JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Integral Approximations in Potential Scattering

P. B. Burt and F. J. Woods
Clemson University, Clemson, South Carolina 29631
(Received 8 April 1971)

A development of the scattering amplitude in potential scattering which is based upon replacing a smooth potential by a sequence of potential steps is given. The Schrödinger equation is solved exactly in each interval over which the potential is constant and by matching boundary conditions an expression relating the coefficients of two linearly independent solutions at small radius to those at large radius is found. From this the scattering amplitude is calculated. The limits of validity are found to be dependent upon the value of the expression

$$(r/2)\frac{d}{dr}\ln\left(\frac{2m}{\hbar^2}[E-V]\right).$$

Limiting cases of the amplitude are shown to be a modified WKB approximation and the Born approximation. A particular application to the Yukawa potential is discussed. The discussion is restricted to attractive potentials.

I. INTRODUCTION

The solution of equations similar to the Schrödinger equation by replacing the potential $V(r)$ by a sequence of step functions has been the subject of several studies.[1-3] In particular, Swan has used this approach to develop expressions for the number of bound states of a potential in the Schrödinger equation.[3] In this paper, this assumption is used to develop a new approximate expression for the scattering amplitude for attractive spherically symmetric potentials. This form of the amplitude has the following important characteristics: The scattering matrix is unitary; the amplitude is an explicit nonlinear function of the potential; the full high energy limit is identical with the result obtained by calculating the Jost function.[4]

II. DEVELOPMENT OF SCATTERING AMPLITUDE

We consider the radial Schrödinger equation with a spherically symmetric potential $V(r)$ which is smooth enough to be written

$$V(r)=\sum_{n=1}^{N}\epsilon(r_n,r)V(r_n), \tag{1}$$

where

$$\epsilon(r_n,r)=\begin{cases}0, & r<r_n,\ r>r_{n+1},\\ 1, & r_n<r<r_{n+1},\end{cases} \tag{2}$$

and $V(r_n)$ is the value of the potential in the nth subinterval. "Smooth enough" is taken to mean that the potential has at least first derivatives. Initially we consider an interval $a\le r\le b$ to be divided into N equal subintervals Δr. Eventually we allow a to approach zero and b to approach infinity while the size of the subinterval approaches zero. Thus, we solve the differential equation

$$\frac{d^2\psi}{dr^2}-\frac{l(l+1)}{r^2}\psi+\frac{2m}{\hbar^2}(E-V(r_n))\psi=0 \tag{3}$$

in each subinterval and then match ψ and its first derivative at the boundaries of each interval. The solutions to Eq. (3) are

$$\psi_n=A_l(n)rh_l^{(1)}(k_nr)+B_l(n)rh_l^{(2)}(k_nr), \tag{4}$$

where $h_l^{(1)}$ and $h_l^{(2)}$ are spherical Hankel functions of the first and second kinds, respectively. These particular forms for the two linearly independent solutions of Eq. (4) are chosen for the boundary conditions of a scattering problem since they are asymptotically spherical waves. In addition, the wave number k_n is given by

$$k_n=\left(\frac{2m}{\hbar^2}[E-V(r_n)]\right)^{1/2}. \tag{5}$$

Satisfying the boundary conditions at r_n relates $A_l(n)$ and $B_l(n)$ to $A_l(n+1)$ and $B_l(n+1)$. Continuing at each boundary eventually leads to an expression for $A_l(a)$ and $B_l(a)$ in terms of $A_l(b)$ and $B_l(b)$. This is

$$\begin{pmatrix}A_l(a)\\B_l(a)\end{pmatrix}=\prod_{n=1}^{N}U^l(n)\begin{pmatrix}A_l(b)\\B_l(b)\end{pmatrix}=M^l(a,b)\begin{pmatrix}A_l(b)\\B_l(b)\end{pmatrix}, \tag{6}$$

where $U^l(n)$ is a matrix whose elements are

$$U_{11}^l(n)=r_n^2\Delta^{-1}(n)\Big\{h_l^{(1)}(k_{n+1}r_n)h_l^{(2)\prime}(k_nr_n)-\frac{k_{n+1}}{k_n}h_l^{(2)}(k_nr_n)h_l^{(1)\prime}(k_{n+1}r_n)\Big\}, \tag{7}$$

$$U_{12}^l(n)=r_n^2\Delta^{-1}(n)\Big\{h_l^{(2)\prime}(k_nr_n)h_l^{(2)}(k_{n+1}r_n)-\frac{k_{n+1}}{k_n}h_l^{(2)}(k_nr_n)h_l^{(2)\prime}(k_{n+1}r_n)\Big\}, \tag{8}$$

$$U_{21}^l=r_n^2\Delta^{-1}(n)\Big\{\frac{k_{n+1}}{k_n}h_l^{(1)}(k_nr_n)h_l^{(1)\prime}(k_{n+1}r_n)-h_l^{(1)\prime}(k_nr_n)h_l^{(1)}(k_{n+1}r_n)\Big\}, \tag{9}$$

$$U_{22}^l=r_n^2\Delta^{-1}(n)\Big\{\frac{k_{n+1}}{k_n}h_l^{(1)}(k_nr_n)h_l^{(2)\prime}(k_{n+1}r_n)-h_l^{(1)\prime}(k_nr_n)h_l^{(2)}(k_{n+1}r_n)\Big\}, \tag{10}$$

and

$$\Delta(n)=r_n^2[h_l^{(1)}(k_nr_n)h_l^{(2)\prime}(k_nr_n)-h_l^{(1)\prime}(k_nr_n)h_l^{(2)}(k_nr_n)]=-2i/k_n^2. \tag{11}$$

The prime denotes differentiation with respect to kr. Now, as the number of intervals N is increased, it is possible to expand these matrix elements in powers of Δr. The details of this expansion are given in the Appendix. The products in Eq. (6) can then be evaluated to lowest order, and the matrix elements of the product are, in the limit as Δr approaches zero,

$$M_{11}^l = (M_{22}^l)^* = 1 - \frac{i}{2}\int_a^b \left[kr^2 \frac{dk}{dr} h_l^{(1)\prime} h_l^{(2)} - k^2 r^3 \frac{dk}{dr}\,(h_l^{(1)\prime} h_l^{(2)\prime} - h_l^{(2)} h_l^{(1)\prime\prime})\right] dr, \tag{12}$$

$$M_{12}^l = (M_{21}^l)^* = \frac{i}{2}\int_a^b \left[- kr^2 \frac{dk}{dr} h_l^{(2)} h_l^{(2)\prime} + k^2 r^3 \frac{dk}{dr}\{(h_l^{(2)\prime})^2 - h_l^{(2)} h_l^{(2)\prime\prime}\}\right] dr, \tag{13}$$

where the argument of the spherical Hankel functions is the variable wave number

$$kr = \left[\frac{2m}{\hbar^2}(E - V)\right]^{1/2} r. \tag{14}$$

In many physical problems, we are interested in extending the range from 0 to ∞. Equations (12)–(13) provide approximate relations between the coefficients $A_l(0)$ and $B_l(0)$ and $A_l(\infty)$ and $B_l(\infty)$ if the potential vanishes at infinity faster than $1/r$, and if it is cut off at some minimum radius ϵ so that $V(r)$ vanishes for $r < \epsilon$. This last condition may be relaxed if $(dV/dr)/V$ is finite at $r = 0$.

Since the wavefunction is to be regular at the origin, we require

$$A_l(0) = B_l(0), \tag{15}$$

and, from this condition, we obtain

$$A_l(\infty) = \frac{M_{22}^l - M_{12}^l}{M_{11}^l - M_{21}^l} B_l(\infty). \tag{16}$$

The scattering matrix can now be calculated using the result of Eq. (16). The wavefunction in the asymptotic region is

$$\psi = \sum_l i^l \frac{(2l+1)}{2} P_l(\cos\theta) \times B_l(\infty)\left[\frac{M_{22}^l - M_{12}^l}{M_{11}^l - M_{21}^l} r h_l^{(1)} + r h_l^{(2)}\right] = B\sum_l i^l \frac{(2l+1)}{2} P_l(\cos\theta)\left[\frac{M_{22}^l - M_{12}^l}{M_{11}^l - M_{21}^l} - 1\right] r h_l^{(1)} + \psi_{\text{inc}}, \tag{17}$$

where B is a normalization constant and ψ_{inc} is the incident plane wave. We have equated $B_l(\infty)$ to B for all l.

Thus, if the scattered wave is written

$$\psi_{\text{scatt}} = \sum_{l=0}^{\infty} f_l(E) \frac{(2l+1)}{2ik} P_l(\cos\theta) e^{ikr}, \tag{18}$$

then

$$f_l(E) = \frac{M_{22}^l - M_{12}^l - M_{11}^l + M_{21}^l}{M_{11}^l - M_{21}^l}. \tag{19}$$

Now it is a simple matter to demonstrate the unitary property of the S matrix, using Eqs. (12), (13), and the definition[5]

$$S_l(E) = 1 + f_l(E) = \frac{M_{22}^l - M_{12}^l}{M_{11}^l - M_{21}^l}. \tag{20}$$

Then we have

$$S_l^*(E) = \frac{(M_{22}^l)^* - (M_{12}^l)^*}{(M_{11}^l)^* - (M_{21}^l)^*} = \frac{M_{11}^l - M_{21}^l}{M_{22}^l - M_{12}^l} = S_l^{-1}. \tag{21}$$

Turning our attention to the partial wave amplitude $f_l(E)$, we find

$$f_l(E) = \frac{-2iN_l(E)}{1 + iN_l(E) + R_l(E)}, \tag{22}$$

where

$$N_l(E) = \frac{m}{\hbar^2}\int_\epsilon^\infty dr\,kr^3 \frac{dV}{dr}[j_{l+1}(kr) j_{l-1}(kr) - j_l^2(kr)], \tag{23}$$

$$R_l(E) = \frac{-m}{\hbar^2}\int_\epsilon^\infty r^2 dr \frac{dV}{dr}[j_l(kr) n_l'(kr) + kr\{j_l(kr) n_l''(kr) - j_l'(kr) n_l'(kr)\}], \tag{24}$$

and j_l and n_l are spherical Bessel and Neumann functions, respectively. We refer to Eqs. (22)–(24) as the integral approximation to the scattering amplitude.

With the expressions for N_l and R_l given in Eqs. (23)–(24), it is a simple matter to determine their behavior near $r = 0$. Specifically, if $r^2 V$ is finite at the origin, we see by inspection of Eq. (23) that the integral for N_l exists (keeping in mind the requirement that $|V| < 1/r$ as $r \to \infty$). The behavior of R_l is determined by the leading term in the expansion of the spherical Bessel functions in Eq. (24) and is

$$R_l = (l + 1/2)\ln[(E - V(0))/E]. \tag{25}$$

Hence, R_l is finite if $V(0)$ is finite. This is a strong restriction except at high energies. Thus, we have assumed, for finite E, that $V(r)$ has the inner cutoff mentioned earlier.

