$\frac{(\gamma+1+n_2-n_1)!}{(\gamma+1+n_2)!} = \frac{(m_{12}-m_{22}+1)!}{(m_{13}-m_{22}+1)}, \quad (31)$$

the *inverse* of h coming into the Eq. (26) because of cancellation of hooks overcounted prior to the application of the lowering operator. Observe also that the binomial coefficients themselves are the *inverse* of the associated probability coefficients. Next we give a direct verification of this combinatorial method for $U(3)$:

$$P_{\max} = \frac{1}{\mathbf{M}_{\max}} : \frac{(m_{13}-m_{33}+2)!\,(m_{23}-m_{33}+1)!}{(m_{13}+2)!\,(m_{23}+1)!\,m_{33}!}$$
$$\times \frac{(m_{13}-m_{23}+1)!}{(m_{13}-m_{33}+1)!\,(m_{23}-m_{33})!\,(m_{13}-m_{23})!},$$

Operator produced parts:
$$\frac{(m_{23}-m_{33})!}{(m_{22}-m_{33})!\,(m_{23}-m_{22})!}\ \text{(missing factor)}$$
$$\times \frac{(m_{13}-m_{23})!}{(m_{12}-m_{23})!\,(m_{13}-m_{12})!}\ \text{(missing factor)}$$
$$\times \frac{(m_{13}-m_{33}+1)!}{(m_{12}-m_{33}+1)!} \times \frac{(m_{12}-m_{22}+1)!}{(m_{13}-m_{22}+1)!}\ \text{(missing factor)},$$

$$P_{\text{s.m.}} = \frac{1}{\mathbf{M}_{\text{s.m.}}} = \frac{(m_{13}-m_{33}+2)!\,(m_{23}-m_{33}+1)!}{(m_{13}+2)!\,(m_{23}+1)!\,m_{33}!}$$
$$\times \frac{(m_{12}-m_{22}+1)!}{(m_{12}-m_{33}+1)!\,(m_{22}-m_{33})!}$$
$$\times \frac{(m_{13}-m_{23}+1)!}{(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!}$$
$$\times \frac{1}{(m_{12}-m_{23})!} \times \frac{1}{(m_{13}-m_{12})!}.$$

Thus

$$P_{\text{s.m.}} = P_{\max}\binom{\beta}{n_2}\binom{\gamma}{n_1}h^{-1}_{\beta-n_2,\gamma+n_2}(1;n_1). \quad (32a)$$

This is a significant result; observe that the contribution from the $U(n-1)$ level, namely,

$$\binom{\beta}{n_2}\binom{\gamma}{n_1}\cdot h^{-1},$$

[18] We discuss this in detail in Paper II. The knowledge that this incomplete part belongs to an hypergeometric probability distribution comes from the fact that $SU(3)$ general states embody an ${}_2F_1$ hypergeometric function that is derived in Paper II by this same lowering procedure.

are all inverses of probabilities so that

$$P_{\text{s.m.}} = \frac{P_{\max}}{P_{\text{due to passage to semimax.}}}. \tag{32b}$$

[Moreover, we shall see in Paper II that in $SU(3)$ the contributions for semi-semimaximal states—namely at the $U(n-2)$ level—to the probability h comes now on the numerator. Thus we see that, in passing to more and more general states of $U(n)$, the overcounted probability contributions are corrected at each stage. This is clearly an indication of a type of the inclusion–exclusion principle[16] of combinatorial analysis. We hope to discuss the connection elsewhere.]

To verify this result, we determine the normalization constants of the lowering operators, namely, that the product of the three contributions

$$\frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max}} = \left[\frac{(m_{13}-m_{33}+2)!\,(m_{23}-m_{33}+1)!\,(m_{13}-m_{23}+1)!}{(m_{13}+2)!\,(m_{23}+1)!\,m_{33}!\,(m_{13}-m_{33}+1)!\,(m_{23}-m_{33})!\,(m_{13}-m_{23})!}\right]^{\frac{1}{2}}, \tag{33}$$

$$\text{operator hook changes} = \frac{(m_{23}-m_{33})!}{(m_{22}-m_{33})!}\cdot\frac{(m_{13}-m_{23})!}{(m_{12}-m_{23})!}\cdot\frac{(m_{13}-m_{33}+1)!}{(m_{12}-m_{33}+1)!}, \tag{34}$$

$$\mathcal{N}^{-1}_{(E_{32})^{n_2}(L_3^1)^{n_1}} = \left[\frac{(m_{12}-m_{22}+1)!\,(m_{12}-m_{23})!\,(m_{12}-m_{33}+1)!}{(m_{13}-m_{12})!\,(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!}\times\frac{(m_{22}-m_{33})!}{(m_{13}-m_{23})!\,(m_{13}-m_{33}+1)!\,(m_{23}-m_{33})!}\right]^{\frac{1}{2}}, \tag{35}$$