Although N_l and R_l are too complex to evaluate analytically even for simple potentials, a numerical evaluation seems straightforward and is being undertaken. Even without explicit evaluation, one important characteristic of the approximation, in addition to its unitarity, is that it contains known, nonlinear functions of the potential strength. In this respect, it is similar to the eikonal and WKB approximations, and its relation to a modification of the latter will be given below. However, Eqs. (22)–(24) also lead to the Born approximation in a high energy limit, so that their validity is not restricted to a semiclassical region of interest. We consider this in somewhat more detail in the next section.

Before considering the limiting forms of Eqs. (22)-(24), it is useful to determine the condition of validity. This condition may be obtained by forming the solutions $\psi_l(r)$ as given in Eq. (4) with $A_l(r)$ and $B_l(r)$ evaluated by calculating the matrix $M(r,\infty)$. Inserting this solution in Eq. (4) gives the condition (see Appendix for detail)

$$r\left|\frac{dk}{dr}/k\right| \ll 1. \tag{26}$$

This may be satisfied if the first derivative of the potential is small or if k is large. It is interesting to note that the assumption that V is small compared with E is unnecessary.

III. HIGH ENERGY LIMITS

There are two distinct limits of the integral approximation—one associated with having k large compared to $r(dk/dr)$, and the other being found for E large compared to V. The first, which resembles the WKB approximation, is best seen by examining the wavefunctions for large kr, i.e.,

$$i^{l+1}krA_l(r)h_l^{(1)}(kr) \approx [M_{11}^l(r,a)A_l(a) + M_{12}^l(r,a)B_l(a)]e^{ikr}, \tag{27}$$

where a is some arbitrary radius at which the wavefunction is assumed to be known. The first term on the right of Eq. (27) represents the contribution to the outgoing wave at r from the outgoing wave at a—it is a measure of transmission—while the second term, arising from the incoming wave at a, describes the contribution of reflection to the outgoing wave. If we ignore the latter, i.e., equate $B_l(a)$ to zero, an approximation similar to the WKB approximation results. If we replace the spherical Hankel functions by their asymptotic forms, we have

$$\begin{aligned} krA_l(r)h_l^{(1)}(kr) &\approx i^{-l-1}A_l(a)e^{ikr}\left[1 + \tfrac{1}{2}i\int_r^a\left(-i\frac{dk}{kdr'} + 2r'\frac{dk}{dr'}\right)dr'\right] \\ &= i^{-l-1}A_l(a)e^{ikr}\left[1 + \tfrac{1}{2}\ln k(a)/k(r) - i\int_r^a kdr' + iak(a) - irk(r)\right] \\ &\approx i^{-l-1}A_l(a)e^{ikr}\exp\left[\tfrac{1}{2}\ln k(a)/k(r) + i\int_a^r kdr' + iak(a) - irk(r)\right] \\ &= A_l(a)i^{-l-1}e^{ik(a)a}\frac{\exp i\int_a^r kdr'}{[k(r)/k(a)]^{1/2}}, \end{aligned} \tag{28}$$

where an integration by parts was performed on the second integrand. The entire expression in brackets has the form $(1+\alpha)$ and has been replaced by $\exp\alpha$. This will be valid for small α. Similar results can be obtained for $krB_l(r)h_l^{(2)}(kr)$.

This expression for the wavefunction has the appearance of a one-dimensional WKB approximation. It differs from the usual WKB approximation to the radial wavefunction, since the function $k(r)$ does not contain the angular momentum term $-l(l+1)r^{-2}$. It is possible to obtain the complete WKB approximation from the integral approximation to the radial wave equation by including from the outset the term $-l(l+1)r^{-2}$ in $k(r)$. In this case, the solutions in each interval $r_n \le r \le r_{n+1}$ are chosen to be $\exp \pm iK'r$, with

$$K' = \left[\frac{2m}{\hbar^2}(E - V(r)) - \frac{l(l+1)}{r^2}\right]^{1/2}. \tag{29}$$

At this point, we should comment that the WKB approximation and the modified WKB approximation represented by Eq. (28) are identical in one dimension (i.e., Cartesian coordinates).

We now examine the second high energy limit of the integral approximation. This may be obtained from Eqs. (23)-(24) by performing integrations by parts for N_l and R_l and then equating V to zero in all k. The expressions are then

$$N_l(K) = \frac{2mK}{\hbar^2}\int_0^\infty r^2dr\,V(r)j_l^2(Kr), \tag{30}$$

$$R_l(K) = -\frac{2mK}{\hbar^2}\int_0^\infty r^2dr\,V(r)j_l(Kr)n_l(Kr), \tag{31}$$

where j_l and n_l are spherical Bessel and Neumann functions respectively, and

$$K = (2mE/\hbar^2)^{1/2}. \tag{32}$$

Using these expressions in Eq. (22), a form for the partial wave amplitude is obtained which is identical to that obtained by calculating the high energy limit of the Jost function and, from that, the scattering amplitude. If the denominator in Eq. (22) is replaced by unity and Eq. (30) is used to calculate the numerator, $f_l(E)$ is identical with the Born approximation.

The expression Eq. (31) for $R_l(K)$ is evidently less singular than the original form given in Eq. (24). The reason for this is that the leading term of Eq. (24) is proportional to $\ln(1 - V(0)/E)$, and vanishes in the high energy approximation. In Eq. (31), there is a term arising from the integration by parts which has been attributed to the leading term of the integral and has been omitted. The basis for this identification is that all succeeding terms beyond the first in Eq. (24) and all terms in Eq. (31) contain physical parameters, while the leading term in Eq. (24) and the integrated term omitted from Eq. (31) have purely numerical coefficients. The expression in Eq. (31) is well defined provided Vr^2 is bounded at the origin.

IV. SCATTERING FROM A YUKAWA POTENTIAL

As a specific example of potential scattering, consider an attractive Yukawa potential

$$V = \begin{cases} (-ve^{-\mu r})/r, & r > \epsilon, \\ 0, & r < \epsilon. \end{cases} \tag{33}$$

The full integral approximation must be evaluated numerically but there are some interesting features exhibited by the high energy limit. From Eqs. (30)–(31), the s-wave amplitude is

$$f_0(K) = \frac{\dfrac{imv}{\hbar^2 K}\ln\left[1+\left(\dfrac{2K}{\mu}\right)^2\right]}{1-\dfrac{imv}{2\hbar^2 K}\ln\left[1+\left(\dfrac{2K}{\mu}\right)^2\right]-\dfrac{mv}{\hbar^2 K}\tan^{-1}\dfrac{2K}{\mu}}. \tag{34}$$

As mentioned earlier, the numerator is identical with the Born approximation, but the denominator can be significant, as it can be zero. In particular, if this amplitude is used to calculate low energy, singlet proton–neutron scattering, experiment requires a coupling constant $v/\hbar c \approx 0.14$, if μ is the inverse Compton wavelength of the pion. The strength obtained by a scattering length calculation is $v/\hbar c \approx 0.08$, while the Born approximation gives $v^B/\hbar c \approx 11$. The origin of the large discrepancy between the Born approximation and the high energy limit of the integral approximation arises because, for $v/\hbar c \approx 0.14$, the denominator of Eq. (34) has a zero on the imaginary K axis at about $-0.03\ \mu$. This enhances the low energy amplitude and consequently reduces the coupling constant necessary to match a given value of the cross section compared with the Born approximation.

V. CONCLUSIONS

The principal results of this work are contained in Eqs. (22)–(24), where the integral approximation to the scattering amplitude is given. If the condition for the validity of this approximation [Eq. (26)] is poorly satisfied, a second interation can be used to calculate the amplitude. The steps in the iterative process are straightforward: From Eqs. (12)–(13), the matrix M^l is calculated for arbitrary r and used to form the first iterations for the wavefunctions. These replace the spherical Hankel functions in the final expressions for the scattering amplitude, Eqs. (22)–(28).

The significant characteristics of any order iteration are: The amplitude satisfies unitarity; each order contains explicit, nonlinear functions of the potential strength; and the validity of the approximation is not dependent upon the ratio of potential strength to energy, but is instead determined by the value of $r(dk/dr)/k$.

ACKNOWLEDGMENTS

We would like to thank W. E. Gettys and J. S. Zmuidzinas for several interesting discussions of this work.

APPENDIX

In this section we include some mathematical details of the expansion of the matrix product appearing in Eq. (6). The expansion and subsequent approximation of this product leads to the expressions for the matrix elements M_{ij} given in Eqs. (12) and (13). Also, details of the determination of the limiting condition found in Eq. (26) are included here.

From inspection of the matrix elements in Eqs. (7)–(10), it is evident that if V is a smooth potential k_{n+1}, then all terms containing it can be expanded about r_n. Thus, the steps leading from Eqs. (7)–(11) to Eqs. (12)–(13) are the following: Expand k_{n+1} about r_n keeping terms of order zero and unity in the interval Δr, then expand all Bessel functions about the argument $k_n r_n$, retaining terms of order zero and unity in Δr. The result for the matrix $U(n)$ will be a sum of matrices with diagonal elements of order zero and unity in Δr and off-diagonal elements of order unity in this quantity. The product of the matrices $U(n)$ will be the unit matrix plus a matrix whose elements are a sum of terms of order Δr. This last matrix will, in the limit as Δr approaches zero, have elements which are the integrals appearing in Eqs. (12)–(13).

Specifically, we have

$$k_{n+1} \approx k_n + \Delta r(dk/dr)_n, \tag{A1}$$

where dk/dr is to be evaluated at r_n. With this result the Hankel functions can be expanded, e.g.,

$$\begin{aligned} h_l^{(1)}(k_{n+1}r_n) &\approx h_l^{(1)}[k_n r_n + \Delta r(dk/dr)_n r_n] \\ &\approx h_l^{(1)}(k_n r_n) + \Delta r(dk/dr)_n r_n h_l^{(1)\prime}(k_n r_n). \end{aligned} \tag{A2}$$

Performing the expansions as indicated for each term in U_{11} and using Eq. (11), we obtain

$$\begin{aligned} U_{11}(n) &= 1 + r_n^2\Delta^{-1}(n)\{h_l^{(1)\prime}(k_n r_n)h_l^{(2)\prime}(k_n r_n)(dk/dr)_n \\ &\quad \times r_n\Delta r - (dk/dr)_n(\Delta r/k_n)h_l^{(2)}(k_n r_n)h_l^{(1)\prime}(k_n r_n) \\ &\quad - (dk/dr)_n r_n h_l^{(2)}(k_n r_n)h_l^{(1)\prime\prime}(k_n r_n)\Delta r\} \\ &= 1 + W_{11}(n)\Delta r. \end{aligned} \tag{A3}$$

The assumption throughout is that $W_{11}(n)\Delta r$ is small compared to unity. For scattering from attractive potentials, this assumption is satisfied subject to the limitations on the potential discussed following Eqs. (14) and (32). Repulsive potentials and bound states ($E < 0$) must be discussed separately and will be considered in a subsequent publication.

Repeating the expansion outlined above for each of the matrix elements displayed in Eqs. (8)–(10) gives an approximate expression for $U(n)$,

$$U(n) \approx 1 + W(n)\Delta r, \tag{A4}$$

where 1 represents the unit matrix and $W(n)\Delta r$ is a matrix whose elements are all small. Finally, the product of matrices in Eq. (6) is approximated by

$$\prod_{n=0}^{N} U(n) \approx \prod_{n=0}^{N} (1 + W(n)\Delta r) \approx 1 + \sum_{n=0}^{N} W(n)\Delta r, \tag{A5}$$

where, as previously, products of terms containing Δr have been neglected. As N becomes large and r approaches zero, the sums in the matrix elements approximate integrals and the expressions given in Eqs. (12)–(13) are obtained.

We now turn to a discussion of the limits of validity of the integral approximation as expressed in Eq. (26). The method of obtaining this result is straightforward. The solution of the Schrödinger equation in the integral approximation is, from Eq. (4),

$$R = r^{-1}\psi = A_l(r)h_l^{(1)}(kr) + B_l(r)h_l^{(2)}(kr) = Au + Bv, \tag{A6}$$

where the index l has been dropped and the arguments suppressed in the last step. R is the radial wavefunction approximant. From Eq. (6) and Eqs. (12)–(13), $A(r)$ and $B(r)$ can be written

$$A(r) = M_{11}(r,b)A(b) + M_{12}(r,b)B(b), \tag{A7}$$

$$B(r) = M_{21}(r,b)A(b) + M_{22}(r,b)B(b), \tag{A8}$$

where b is some arbitrary point at which R is assumed to be known. $A(b)$ and $B(b)$ are coefficients determined by the boundary conditions on R and may be considered arbitrary until these conditions are stated explicitly.

The limits of validity are obtained by inserting the solution for R given in Eq. (A6) in the radial Schrödinger equation. Since this is an approximation, there will be a remainder term. The condition that the remainder be small will determine the limits of validity of the approximation. Thus, we have

$$\begin{aligned}[]&[d^2/dr^2 + (2/r)d/dr + k^2 - l(l+1)/r^2]R \\ &\quad = [d^2/dr^2 + (2/r)d/dr + k^2 - l(l+1)/r^2] \\ &\qquad \times [A(r)u + B(r)v] \approx 0.\end{aligned} \tag{A9}$$

Using Eqs. (A7) and (A8) and the expressions in Eqs. (12) and (13) for M_{11} and M_{21} and performing the operations indicated in Eq. (A9), we obtain

$$\begin{aligned} A(b)\{&M_{11}d^2u/dr^2 + 2(du/dr)dM_{11}/dr + ud^2 \\ &\times M_{11}/dr^2 + (2/r)M_{11}du/dr + (2u/r)dM_{11}/dr \\ &+ [k^2 - l(l+1)r^{-2}]M_{11}u + M_{21}d^2v/dr^2 \\ &+ 2(dM_{21}/dr)dv/dr + vd^2M_{21}/dr^2 + (2/r) \\ &\times M_{21}dv/dr + (2v/r)dM_{21}/dr + [k^2 - l(l+1) \\ &\times r^{-2}]vM_{21}\} \approx 0.\end{aligned} \tag{A10}$$

The coefficient of $B(b)$ is the complex conjugate of that of $A(b)$. Since A and B are considered arbitrary, each coefficient must vanish separately.

The sense of the approximation is that the deviations of R from the functions u and v is to be small. Consequently, in the terms in Eq. (A10) which do not contain derivatives of M_{11} or M_{21}, we write

$$M_{11} \approx 1, \tag{A11}$$

$$M_{21} \approx 0. \tag{A12}$$

With this simplification the condition for the validity of the approximation is

$$\begin{aligned} k^{-2}[&(4dk/dr + rd^2k/dr^2)u' + \{2krdk/dr \\ &+ r^2(dk/dr)^2\}u'' + 2(du/dr)dM_{11}/dr \\ &+ ud^2M_{11}/dr^2 + (2dv/dr)dM_{21}/dr \\ &+ vd^2M_{21}/dr^2 + (2u/r)dM_{11}/dr \\ &+ (2v/r)dM_{21}/dr] \approx 0.\end{aligned} \tag{A13}$$

The factor k^{-2} has been included to make the coefficient dimensionless. In Eq. (A13) the terms which do not contain M_{11}, M_{21} or their derivatives appear because u satisfies Bessel's equation of order l in the variable kr. Performing the differentiations and using the result that the Wronskian of u and v is

$$uv' - u'v = -2i/(kr)^2, \tag{A14}$$

we obtain (recalling that prime denotes differentiation with respect to kr)

$$u''(rk^{-1}dk/dr)^2 + k^{-2}(dk/dr)u' \approx 0. \tag{A15}$$

Equation (A15) is the condition for the validity of the approximation.

Finally, Eq. (A15) may be evaluated in the limit of large kr, where u'' approaches $-u$ and u' approaches iu. Thus, to lowest order in $1/kr$, Eq. (A15) reduces to

$$|rk^{-1}dk/dr| \ll 1. \tag{A16}$$

The condition expressed in Eq. (A16) can be satisfied by potentials with small gradients or by potentials which are small compared with the incident kinetic energy. In the former circumstance this is similar to the condition for the validity of the WKB approximation, while in the latter it is analogous to the requirement for the validity of the Born approximation.

[1] H. Bremmer, Commun. Pure Appl. Math. 4, 105 (1951).
[2] P. Swan, Phys. Rev. 153, 1379 (1967).
[3] P. B. Burt, J. Plasma Phys. (U.K.) 3, 417 (1969).
[4] D. Park, *Introduction to Strong Interactions* (Benjamin, New York, 1966).
[5] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

The Unitary Group U(m) as the Symmetry Group of Curved Phase Space

Said Heskia
Birkbeck College, University of London, England
and
S. A. Sofroniou
Enfield College of Technology, Enfield, England
(Received 24 March 1971)

By describing $U(m)$ as the symmetry group of a curved phase space, namely, by describing $U(m)$ as the group of holonomy of a Hamiltonian space endowed with a Riemannian metric, it is shown that the Lie algebra of such a group is prior to any explicit Hamiltonian assumption.

INTRODUCTION

The purpose of this paper is to discuss a treatment of the unitary group $U(m)$ as the symmetry group of phase space in the absence of any Hamiltonian information. This is done by obtaining the group $U(m)$ as a symmetry group of a curved phase space, i.e., the group of holonomy of phase space, which implies that the Hamiltonian space is characterized by a Riemann connection. This is in analogy to the holonomy group $O(3, 1)$ of the four-dimensional space–time of general relativity.

In this context, we shall start in Sec. 1 with the usual "flat-space" description of the group $U(m)$ and show that the description of this group as the symmetry group of a $2m$-dimensional flat Hamiltonian space is possible, provided we consider those canonical transformations which preserve the angle between the dynamical variables, i.e., provided the Hamiltonian space is endowed with an orthogonal metric, and provided we also restrict the Hamiltonian (or the generating function) so as to be at most quadratic in the dynamical variables.

In Sec. 2, we shall show that another point of view is possible which does not depend on the ad hoc introduction of the quadratic Hamiltonian for its Lie algebra. This is done by deriving the group $U(m)$ as the symmetry group of a $2m$-dimensional curved phase space, i.e., the group of holonomy of a Hamiltonian space endowed with a Riemann metric. In this case the Lie algebra of the group is seen to arise quite naturally from the $\substack{\alpha \\ \beta}$-domain of a set of $m \times m$ curvature matrices $R_{\alpha\beta} = R_{\alpha\beta ij} dx^i \wedge dx^j$ [of the linear Hermitian tangent space of the curved phase space $M_{2m}(x^i)$], just as the Lie algebra of the flat phase space is spanned by the $\substack{\alpha \\ \beta}$-domain of the initially assumed Hamiltonian matrix $\hat{H}_{\alpha\beta}$ of the quadratic Hamiltonian $H = \hat{H}_{\alpha\beta} z^\alpha \overset{*}{z}{}^\beta$ $(z^\alpha = x^\alpha + i p_\alpha)$ of the Hermitian flat phase space $\hat{M}_{2m}(z^\alpha, \overset{*}{z}{}^\alpha)$.

1. GEOMETRY OF PHASE SPACE—$U(m)$ AS THE SYMMETRY GROUP OF FLAT PHASE SPACE

With a view to describing the internal symmetry group $U(m)$ as a symmetry group of a $2m$-dimensional classical phase space M_{2m}, we shall first briefly describe the geometry of the space and in particular its finite group of canonical transformations, i.e., the symplectic group $SP(m)$ as $U(m)$ happens to be a subgroup of this group.

Following Lee,[1] we shall begin with a $2m$-dimensional manifold M_{2m} covered with a system of coordinate neighborhoods $x^i (i, j, k, \ldots = 1, \ldots, 2m)$, and we shall introduce a_{ij} as a skew symmetric nonsingular covariant tensor in M_{2m}, whose components are to be analytic function of the x's. In terms of exterior calculus, there is associated with a_{ij} the exterior differential form of degree two, i.e.,

$$\Omega = \tfrac{1}{2} a_{ij} dx^i \wedge dx^j, \tag{1.1}$$

which is called the fundamental form of M_{2m}. Application of exterior derivative to Ω yields

$$d\Omega = \tfrac{1}{6} K_{ijk} dx^i \wedge dx^j \wedge dx^k, \tag{1.2}$$

where

$$K_{ijk} = \frac{\partial a_{ij}}{\partial x^k} + \frac{\partial a_{jk}}{\partial x^i} + \frac{\partial a_{ti}}{dx^j} \tag{1.3}$$

is called the "curvature tensor," although it has quite a different structure from the Riemann curvature tensor which arises from the Riemann metric, i.e., the symmetric metric G_{ij}. M_{2m} is flat when $K_{ijk} = 0$, i.e., when $d\Omega = 0$, so that by the converse of Poincaré's lemma, Ω itself is the exterior derivative of a Pfaffian form $\eta = \eta_i dx^i$, such that

$$\Omega = d\eta = \tfrac{1}{2}\left(\frac{\partial \eta_i}{\partial x^j} - \frac{\partial \eta_j}{dx^i}\right) dx^i \wedge dx^j, \tag{1.4}$$

[1] H. Bremmer, Commun. Pure Appl. Math. 4, 105 (1951).
[2] P. Swan, Phys. Rev. 153, 1379 (1967).
[3] P. B. Burt, J. Plasma Phys. (U.K.) 3, 417 (1969).
[4] D. Park, *Introduction to Strong Interactions* (Benjamin, New York, 1966).
[5] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

The Unitary Group U(m) as the Symmetry Group of Curved Phase Space

Said Heskia
Birkbeck College, University of London, England

and

S. A. Sofroniou
Enfield College of Technology, Enfield, England

(Received 24 March 1971)

By describing $U(m)$ as the symmetry group of a curved phase space, namely, by describing $U(m)$ as the group of holonomy of a Hamiltonian space endowed with a Riemannian metric, it is shown that the Lie algebra of such a group is prior to any explicit Hamiltonian assumption.