which must, and do, give

$$\frac{1}{\mathbf{M}^{\frac{1}{2}}_{\substack{\text{s.m.}\\U_3}}} = \left[\frac{(m_{13}-m_{33}+2)!\,(m_{23}-m_{33}+1)!\,(m_{12}-m_{22}+1)!\,(m_{13}-m_{23}+1)!}{(m_{13}+2)!\,(m_{23}+1)!\,m_{33}!\,(m_{12}-m_{33}+1)!\,(m_{22}-m_{33})!\,(m_{13}-m_{22}+1)!\,(m_{23}-m_{22})!}\times\frac{1}{(m_{12}-m_{23})!}\times\frac{1}{(m_{13}-m_{12})!}\right]^{\frac{1}{2}}. \tag{36}$$

We have thus shown that, for $U(3)$ semimaximal states, the probability approach is equivalent to the use of normalized lowering operators.

Let us also demonstrate that the combinatorial approach determines the normalization constant of the $(L_3^2)^{n_2}$ and $(L_3^1)^{n_1}$ operator of $U(3)$. We have the general rule

$$P_{\substack{\text{lowered}\\\text{state}}} = P_{\max}\times\text{operator produced parts}\times\text{missing factors}, \tag{37a}$$

$$= \frac{1}{\mathbf{M}_{\max}}\times(\text{operator produced parts})^2\times(\mathcal{N}^{-1}_{(L_j^i)^n})^2, \tag{37b}$$

whence

$$\mathcal{N}^{-1}_{(L_j^i)^n} = \left[\frac{\text{missing factors}}{\text{operator produced parts}}\right]^{\frac{1}{2}}. \tag{38}$$

Thus, for $(E_{22})^{n_2}$ we have

$$\mathcal{N}^{-1}_{(E_{32})^{n_2}} = \left[\frac{1}{\dfrac{(m_{23}-m_{22})!}{(m_{23}-m_{33})!}\dfrac{}{}\dfrac{}{(m_{22}-m_{33})!}}\right]^{\frac{1}{2}}, \tag{39}$$

which agrees with Eq. (35) when $n_1 \equiv m_{13}-m_{12}=0$.

Also

$$\mathcal{N}^{-1}_{(L_3^1)^{n_1}} = \left[\frac{1}{(m_{13}-m_{12})!}\cdot\frac{(m_{12}-m_{23}+1)!}{(m_{13}-m_{23}+1)!}\cdot\frac{(m_{13}-m_{23})!}{(m_{12}-m_{23})!}\cdot\frac{(m_{13}-m_{33}+1)!}{(m_{12}-m_{33}+1)!}\right]^{\frac{1}{2}}, \tag{40}$$

which again agrees with Eq. (35) when $n_2 \equiv m_{23}-m_{22}=0$.

The Semimaximal states of $U(4)$ and $U(n)$

We now derive the semimaximal $U(4)$ states in a manner which demonstrates the validity of the results for the semimaximal states of *all* $U(n)$.

Starting with the maximal $U(4)$ state

$$\frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max}}(a_{1234})^{m_{44}}(a_{123})^{m_{34}-m_{44}}(a_{12})^{m_{24}-m_{34}}(a_1)^{m_{14}-m_{24}}|0\rangle, \tag{41}$$

we use the lowering operators

$$(L_4^3)^{m_{34}-m_{33}}(L_4^2)^{m_{24}-m_{23}}(L_4^1)^{m_{14}-m_{13}} \tag{42}$$

on this maximal state; letting for convenience (see

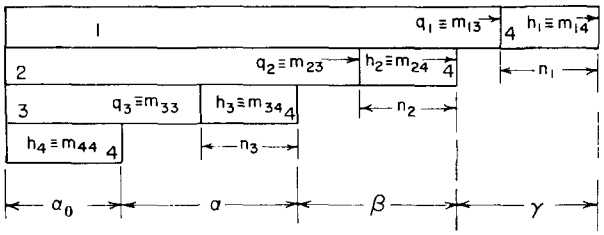


FIG. 8. The generalized diagram for $U(4)$ states giving the hook-chain rule of Eq. 43.

Fig. 8):

$$n_1 \equiv m_{14} - m_{13}, \quad \alpha_0 \equiv m_{44}, \quad h_1 \equiv m_{14}, \quad q_1 \equiv m_{13},$$
$$n_2 \equiv m_{24} - m_{23}, \quad \alpha \equiv m_{34} - m_{44},$$
$$h_2 \equiv m_{24}, \quad q_2 \equiv m_{23},$$
$$n_3 \equiv m_{34} - m_{33}, \quad \beta \equiv m_{24} - m_{24},$$
$$h_3 \equiv m_{34}, \quad q_3 \equiv m_{33},$$
$$\gamma \equiv m_{14} - m_{24},$$
$$h_4 \equiv m_{44}.$$

We obtain

$$(L_4^3)^{n_3}(L_4^2)^{n_2}(L_4^1)^{n_1} \frac{1}{M^{\frac{1}{2}}_{\max U_4}} (a_{1234})^{\alpha_0}(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma} |0\rangle$$
$$= \left\{\frac{\gamma!}{(\gamma - n_1)!} \frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!} \frac{(\gamma+\beta+\alpha+2)!}{(\gamma+\beta+\alpha+2-n_1)!}\right\}$$
$$\times \left\{\frac{\beta!}{(\beta - n_2)!} \frac{(\beta+\alpha+1)!}{(\beta+\alpha+1-n_2)!}\right\} \times \left\{\frac{\alpha!}{(\alpha - n_2)!}\right\}$$
$$\frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max U_4}} \times (a_{1234})^{\alpha_0}(a_{123})^{\alpha - n_3}(a_{124})^{n_3}$$
$$\times (a_{12})^{\beta - n_2}(a_{14})^{n_2}(a_1)^{\gamma - n_1}(a_4)^{n_1} |0\rangle, \tag{43}$$

in the following manner.

First observe the pattern of the expressions for $U(2)$, $U(3)$, $U(4)$ when the L_2^1, L_3^1, L_4^1 operators operate on the operators of the maximal $U(2)$, $U(3)$, $U(4)$ states, respectively:

$$L_2^1(a_1)^{\gamma} |0\rangle = \gamma(a_1)^{\gamma-1}a_2 |0\rangle$$
$$L_3^1(a_{12})^{\beta}(a_1)^{\gamma} |0\rangle = \gamma(\gamma+\beta+1)(a_{12})^{\beta}(a_1)^{\gamma-1}a_3 |0\rangle$$
$$L_4^1(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma} = \gamma(\gamma+\beta+1)(\gamma+\beta+\alpha+2)$$
$$\times (a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma-1}a_4 |0\rangle, \tag{44}$$

etc. (to be called the hook chain rule), with

$$[L_2^1, a_{12}] = 0; \quad [L_2^1, a_2] = 0,$$
$$[L_3^1, a_{123}] = 0; \quad [L_3^1, a_3] = 0, \tag{45}$$
$$[L_4^1, a_{1234}] = 0; \quad [L_4^1, a_4] = 0.$$

Whence,

$$(L_2^1)^n(a_{12})^{\beta}(a_1)^{\gamma} |0\rangle$$
$$= \frac{\gamma!}{(\gamma - n)!}(a_{12})^{\beta}(a_1)^{\gamma-n}(a_2)^n |0\rangle$$
$$(L_3^1)^n(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma} |0\rangle$$
$$= \frac{\gamma!}{(\gamma - n)!} \frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n)!}$$
$$\times (a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma-n}(a_3)^n |0\rangle$$
$$(L_4^1)^{n_1} \frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max U_4}} (a_{1234})^{\alpha_0}(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma} |0\rangle$$
$$= \frac{\gamma!}{(\gamma - n_1)!} \frac{(\gamma+\beta+1)!}{(\gamma+\beta+1-n_1)!} \frac{(\gamma+\beta+\alpha+2)!}{(\gamma+\beta+\alpha+2-n_1)!}$$
$$\times \frac{1}{\mathbf{M}^{\frac{1}{2}}_{\max U_4}} (a_{1234})^{\alpha_0}(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma-n_1}(a_4)^{n_1} |0\rangle. \tag{46}$$

Next observe that $[L_4^2, a_1] = 0$ as well as $[L_4^2, a_4]$ and, therefore, L_4^2 does not "see" the a_1 operator nor the a_4 operator created by the previous lowering operator L_4^1. The result is reflected in the associated tableau. Again by the hook chain rules, Eq. (44),

$$L_3^2(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma-1}a_3 |0\rangle$$
$$= (a_{123})^{\alpha}(a_1)^{\gamma-1}a_3L_3^2(a_{12})^{\beta} |0\rangle,$$
$$L_3^2(a_{12})^{\beta} = \beta(a_{12})^{\beta-1}a_{13} |0\rangle,$$
$$L_4^2(a_{1234})^{\alpha_0}(a_{123})^{\alpha}(a_{12})^{\beta}(a_1)^{\gamma-1}a_4 |0\rangle$$
$$= (a_{1234})^{\alpha_0}(a_1)^{\gamma-1}a_4L_4^2(a_{123})^{\alpha}(a_{12})^{\beta} |0\rangle,$$
$$L_4^2(a_{123})^{\alpha}(a_{12})^{\beta} |0\rangle$$
$$= \beta(\beta+\alpha+1)(a_{123})^{\alpha}(a_{12})^{\beta-1}a_{14} |0\rangle. \tag{47}$$