INTRODUCTION

The purpose of this paper is to discuss a treatment of the unitary group $U(m)$ as the symmetry group of phase space in the absence of any Hamiltonian information. This is done by obtaining the group $U(m)$ as a symmetry group of a curved phase space, i.e., the group of holonomy of phase space, which implies that the Hamiltonian space is characterized by a Riemann connection. This is in analogy to the holonomy group $O(3, 1)$ of the four-dimensional space–time of general relativity.

In this context, we shall start in Sec. 1 with the usual "flat-space" description of the group $U(m)$ and show that the description of this group as the symmetry group of a $2m$-dimensional flat Hamiltonian space is possible, provided we consider those canonical transformations which preserve the angle between the dynamical variables, i.e., provided the Hamiltonian space is endowed with an orthogonal metric, and provided we also restrict the Hamiltonian (or the generating function) so as to be at most quadratic in the dynamical variables.

In Sec. 2, we shall show that another point of view is possible which does not depend on the ad hoc introduction of the quadratic Hamiltonian for its Lie algebra. This is done by deriving the group $U(m)$ as the symmetry group of a $2m$-dimensional curved phase space, i.e., the group of holonomy of a Hamiltonian space endowed with a Riemann metric. In this case the Lie algebra of the group is seen to arise quite naturally from the $^{\alpha}_{\beta}$-domain of a set of $m \times m$ curvature matrices $R_{\alpha\beta} = R_{\alpha\beta ij}dx^i \wedge dx^j$ [of the linear Hermitian tangent space of the curved phase space $M_{2m}(x^i)$], just as the Lie algebra of the flat phase space is spanned by the $^{\alpha}_{\beta}$-domain of the initially assumed Hamiltonian matrix $\hat{H}_{\alpha\beta}$ of the quadratic Hamiltonian $H = \hat{H}_{\alpha\beta}z^{\alpha}\overset{*}{z}^{\beta}$ $(z^{\alpha} = x^{\alpha} + ip_{\alpha})$ of the Hermitian flat phase space $\hat{M}_{2m}(z^{\alpha}, \overset{*}{z}^{\alpha})$.

1. GEOMETRY OF PHASE SPACE—$U(m)$ AS THE SYMMETRY GROUP OF FLAT PHASE SPACE

With a view to describing the internal symmetry group $U(m)$ as a symmetry group of a $2m$-dimensional classical phase space M_{2m}, we shall first briefly describe the geometry of the space and in particular its finite group of canonical transformations, i.e., the symplectic group $SP(m)$ as $U(m)$ happens to be a subgroup of this group.

Following Lee,[1] we shall begin with a $2m$-dimensional manifold M_{2m} covered with a system of coordinate neighborhoods $x^i (i, j, k, \ldots = 1, \ldots, 2m)$, and we shall introduce a_{ij} as a skew symmetric nonsingular covariant tensor in M_{2m}, whose components are to be analytic function of the x's. In terms of exterior calculus, there is associated with a_{ij} the exterior differential form of degree two, i.e.,

$$\Omega = \tfrac{1}{2}a_{ij}dx^i \wedge dx^j, \tag{1.1}$$

which is called the fundamental form of M_{2m}. Application of exterior derivative to Ω yields

$$d\Omega = \tfrac{1}{6}K_{ijk}dx^i \wedge dx^j \wedge dx^k, \tag{1.2}$$

where

$$K_{ijk} = \frac{\partial a_{ij}}{\partial x^k} + \frac{\partial a_{jk}}{\partial x^i} + \frac{\partial a_{ti}}{dx^j} \tag{1.3}$$

is called the "curvature tensor," although it has quite a different structure from the Riemann curvature tensor which arises from the Riemann metric, i.e., the symmetric metric G_{ij}. M_{2m} is flat when $K_{ijk} = 0$, i.e., when $d\Omega = 0$, so that by the converse of Poincaré's lemma, Ω itself is the exterior derivative of a Pfaffian form $\eta = \eta_i dx^i$, such that

$$\Omega = d\eta = \tfrac{1}{2}\left(\frac{\partial \eta_i}{\partial x^j} - \frac{\partial \eta_j}{dx^i}\right)dx^i \wedge dx^j, \tag{1.4}$$

where a_{ij} is given by

$$a_{ij} = \left(\frac{\partial \eta_i}{\partial x^j} - \frac{\partial \eta_j}{\partial x^i}\right). \tag{1.5}$$

By a change of coordinates, this Pfaffian form can be put in its well-known canonical form, i.e., on setting

$$x^i = \begin{pmatrix} x^\alpha \\ x^{\bar\alpha} \end{pmatrix}, \quad \eta_i = \begin{pmatrix} p_\alpha \\ 0 \end{pmatrix}, \quad x^{\bar\alpha} = p_\alpha, \quad \bar\alpha = m + \alpha, \quad 2m = 6, \tag{1.6}$$

we find that in the new coordinate system the fundamental tensor assumes the symplectic form

$$a_{ij} = \begin{pmatrix} 0 & \delta\alpha\beta \\ -\delta\alpha\beta & 0 \end{pmatrix} = -a_{ji}, \tag{1.7}$$

where

$$a_{ij} = a^{ji}, \quad a_{ij}a^{jk} = \delta^k_i.$$

A locally flat M_{2m} is in particular a Hamiltonian manifold; for, if we consider a system of curves in M_{2m} defined by a system of ordinary differential equations of the form

$$\frac{dx^i}{dt} - a^{ij}\frac{\partial H}{\partial x^j} = 0, \tag{1.8}$$

where H is a given function of x^i and t. This last equation, on account of (1.7), may be written in the form

$$\dot{x}^\alpha = \partial H/\partial p_\alpha, \quad \dot{p}_\alpha = -\partial H/\partial x^\alpha, \tag{1.9}$$

which gives the pair of the well-known Hamiltonian equations with x^α and p_α as canonically conjugate dynamical variables.

Consider a dynamical system with Hamiltonian H. In time δt, we have

$$\delta x^\alpha = \delta t(\partial H/\partial p_\alpha), \quad \delta p_\alpha = -\delta t(\partial H/\partial x^\alpha), \tag{1.10}$$

so that the motion from the position at time $t = 0$ to that at time δt is an infinitesimal canonical transformation, such that

$$x'^\alpha = x^\alpha + \delta t(\partial H/\partial p_\alpha), \quad p'_\alpha = p_\alpha - \delta t(\partial H/\partial x^\alpha), \tag{1.11}$$

where x^α, p_α stand for the coordinates and momenta at time $t = 0$, while primed quantities refer to time δt. The most general infinitesimal canonical transformation is, however, given by

$$x'^\alpha = x^\alpha + \delta\epsilon(\partial F/\partial p_\alpha), \quad p'_\alpha = p_\alpha - \delta\epsilon(\partial F/\partial x^\alpha), \tag{1.12}$$

where $\delta\epsilon$ is an infinitesimal parameter and F is a function of (x^α, p_α).

It can be shown that the canonical transformations form an infinite Lie group if F is a one-valued analytic function[2] of (x^α, p_α).

The change in a function $G(x^\alpha, p_\alpha)$ as a result of an infinitesimal canonical transformation is then given by

$$\delta G = \delta\epsilon\{G, F\}, \tag{1.13}$$

where $\{\ ,\ \}$ is the Poisson bracket.

An "invariance group" of a dynamical system is defined as any subgroup of the canonical transformations, which leave the Hamiltonian invariant; that is, transformations such that

$$\delta H = \delta t\{H, F\} = 0. \tag{1.14}$$

In such cases, one considers only those systems whose Hamiltonian is time-independent. The invariance dynamical group is then generated by the one-valued constants of motion.

Now the group of canonical transformations is, so to speak, the "symmetry group" of classical mechanics as a whole, before any one explicit system is considered. To describe what is meant by "classical mechanics" in physics, one must focus attention on the subalgebra of F. For example, in Newtonian mechanics, one is usually given one observable (the "energy" or "Hamiltonian") in a distinguished role,[3] and several other observables, which have relatively simple commutation relations with H playing the role of the linear and angular momenta. Note that the observables, i.e., the F's (or the H's)[4] that are at most quadratic in the x^α and p_α, together, form a Lie algebra, i.e., those of the form[5]

$$F = F_i x^i + F_{ij}x^i x^j, \tag{1.15}$$

where F_i, F_{ij} are constant coefficients with the following matrix representation

$$F_i = \begin{pmatrix} F_\alpha \\ F_{\bar\alpha} \end{pmatrix} F_{ij} = \begin{pmatrix} F_{\alpha\beta} & F_{\alpha\bar\beta} \\ F_{\bar\alpha\beta} & F_{\bar\alpha\bar\beta} \end{pmatrix}. \tag{1.16}$$

Those with $F_i = 0$, however, generate the real symplectic group $SP(2m)$. They will also generate its unitary subgroup $U(m)$ provided the angle between the dynamical variables is preserved.

Let us first consider the symplectic group. If we substitute $F = F_{ij}x^i x^j$ in the infinitesimal canonical transformation (1.12), which may also be expressed in terms of a single coordinate x^i, i.e., as

$$\begin{aligned} x'^i &= x^i + \delta x^i \\ &= x^i + \delta\epsilon a^{ij}(\partial F/\partial x^j), \end{aligned} \tag{1.17}$$

we get

$$\begin{aligned} x'^i &= (\delta^i_j + \epsilon a^{ik}F_{kj})x^j \\ &= (\delta^i_j + \epsilon F^i_j)x^j \\ &= \gamma^i_j x^j, \end{aligned} \tag{1.18}$$

where for notational reasons we have replaced $\delta\epsilon$ by ϵ and where $\gamma^i_j = (\delta^i_j + \epsilon F^i_j)$ is a $2m \times 2m$ constant matrix with

$$\partial\gamma^i_j/\partial x^k = 0. \qquad (1.19)$$

Consequently, if there exists a linear motion given by $dx'^i = \gamma^i_j dx^j$, such that the bilinear form $\Omega = a_{ij}dx^i \wedge dx^j$ is left invariant (as required by the group of canonical transformations), we must have

$$\eta' = \gamma\eta\gamma^t, \qquad (1.20)$$

where γ^t denotes the transpose of the matrix $\gamma = (\gamma^i_j)$.