Operating $(L_4^2)^{n_2}$ on the right-hand side of Eq. (46) gives the second collection of factors in curly brackets on the right-hand side of Eq. (43), and the respective operator changes effected by the power of n_2. Again the L_4^3 operator in Eq. (43) does not "see" the a_{12}, a_1 operators that the preceeding L_4^2, L_4^1 operators "see," nor does it see the operators a_{14}, a_3^1 that the L_4^2, L_4^1 operators have created; the hook chain rule again applies, and finally one obtains Eq. (43); it is clear that this process gives the semimaximal states of *all* $U(n)$. The operator part is simply read off the tableau given above; we next show that the coefficients are precisely the required hook changes from the maximal states to give the semimaximal branching

law; this is demonstrated as follows:

$$\frac{1}{\mathbf{M}_{\max U_4}} = \frac{(h_1-h_4+3)!\,(h_2-h_4+2)!\,(h_3-h_4+1)!}{(h_1+3)!\,(h_2+2)!\,(h_3+1)!\,h_4!} \times \frac{(h_1-h_3+2)!\,(h_2-h_3+1)!}{(h_1-h_4+2)!\,(h_2-h_4+1)!\,(h_3-h_4)!} \times \frac{(h_1-h_2+1)!}{(h_1-h_3+1)!\,(h_2-h_3)!} \times \frac{1}{(h_1-h_2)!}, \tag{48}$$

$$\text{operator produced parts} = \frac{(h_1-h_2)!}{(q_1-h_2)!}\frac{(h_1-h_3+1)!}{(q_1-h_3+1)!}\frac{(h_1-h_4+2)!}{(q_1-h_4+2)!} \times \frac{(h_2-h_3)!}{(q_2-h_3)!}\frac{(h_2-h_4+1)!}{(q_2-h_4+1)!}\frac{(h_3-h_4)!}{(q_3-h_4)!}, \tag{49}$$

$$\text{missing factors} = \frac{1}{(h_1-q_1)!}\frac{(q_1-q_2+1)!}{(h_1-q_2+1)!}\frac{(q_1-q_3+2)!}{(h_1-q_3+2)!} \times \frac{1}{(h_2-q_2)!}\frac{(q_2-q_3+1)!}{(h_2-q_3+1)!}\frac{1}{(h_3-q_3)!}. \tag{50}$$

Whence

$$\frac{1}{\mathbf{M}_{\text{s.m.}}} = \frac{(h_1-h_4+3)!\,(h_2-h_4+2)!\,(h_3-h_4+1)!}{(h_1+3)!\,(h_2+2)!\,(h_3+1)!\,h_4!} \times \frac{(q_1-q_3+2)!\,(q_2-q_3+1)!}{(q_1-h_4+2)!\,(q_2-h_4+1)!\,(q_3-h_4)!} \times \frac{(h_1-h_3+2)!\,(h_2-h_3+1)!}{(h_1-q_3+2)!\,(h_2-q_3+1)!\,(h_3-q_3)!} \times \frac{(q_1-q_2+1)!}{(q_1-h_3+1)!\,(q_2-h_3)!} \times \frac{(h_1-h_2+1)!}{(h_1-q_2+1)!\,(h_2-q_2)!} \times \frac{1}{(q_1-h_2)!}\frac{1}{(h_1-q_1)!}. \tag{51}$$

As before in Eq. (32a), we complete the combinatorial coefficients in Eq. (43) by supplying the missing terms; again the same result can be obtained if the method of using the appropriate normalization constants of the lowering operators are used, but this latter method is unnecessary and less illuminating.

In fact, the completion of the missing factors, corresponding to any of the given lowering operators, gives the normalization constant of that operator. By the process of passing from any U_μ maximal to $U_{\mu-1}$ maximal states, one obtains the normalization constant of *any* U_μ lowering operator immediately, without intermediary calculations. Equation (47) is the same as the expression obtained by the hook algorithm; the procedure is valid, *mutatis mutandis*, for all $U(n)$ and thus constitutes a general proof of the algorithm.

We conclude that we have proven the validity of the hook algorithm which gives the boson-operator realization of semimaximal states. Furthermore, the details of the above constructive algebraic proof of the algorithm has demonstrated that the hook is a useful combinatorial entity and elucidates the structure of these $U(n)$ states.