If we write

$$\gamma = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad \begin{array}{l} A = (\gamma^{\alpha}_{\beta}), C = (\gamma^{\bar{\alpha}}_{\beta}), \\ B = (\gamma^{\alpha}_{\bar{\beta}}), D = (\gamma^{\bar{\alpha}}_{\bar{\beta}}), \end{array} \qquad (1.21)$$

then (1.20) implies

$$\begin{aligned} A^tC - C^tA &= 0, \\ D^tB - B^tD &= 0, \\ A^tD - C^tB &= I, \end{aligned} \qquad (1.22)$$

The following identity follows easily:

$$\gamma^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} D^t & -B^t \\ -C^t & A^t \end{pmatrix}. \qquad (1.23)$$

The above matrices define the so-called symplectic group. (See for example Weyl[6]).

If further γ is unitary,

$$\gamma^{-1} = (\gamma^*)^t$$

or

$$\begin{pmatrix} D^t & -B^t \\ -C^t & A^t \end{pmatrix} = \begin{pmatrix} A^t & C^t \\ B^t & D^t \end{pmatrix}, \qquad (1.24)$$

one finds, from (1.24),

$$A = D, \quad B = -C. \qquad (1.25)$$

Hence, of course, we also verify that the following relations:

$$\begin{aligned} F^{\alpha}_{\beta} &= F^{\bar{\alpha}}_{\bar{\beta}} = M^{\alpha}_{\beta}, \\ F^{\bar{\alpha}}_{\beta} &= -F^{\alpha}_{\bar{\beta}} = N^{\alpha}_{\beta}, \end{aligned} \qquad (1.26)$$

or

$$F^i_j = \begin{pmatrix} M^{\alpha}_{\beta} & -N^{\alpha}_{\beta} \\ N^{\alpha}_{\beta} & M^{\alpha}_{\beta} \end{pmatrix}, \quad \text{where } \left\{ \begin{array}{l} M^{\alpha}_{\beta} = M^{\beta}_{\alpha} \\ N^{\alpha}_{\beta} = -N^{\beta}_{\alpha} \end{array} \right. . \qquad (1.27)$$

will hold.

The general form of the real unitary matrix is therefore of the form

$$\gamma^i_j = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}, \qquad (1.28)$$

which satisfies

$$\begin{aligned} A^tB - B^tA &= 0, \\ A^tA + B^tB &= I, \end{aligned} \qquad (1.29)$$

on account of the relations (1.22). Hence if we introduce a constant matrix

$$S = \frac{1}{\sqrt{2}}\begin{pmatrix} iI & -iI \\ I & I \end{pmatrix}, \qquad (1.30)$$

we can easily verify that the following relations hold:

$$S^{-1}\gamma S = \begin{pmatrix} A + iB & 0 \\ 0 & A - iB \end{pmatrix}. \qquad (1.31)$$

The last equation shows that the $m \times m$ matrix $(A + iB)$ is complex unitary, i.e.,

$$U = A + iB \qquad (1.32)$$

satisfies [by (1.29)]

$$(U^*)^tU = U^{\dagger}U = I. \qquad (1.33)$$

It must be noted that the reduction of the group of canonical transformations $SP(2m)$ to its unitary subgroup $U(m)$, presupposes the introduction of an orthogonal metric, i.e., a constant symmetric metric into the Hamiltonian space. For if

$$O_{ij} = \begin{pmatrix} \delta_{\alpha\beta} & 0 \\ 0 & \delta_{\alpha\beta} \end{pmatrix} \qquad (1.34)$$

is the metric tensor which preserves the angle between the dynamical variables, then under an arbitrary coordinate transformation $x'^i = f(x)$, not only the volume element but also the line element, i.e., both

$$\Omega = a_{ij}dx^i \wedge dx^j \quad \text{and} \quad ds^2 = O_{ij}dx^i dx^j \qquad (1.35)$$

remain invariant; from this fact, we deduce that

$$a'_{ij} = a_{kl}\frac{\partial x^k}{\partial x'^i}\frac{\partial x^l}{\partial x'^j}, \qquad O_{ij} = O_{kl}\frac{\partial x^k}{\partial x'^i}\frac{\partial x^l}{\partial x'^j}. \qquad (1.36)$$

It is easily verified that the transformations

$$x'^i = \gamma^i_j x^j, \qquad \gamma^i_j\gamma^j_k = \delta^i_k,$$
$$\overset{*}{\gamma}{}^i_j = \gamma^i_j, \qquad (\partial\gamma^i_j/\partial x^k) = 0,$$

with γ given by the matrix

$$\gamma = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}$$

satisfying

$$\begin{aligned} A^tB - B^tA &= 0, \\ A^tA + B^tB &= I, \end{aligned}$$

can be considered as the most general transformations satisfying Eq. (1.36). Needless to say, the subgroup of the general linear group $GL(2m, R)$ which leaves invariant a_{ij} is, by definition, the symplectic group $SP(2m)$, whilst that leaving invariant

O_{ij} is, by definition, the orthogonal group $O(2m)$. But the subgroup of the general linear group which leaves invariant both a_{ij} and O_{ij} is the intersection of the two groups $SP(2m)$ and $O(2m)$, [i.e., $U(m) = SP(2m) \cap O(2m)$] and is known as the real representation of the unitary group. However, since for particle physics it is the complex representation of the group $U(m)$ which plays a fundamental role, we shall proceed to discuss the complex representation of the group.

Such a representation is obtained by setting

$$z^\alpha = x^\alpha + ip_\alpha, \qquad \overset{*}{z}{}^\alpha = x^\alpha - ip_\alpha, \tag{1.37}$$

so that the real phase space M_{2m} is now equivalent to the complex phase space $\hat{M}_{2m}$. In terms of the new variables, the equations of motion equivalent to (1.8) assume the complex form

$$\frac{dz^i}{d\epsilon} - \hat{a}^{ij}\frac{\partial F}{\partial z^j} = 0, \tag{1.38}$$

where

$$\frac{dz^\alpha}{d\epsilon} = -i\delta^{\alpha\beta}\frac{\partial F}{\partial \overset{*}{z}{}^\beta} = -i\frac{\partial F}{\partial z^*_\alpha}, \tag{1.39a}$$

$$\frac{d\overset{*}{z}{}^\alpha}{d\epsilon} = id^{\alpha\beta}\frac{\partial F}{\partial z^\beta} = i\frac{\partial F}{\partial z_\alpha}, \tag{1.39b}$$

is their explicit representation, since

$$\hat{a}^{ij} = \begin{pmatrix} 0 & -i\delta^{\alpha\beta} \\ i\delta^{\alpha\beta} & 0 \end{pmatrix}, \qquad z^i = \begin{pmatrix} z^\alpha \\ \overset{*}{z}{}^\alpha \end{pmatrix}. \tag{1.40}$$

In Eq. (1.39), the generating function F has to be regarded as a function of $z^\alpha, \overset{*}{z}{}^\alpha$ satisfying the reality condition

$$F(z^\alpha, \overset{*}{z}{}^\alpha) = [F(z^\alpha, \overset{*}{z}{}^\alpha)]^* = F^*(z^\alpha, \overset{*}{z}{}^\alpha). \tag{1.41}$$

For the specific case of the quadratic F under consideration, namely, $F = F_{ij}x^i x^j$, the function $F(z^\alpha, \overset{*}{z}{}^\alpha)$ assumes the form

$$F = \hat{F}_{\alpha\beta} z^\alpha \overset{*}{z}{}^\beta, \tag{1.42}$$

where

$$\hat{F}_{\alpha\beta} = M_{\alpha\beta} - iN_{\alpha\beta} = \hat{F}^{**}_{\beta\alpha} \tag{1.43}$$

is a set of m^2 linearly independent Hermitian matrices. When the above special function (1.42) is inserted into the equations of motion (1.39a), we obtain

$$\frac{dz^\alpha}{d\epsilon} = -i\hat{F}^\alpha_\beta z^\beta, \tag{1.44}$$

which is the equation of motion for m coupled harmonic oscillators.

For an infinitesimal transformation, we have

$$\begin{aligned} z'^\alpha &= z^\alpha + \delta z^\alpha \\ &= z^\alpha - i\epsilon^{(a)}\hat{F}^\alpha_{(a)\beta} z^\beta \\ &= (\delta^\alpha_\beta - i\epsilon^{(a)}\hat{F}^\alpha_{(a)\beta}) z^\beta \\ &= U^\alpha_\beta z^\beta, \end{aligned} \tag{1.45}$$

which defines the complex representation of the real unitary transformations, i.e., the transformations defined by $x'^i = \gamma^i_j x^j$ with $\hat{F}_{(a)}$ ($^\alpha_\beta$-indices suppressed) as a set of m^2 Hermitian matrices spanning the Lie algebra of the complex unitary group as they satisfy the following commutation relations

$$[\hat{F}_{(a)}, \hat{F}_{(b)}] = if^{(c)}_{(a)(b)}\hat{F}_{(c)}. \tag{1.46}$$

2. THE GROUP $U(m)$ AS THE SYMMETRY GROUP OF THE CURVED PHASE SPACE

We shall now replace the orthogonal metric of the phase space M_{2m} by a Riemannian metric and thus show that the Lie algebra of the group $U(m)$ is no longer dependent on an ad hoc stipulation of the quadratic generating function. For in our case, the Lie algebra of the group $U(m)$ (which is the group of holonomy of M_{2m} is spanned by the α_β domain of the anti-Hermitian curvature tensor $R^\alpha_{\beta ij}$ of the tangent-bundle of the base manifold M_{2m}. The group $U(m)$ will thus arise as the symmetry group of the curved phase space.

We thus begin with a curved phase manifold M_{2m}, namely, a Hamiltonian manifold endowed with a Riemannian metric given by the square of the line element

$$ds^2 = G_{ij}dx^i dx^j. \tag{2.1}$$

The Riemannian metric gives rise to the Christoffel connection

$$\Gamma^i_{jk} = \left\{ {i \atop jk} \right\} = \tfrac{1}{2}G^{il}\left(\frac{\partial G_{lj}}{\partial x^k} + \frac{\partial G_{lk}}{\partial x^j} - \frac{\partial G_{jk}}{\partial x^l}\right), \tag{2.2}$$

which we shall assume to be nonintegrable, i.e., nonflat. If we denote by ∇_k the operation of the covariant derivative of the metric a_{ij} of M_{2m} with respect to the symmetric connection Γ^i_{jk}, we have

$$\nabla_k a_{ij} = \frac{\partial a_{ij}}{\partial x^k} - \Gamma^l_{ik}a_{lj} - \Gamma^l_{jk}a_{li} \tag{2.3}$$

from which

$$K_{ijk} = \nabla_k a_{ij} + \nabla_i a_{jk} + \nabla_j a_{ki}, \tag{2.4}$$

where once again

$$K_{ijk} = \frac{\partial a_{ij}}{\partial x^k} + \frac{\partial a_{jk}}{\partial x^i} + \frac{\partial a_{ki}}{\partial x^j} = 0. \tag{2.5}$$

A phase manifold with the above metrical properties is known as an almost Kahlerian manifold.[7]

The nonintegrability of the Riemann connection of M_{2m} will give rise to the Riemann curvature tensor

$$R^i_{jkl} = \frac{\partial \Gamma^i_{jk}}{\partial x^l} - \frac{\partial \Gamma^i_{jl}}{\partial x^k} + \Gamma^m_{jl}\Gamma^i_{mk} - \Gamma^m_{jk}\Gamma^i_{ml}, \quad (2.6)$$

which will, however, prevent us from obtaining a group of unitary transformations on such a space since this would require a coordinate system in which $G_{ij} = O_{ij}$ everywhere on a finite domain and hence $R^i_{jkl} = 0$. To remedy this situation, we introduce at each point P of M_{2m} a "tetrad" of $2m$ independent vectors

$$e^A_i = \begin{pmatrix} e^\alpha_i \\ e^{\bar\alpha}_i \end{pmatrix}$$

and their duals

$$e^i_A = \begin{pmatrix} e^i_\alpha \\ e^i_{\bar\alpha} \end{pmatrix},$$

where the duality is defined by either of the equivalent relations:

$$e^A_i e^j_A = \delta^j_i, \quad e^A_i e^i_B = \delta^A_B, \qquad A, B, C, \ldots = 1, \ldots, 2m, \quad (2.7)$$

with

$$e^i_\mu e^\lambda_i = 0, \quad e^i_\mu e^\lambda_i = \delta^\lambda_\mu, \quad e^i_{\bar\mu} e^\lambda_i = 0, \qquad e^i_{\bar\mu} e^{\bar\lambda}_i = \delta^{\bar\lambda}_{\bar\mu}, \quad e^i_\mu e^\mu_j + e^i_{\bar\mu} e^{\bar\mu}_j = \delta^i_j, \quad (2.8)$$

as their equivalent representation.

The $2m$ independent vectors e^A_i, and their duals, then serve to define

$$O_{AB} = e^i_A e^j_B G_{ij}, \quad a_{AB} = e^i_A e^j_B a_{ij}, \quad (2.9)$$

where

$$O_{AB} = \begin{pmatrix} \delta_{\alpha\beta} & 0 \\ 0 & \delta_{\alpha\beta} \end{pmatrix}, \quad a_{AB} = \begin{pmatrix} 0 & \delta_{\alpha\beta} \\ -\delta_{\alpha\beta} & 0 \end{pmatrix} \quad (2.10)$$

are the orthogonal and symplectic metric tensors of the linear tangent space T_{2m} attached to each point P of M_{2m}.

If we consider another "tetrad" at the same point P and put[7]

$$e'^i_A = \gamma^B_A e^i_B, \quad (2.11)$$

then

$$O'_{AB} = \gamma^C_A \gamma^D_B O_{CD}, \quad a'_{AB} = \gamma^C_A \gamma^D_B a_{CD} \quad (2.12)$$

should have again the form (2.11) from which fact we conclude that the matrix γ should be of the form

$$\gamma = \begin{pmatrix} A & -B \\ B & A \end{pmatrix} \quad (2.13)$$

satisfying

$$A^tB - B^tA = 0, \qquad A^tA + B^tB = I. \quad (2.14)$$

This means that γ is a real representation of the unitary transformation.

The complex representation of the above group is obtained, as before, by setting

$$v^i_\alpha = \frac{1}{\sqrt{2}} (e^i_\alpha - ie^i_{\bar\alpha}) \quad (2.15)$$

and applying similarity transformation to γ, i.e.,

$$S^{-1}\gamma S = \begin{pmatrix} U & 0 \\ 0 & \overset{*}{U} \end{pmatrix}, \quad (2.16)$$

where

$$v^i_\alpha v^\beta_i = \delta^\beta_\alpha, \quad v^i_{\overset{*}{\alpha}} v^{\overset{*}{\beta}}_i = \delta^{\overset{*}{\beta}}_{\overset{*}{\alpha}}, \quad v^i_\alpha v^{\overset{*}{\beta}}_i = 0, \qquad v^i_\alpha v^\alpha_j + v^i_{\overset{*}{\alpha}} v^{\overset{*}{\alpha}}_j = \delta^i_j, \quad (2.17)$$

and

$$U = A + iB \quad (2.18)$$

and where the latter matrix is unitary since it obeys the unitarity conditions

$$U^\dagger U = I \quad (2.19)$$

on account of the relations (2.14). The real unitary transformations (2.11) are thus equivalent to

$$v'^i_\lambda = U^\alpha_\lambda v^i_\alpha. \quad (2.20)$$

It now remains to show that the Lie algebra of the above group is spanned by the $\frac{\alpha}{\beta}$-domain of the curvature of $R^\alpha_{\beta ij}$ of the complex tangent-bundle. For this purpose we must apply covariant derivation on the "tetrad" v^i_α. Thus, we obtain

$$\nabla_k v^i_\alpha = (\partial v^i_\alpha / \partial x^K) + \Gamma^i_{jk} v^j_\alpha = w^\beta_{\alpha k} v^i_\beta, \quad (2.21)$$

where $w^\beta_{\alpha k}$ is the connection in the tangent-bundle obeying the following anti-Hermiticity conditions

$$w^\beta_{\alpha k} + w^{\overset{*}{\alpha}}_{\overset{*}{\beta} k} = 0. \quad (2.22)$$

The last relation is a consequence of the fact that

$$\nabla_k \hat{O}_{AB} = \frac{\partial \hat{O}_{AB}}{\partial x^k} + \hat{w}^C_{Ak} \hat{O}_{CB} - \hat{w}^C_{Bk} \hat{O}_{CA} = 0, \quad (2.23)$$

where

$$\hat{O}_{AB} = \begin{pmatrix} 0 & \delta_{\alpha\beta} \\ \delta_{\alpha\beta} & 0 \end{pmatrix}, \quad \hat{w}^B_{Ak} = \begin{pmatrix} w^\beta_{\alpha k} & 0 \\ 0 & w^{\overset{*}{\beta}}_{\overset{*}{\alpha} k} \end{pmatrix}. \quad (2.24)$$

As covariant derivatives do not commute, in general, we have

$$\nabla_l \nabla_k v^i_\alpha - \nabla_k \nabla_l v^i_\alpha = -R^\beta_{\alpha kl} v^i_\beta, \quad (2.25)$$

where

$$R^{\beta}_{\alpha kl} = \frac{\partial w^{\beta}_{\alpha k}}{\partial x^{l}} - \frac{\partial w^{\beta}_{\alpha l}}{\partial x^{k}} + w^{\lambda}_{\alpha k} w^{\beta}_{\lambda l} - w^{\lambda}_{\alpha l} w^{\beta}_{\lambda k} \tag{2.26}$$

is the curvature tensor of the tangent-bundle satisfying

$$R^{\beta}_{\alpha kl} + R^{\overset{*}{\alpha}}_{\overset{*}{\beta} kl} = 0. \tag{2.27}$$

On the other hand, we have by Ricci's identity[8]

$$\nabla_l \nabla_k v^i_\alpha - \nabla_k \nabla_l v^i_\alpha = - R^i_{jkl} v^i_\alpha, \tag{2.28}$$

where R^i_{jkl} is the Riemann curvature tensor of M_{2m}.

Hence

$$R^{\beta}_{\alpha kl} = R^i_{jkl} v^j_\alpha v^\beta_i. \tag{2.29}$$

If we now take a complex tangent vector $\phi^\alpha = v^\alpha_i(\partial/\partial x^i)$ around an infinitesimal loop from a point P of the base space back to itself, we shall arrive at a new tangent vector ϕ'^α related to the old one by the infinitesimal transformation

$$\begin{aligned} \phi'^\alpha &= \phi^\alpha + \delta\phi^\alpha \\ &= \phi^\alpha - \tfrac{1}{2} R^\alpha_{\beta kl} \phi^\beta dx^k \wedge dx^l, \end{aligned} \tag{2.30}$$

where $dx^k \wedge dx^l$ is the oriented surface enclosed by the loop. The above transformation is, in fact, a unitary transformation, i.e.,

$$\begin{aligned} \phi'^\alpha &= (\delta^\alpha_\beta - \tfrac{1}{2} R^\alpha_{\beta kl} dx^k \wedge dx^l)\phi^\beta \\ &= U^\alpha_\beta \phi^\beta \end{aligned} \tag{2.31}$$

on account of the anti-Hermiticity of the curvature (2.27). The set of all such transformations constitutes the holonomy group[9] of M_{2m}, where the ${}^\beta_\alpha$-domain of the curvature $R^\alpha_{\beta kl}$ spans the Lie algebra of this group. Thus there exists a decomposition of the curvature

$$R^\alpha_{\beta kl} = i B^{(a)}_{kl} \hat{F}^\alpha_{(a)\beta}, \tag{2.32}$$

such that $\hat{F}_{(a)}$ are the generators of the group $U(m)$, obeying the bracket operation

$$[\hat{F}_{(a)}, \hat{F}_{(b)}] = i f^{(c)}_{(a)(b)} \hat{F}_c, \tag{2.33}$$

where ${}^\alpha_\beta$-indices have been suppressed.

Substituting the expansion of the curvature in the infinitesimal transformation (2.31), we obtain

$$\phi'^\alpha = (\delta^\alpha_\beta - i\epsilon^{(a)} \hat{F}^\alpha_{(a)\beta})\phi^\beta, \tag{2.34}$$

where

$$\epsilon^{(a)} = \tfrac{1}{2} B^{(a)}_{kl} dx^k \wedge dx^l \tag{2.35}$$

is the infinitesimal element of the holonomy group $U(m)$. The transformation (2.34) has the form of the infinitesimal transformation

$$z'^\alpha = (\delta^\alpha_\beta - i\epsilon^{(a)} \hat{F}^\alpha_{(a)\beta}) z^\beta \tag{2.36}$$

of the flat phase space considered earlier. Indeed, the infinitesimal increment (with $\epsilon^{(a)}$ replaced by $\delta\epsilon^{(a)}$),

$$\delta\phi^\alpha = - i\delta\epsilon^{(a)} \hat{F}^\alpha_{(a)\beta}\phi^\beta \tag{2.37}$$

leads to the equations of motion

$$d\phi^\alpha/d\epsilon = - i\hat{F}^\alpha_\beta \phi^\beta, \tag{2.38}$$

which are of the same form as the equations of a coupled harmonic oscillator

$$dz^\alpha/d\epsilon = - i\hat{F}^\alpha_\beta z^\beta \tag{2.39}$$

of the flat phase space. Moreover, by introducing the generating function

$$F = \hat{F}_{\alpha\beta} \phi^\alpha \overset{*}{\phi}{}^\beta, \tag{2.40}$$

we can see that the equations of motion (2.38) assume the form

$$\frac{d\phi^\alpha}{d\epsilon} = - i \frac{\partial F}{\partial \phi^*_\alpha}, \tag{2.41}$$

which is the same as that of the equations of motion

$$\frac{dz^\alpha}{d\epsilon} = - i \frac{\partial F}{\partial z^*_\alpha} \tag{2.42}$$

of flat phase space.

The above derivation shows that the generating function (2.40) in the curved phase space can play the role of the quadratic generating function of the flat phase space. In this approach the generating function is not introduced as an initial assumption but has been shown to be a manifestation of the underlying geometry. This approach has the additional merit of enabling one to give a geometric description of the gauge fields as fields arising from the Christoffel connection of the curved phase space. In this case the holonomy group is an internal holonomy group of the space–time as it is generated through a displacement of a vector around a loop in the event space, rather than the curved phase space. The details of this viewpoint have been expounded elsewhere.[10]

---

1 H. C. Lee, Am. J. Math. 65, 433 (1943). See also N. Mukunda and E. G. Sudarshan, J. Math. Phys. 9, 411 (1968).

2 E. P. Eisenhart, *Continuous Groups of Transformations* (Dover, New York, 1961), p. 252.

3 In Newtonian Mechanics one usually considers Hamiltonians $H(x,p)$ of the form $H = \frac{1}{2}p^2 + V(x)$, where $V(x)$ is the potential.

4 In general, if H is a Hamiltonian of a specific system, one may consider the "symmetries" of H in the broad sense as the set of F's such that $\{F, H\} = 0$. Then one-parameter groups generated by F can be put to work to find the group generated by H.

[5] The generating function F (or H) has the power series expansion $F = F_1 + F_2 + \cdots$, where F_k is a homogenous polynomial of degree k in the independent variables

$$x^i = \begin{pmatrix} x^\alpha \\ p^\alpha \end{pmatrix}$$

and where in particular we have

$$F_1 = F_i x^i, \quad F_2 = F_{ij} x^i x^j.$$

[6] H. Weyl, *The Classical Groups and their Invariant Representations* (Princeton U. P., Princeton, N. J., 1939).
[7] K. Yano, *Differential Geometry on Complex and Almost Complex Spaces* (Pergamon, New York, 1965).
[8] E. P. Eisenhart, Am. Math. Soc. Coll. Pub. 8, 12 (1927).
[9] J. A. Schouten, *Ricci Calculus* (Springer-Verlag, Berlin, 1954), 2nd ed., p. 375.
[10] S. Heskia, Nuovo Cimento 3A, 625 (1971).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Correlation Length in a Nonequilibrium Gas

Y. Pomeau
Laboratoire de Physique des Plasmas, Faculté des Sciences, 91-Orsay-France
(Received 20 October 1970)

We demonstrate on a gas model that, if three-body events are neglected, the nonequilibrium correlations extend over a distance proportional to the relaxation time of the one-body distribution function. For homogeneous perturbations this correlation length is the mean free path, the relaxation time being the mean free flight time. In the hydrodynamical limit both the relaxation time of nonhomogeneous perturbations and the correlation length become infinite. This resolves the apparent contradistinction between the recent claim of a finite correlation length for nonequilibrium (but homogeneous) gases and the occurrence of correlations with an infinite range leading to divergences in the virial expansion of transport coefficients which precisely describe hydrodynamical perturbations.

1. INTRODUCTION

The question of the range of the correlations in nonequilibrium gases plays a crucial role in the problem of the virial expansion of transport coefficients.[1] In fact, the divergences occurring in this expansion are closely connected to the correlations with an inifinite range appearing at the Boltzmann approximation,[2] namely, when three-body events are not accounted for. This last point, which is more or less implicit in the previous reference,[2] will be wholly confirmed here (Sec. 5). Henceforth, the recent discovery[3] of correlation functions with a *finite* range in a modeled kinetic theory of gases may appear as being in contradistinction with the results found in the search of a virial expansion for the collision operator.

In fact the nonequilibrium correlations with an infinite range appear when one assumes, after Bogoliubov,[4] a "synchronization" between the one- and two-body distribution functions, the two-body distribution functions being calculated by considering the one-body distribution function as stationary, although a nonequilibrium distribution function is certainly *non*stationary in the absence of any constant external source of disturbance, as usually assumed. And it is not surprising that the correlation with an infinite range may be removed by dropping this synchronization assumption, and by solving simultaneously the equations relating the one- and two-body distribution functions in the low density limit. This has been done[5] for particular models, and correlations with a finite range have actually appeared.

However, it may be emphasized that, in these works,[3,5] the range of the nonequilibrium correlations appears to be roughly proportional to the relaxation time of the one-body distribution function, when three-body events are neglected. This can be understood as follows: When one neglects three-body events and makes the stosszahlansatz, two particles which collide become correlated *after* the collision in a nonequilibrium gas and remain indefinitely correlated after this collision if the effect of the other particles is neglected. In this way[6] binary collisions constitutes in a nonequilibrium system a "source" of correlations located at $|\mathbf{r}_1 - \mathbf{r}_2| \sim r_0 (r_0 =$ range of the intermolecular forces). If three-body collisions are not accounted for, there is no "sink" for these nonequilibrium correlations which, once they have been created at a relative distance r_0, propagate freely among the rectilinear free motion. That explains why, in this approximation (with no three-body events), the undamped peak of correlation corresponds to a relative distance increasing as $|\mathbf{v}_1 - \mathbf{v}_2| t$, the spatial width of this peak being of order $|\mathbf{v}_1 - \mathbf{v}_2| t_r$, t_r being the relaxation time of the system: In fact, the "source" of correlation has a lifetime t_r, since it disappears when the equilibrium state is reached. Calling "correlation length" the spatial width of the peak of maximum correlation, this correlation length is proportional to the relaxation time of the system. Hence, the existence of correlations with an infinite range is connected with the infinite relaxation times which may appear in nonequilibrium phenomena. When the nonequilibrium state is homogeneous, namely, when the one-body distribution function does not depend on the position, the gas reaches an equilibrium state with a finite time rate, of order of the mean free flight time, so that the assumption of synchronization is incorrect for correlation range of order or larger than the mean free path. On the contrary, when one studies the relaxation of a perturbed one-body distribution function which depends on the position, e.g., as $e^{i\mathbf{k}\cdot\mathbf{r}}$, one finds in the hy-

[5] The generating function F (or H) has the power series expansion $F = F_1 + F_2 + \cdots$, where F_k is a homogenous polynomial of degree k in the independent variables

$$x^i = \binom{x^\alpha}{p^\alpha}$$

and where in particular we have

$$F_1 = F_i x^i, \quad F_2 = F_{ij} x^i x^j.$$

[6] H. Weyl, *The Classical Groups and their Invariant Representations* (Princeton U.P., Princeton, N.J., 1939).
[7] K. Yano, *Differential Geometry on Complex and Almost Complex Spaces* (Pergamon, New York, 1965).
[8] E. P. Eisenhart, Am. Math. Soc. Coll. Pub. 8, 12 (1927).
[9] J. A. Schouten, *Ricci Calculus* (Springer-Verlag, Berlin, 1954), 2nd ed., p. 375.
[10] S. Heskia, Nuovo Cimento 3A, 625 (1971).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Correlation Length in a Nonequilibrium Gas

Y. Pomeau
Laboratoire de Physique des Plasmas, Faculté des Sciences, 91-Orsay-France
(Received 20 October 1970)

We demonstrate on a gas model that, if three-body events are neglected, the nonequilibrium correlations extend over a distance proportional to the relaxation time of the one-body distribution function. For homogeneous perturbations this correlation length is the mean free path, the relaxation time being the mean free flight time. In the hydrodynamical limit both the relaxation time of nonhomogeneous perturbations and the correlation length become infinite. This resolves the apparent contradistinction between the recent claim of a finite correlation length for nonequilibrium (but homogeneous) gases and the occurrence of correlations with an infinite range leading to divergences in the virial expansion of transport coefficients which precisely describe hydrodynamical perturbations.

1. INTRODUCTION

The question of the range of the correlations in nonequilibrium gases plays a crucial role in the problem of the virial expansion of transport coefficients.[1] In fact, the divergences occurring in this expansion are closely connected to the correlations with an inifinite range appearing at the Boltzmann approximation,[2] namely, when three-body events are not accounted for. This last point, which is more or less implicit in the previous reference,[2] will be wholly confirmed here (Sec. 5). Henceforth, the recent discovery[3] of correlation functions with a *finite* range in a modeled kinetic theory of gases may appear as being in contradistinction with the results found in the search of a virial expansion for the collision operator.

In fact the nonequilibrium correlations with an infinite range appear when one assumes, after Bogoliubov,[4] a "synchronization" between the one- and two-body distribution functions, the two-body distribution functions being calculated by considering the one-body distribution function as stationary, although a nonequilibrium distribution function is certainly *non*stationary in the absence of any constant external source of disturbance, as usually assumed. And it is not surprising that the correlation with an infinite range may be removed by dropping this synchronization assumption, and by solving simultaneously the equations relating the one- and two-body distribution functions in the low density limit. This has been done[5] for particular models, and correlations with a finite range have actually appeared.

However, it may be emphasized that, in these works,[3,5] the range of the nonequilibrium correlations appears to be roughly proportional to the relaxation time of the one-body distribution function, when three-body events are neglected. This can be understood as follows: When one neglects three-body events and makes the stosszahlansatz, two particles which collide become correlated *after* the collision in a nonequilibrium gas and remain indefinitely correlated after this collision if the effect of the other particles is neglected. In this way[6] binary collisions constitutes in a nonequilibrium system a "source" of correlations located at $|\mathbf{r}_1 - \mathbf{r}_2| \sim r_0 (r_0 =$ range of the intermolecular forces). If three-body collisions are not accounted for, there is no "sink" for these nonequilibrium correlations which, once they have been created at a relative distance r_0, propagate freely among the rectilinear free motion. That explains why, in this approximation (with no three-body events), the undamped peak of correlation corresponds to a relative distance increasing as $|\mathbf{v}_1 - \mathbf{v}_2| t$, the spatial width of this peak being of order $|\mathbf{v}_1 - \mathbf{v}_2| t_r$, t_r being the relaxation time of the system: In fact, the "source" of correlation has a lifetime t_r, since it disappears when the equilibrium state is reached. Calling "correlation length" the spatial width of the peak of maximum correlation, this correlation length is proportional to the relaxation time of the system. Hence, the existence of correlations with an infinite range is connected with the infinite relaxation times which may appear in nonequilibrium phenomena. When the nonequilibrium state is homogeneous, namely, when the one-body distribution function does not depend on the position, the gas reaches an equilibrium state with a finite time rate, of order of the mean free flight time, so that the assumption of synchronization is incorrect for correlation range of order or larger than the mean free path. On the contrary, when one studies the relaxation of a perturbed one-body distribution function which depends on the position, e.g., as $e^{i\mathbf{k}\cdot\mathbf{r}}$, one finds in the hydrodynamical limit ($k \to 0$) some relaxation processes whose time rate goes to infinity as k^{-2}. And in this hydrodynamical limit, the assumption of synchronization can be considered as valid, since the one-body distribution function is stationary with an accuracy as great as desired. This remark is of a crucial importance for the study of the transport coefficients, since it can be easily seen[7] that one is dealing with a nonequilibrium *hydrodynamical* state when one tries to obtain these transport coefficients by means of the Chapman-Enskog method. Hence the synchronization assumption is convenient for this case.

The aim of this paper is twofold: first, the preceding statements about the range of correlations at the Boltzmann order are verified on a gas model both for a homogeneous and a hydrodynamic nonequilibrium state; it is shown further that the divergences of the virial expansion of the collision operator may be considered as originating from the correlations with an infinite range appearing at the Boltzmann order.

Two features of the studied model render it very suitable for this study:

(1) The interaction law is of the "hard-core" type, so that, at the Boltzmann approximation, the collision operator is exactly Markovian and no "synchronization" assumption is needed to derive the collision operator in the low density limit;

(2) The correlation function may be readily deduced from the one-body distribution function. Further, in order to minimize difficulties usually encountered by solving the complete Boltzmann equation, we have chosen one of the simplest model of gas; the Lorentz gas of light particles colliding with fixed hard spheres. This model has been the subject of detailed investigations[8]; the transport equation may be solved for perturbation varying in space as $e^{i\mathbf{k}\cdot\mathbf{r}}$, and this solution joins the usual diffusion solution decaying as e^{-k^2Dt} in the hydrodynamic limit $k \to 0$. The Boltzmann equation of this model will be given in Sec. 2, and it will be explained how to deduce the correlation function from the one-body distribution functions when three-body events are neglected.

In Sec. 3, it will be shown that, for homogeneous perturbations, the correlation length is actually finite of the order of mean free path.

In Sec. 4, the Boltzmann equation is solved for a perturbed one-body distribution function varying in space as $e^{i\mathbf{k}\cdot\mathbf{r}}$, and it will be shown that, in the limit $k \to 0$, the perturbation decreases at $t \to \infty$ as e^{-Dk^2t}, yielding nonequilibrium correlation with an infinite range.

In Sec. 5, we shall relate the divergences appearing in the virial expansion of the collision operator and the infinite range of the Boltzmann order correlations, which actually exists in nonhydrodynamic nonequilibrium states, as shown in Sec. 4. For that purpose we shall use a recent derivation[2] of the Ring collision operator, this collision operator being the sum of the most diverging terms appearing at each order in the virial expansion of the collision operator. In particular, we shall be able to express in a closed form this collision operator from the Boltzmann order correlation function. Studying further the density expansion of this collision operator, we shall find a divergence at the order n^3 which is removed when an upper bound for the range of the Boltzmann order correlations is arbitrarily introduced.

In the conclusion, we examine briefly the problem of the actual existence of these infinite-range correlations, and the question whether the introduction of three- and many-body events do really cut the nonequilibrium correlation at a microscopic distance.

2. KINETIC THEORY OF A LORENTZ GAS OF HARD SPHERES

In this section, it will be shown that for a Lorentz gas of hard spheres, the one-body distribution function (or distribution function of a light particle) is given by the solution of a self-consistent Markovian equation; furthermore, the correlation function will be given as an explicit function of the distribution function of a light particle.

Let us consider a system of light particles moving in an array of N stationary and identical hard spheres of radius r_0. The positions of the hard spheres are distributed at random, and there is no mutual interaction between the spheres. Let $\mathbf{R}_i$ and $\mathbf{R}_j$ be the positions of the centers of two hard spheres (we do not exclude the possibility of an "overlapping" situation with $|\mathbf{R}_i - \mathbf{R}_j| < 2r_0$). Furthermore, we assume that there is no mutual interaction between the light particles, which are of zero extension. Let $\mathbf{R}_1, \ldots, \mathbf{R}_N$ be the positions of the hard spheres, and $\mathbf{r}$ and $\mathbf{v}$ the position and the velocity of a light particle. The Liouville equation for this system of $(N+1)$ particles, deduced by slightly modifying the Liouville equation for a system of identical hard spheres[9] is

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}} + \sum_{i=1}^{N} \kappa_i\right) D = 0, \qquad (2.1)$$

where D is the Gibbs distribution function in phase space of the light particle and the hard spheres, D being a function of $\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \ldots, \mathbf{R}_N$ and t, κ_i is a singular operator which acts on D as

$$\begin{aligned}\kappa_i D(\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \ldots, \mathbf{R}_N | t) &= (\mathbf{u}\cdot\mathbf{v})\delta(\mathbf{r} - \mathbf{R}_i + r_0\mathbf{u}) D(\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \ldots, \mathbf{R}_N | t) \\ &\quad - (\mathbf{u}\cdot\mathbf{v})\delta(\mathbf{r} - \mathbf{R}_i - r_0\mathbf{u}) D(\mathbf{r}, \mathbf{v}^*; \mathbf{R}_1, \ldots, \mathbf{R}_N | t).\end{aligned} \qquad (2.2)$$

In (2.2):

$$u = \frac{\mathbf{r} - \mathbf{R}_i}{|\mathbf{r} - \mathbf{R}_i|},$$
$$\mathbf{v}^* = -\mathbf{v}\left(1 - \frac{2b^2}{r_0^2}\right) + \frac{2\mathbf{b}}{r_0} v \left(1 - \frac{b^2}{r_0^2}\right)^{1/2}, \tag{2.3}$$

b being the impact parameter:

$$\mathbf{b} = r_0 \mathbf{u} - \frac{\mathbf{u}\cdot\mathbf{v}}{v^2}\mathbf{v}. \tag{2.4}$$

Since (2.1) is a Liouville equation, D is normalized at any time by

$$\int d\mathbf{r} \int d\mathbf{v} \int d\mathbf{R}_1, \ldots, \int d\mathbf{R}_N D(t=0) = 1.$$

We shall furthermore suppose that D is a symmetrical function of $\mathbf{R}_1, \ldots, \mathbf{R}_N$. In order to avoid nonphysical situations in which a light particle would lie at time $t = 0$ inside a hard sphere, we suppose that at $t = 0$ any light particle lies outside any hard sphere, that is

$$D(\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \ldots, \mathbf{R}_N \,|\, t = 0) = 0, \tag{2.5}$$

if there exists a label $i (1 \le i \le N)$ such as

$$|\mathbf{r} - \mathbf{R}_i| < r_0.$$

Solving the Liouville Eq. (2.1) by the method of trajectories, we find at once that at any time $t \ge 0$, the exclusion condition (2.6) remains fulfilled. Let us now define the j-body distribution function f_j as

$$f_j(\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \ldots, \mathbf{R}_{j-1} | t) = \left(\frac{\Omega}{N}\right)^{j-1} \frac{N!}{(N-j+1)!} \int d\mathbf{R}_{j+1}, \ldots, \int d\mathbf{R}_N D, \tag{2.6}$$

Ω being the volume of the box containing the system.

The equations of the BBGKY hierarchy yield for the lowest orders:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right) f_1(\mathbf{r}, \mathbf{v} | t) = nv \int d\mathbf{b} \{ f_2(\mathbf{r}, \mathbf{v}^*; \mathbf{r} + r_0 \mathbf{u} | t) - f_2(\mathbf{r}, \mathbf{v}; r - r_0 \mathbf{u} | t) \}, \tag{2.7}$$

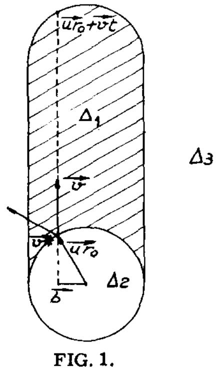

FIG. 1.

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}} + \kappa_1\right) f_2(\mathbf{r}, \mathbf{v}; \mathbf{R}_1 | t) = nv \int d\mathbf{b} \{ f_3(\mathbf{r}, \mathbf{v}^*; \mathbf{R}_1, \mathbf{r} + r_0 \mathbf{u} | t) - f_3(\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \mathbf{r} - r_0 \mathbf{u} | t) \}, \tag{2.8}$$

where the integration on the right-hand side of (2.7) and (2.8) extends over the impact parameter **b**, a vector limited to a circle of radius r_0 in the plane perpendicular to **v**; n is the number density of hard spheres ($n = N/\Omega$), **u** is the function of **v** and **b** defined in

$$r_0 \mathbf{u} = \mathbf{b} + (\mathbf{v}/v)(r_0^2 - b^2)^{1/2},$$

and $\mathbf{v}^*$ is the function of **b** and **v** defined in Eq. (2.3).

The system of Eqs. (2.7) and (2.8) is open, since the function f_3 cannot yet be calculated from f_1 and f_2.

However, in the low density limit, one may derive (see Appendix A) from (2.7) and (2.8) a Boltzmann equation for f_1 which is Markovian. Let us point out that this can be done without recourse to some synchronization assumption, and by assuming that at $t = 0$, the only correlations present in the gas stem from the exclusion condition (2.5). This Boltzmann kinetic equation reads for $t \ge 0$:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right) f_1(\mathbf{r}, \mathbf{v} | t) = nv \int d\mathbf{b} [f_1(\mathbf{r}, \mathbf{v}^* | t) - f_1(\mathbf{r}, \mathbf{v} | t)]. \tag{2.9}$$

Furthermore, in the same approximation, the correlation function $g(\mathbf{r}, \mathbf{v}; \mathbf{R} | t)$ defined by

$$g(\mathbf{r}, \mathbf{v}; \mathbf{R} | t) = f_2(\mathbf{r}, \mathbf{v}; \mathbf{R} | t) - f_1(\mathbf{r}, \mathbf{v} | t), \tag{2.10a}$$

may be deduced from f_1 in a rather simple way (see Appendix A). This correlation function at the Boltzmann order g_B is a linear functional of f_1, the form of which depends on the domain of phase space $(\mathbf{r}, \mathbf{v}; \mathbf{R})$ in which g_B takes its value. This functional can be described as follows:

(i) Let us consider the domain Δ_1 (shaded region in Fig. 1) defined by

$$\mathbf{v}\cdot\mathbf{u} \ge 0 \tag{2.10b}$$

and

$$r_0 \mathbf{u}\cdot\mathbf{v} \le \mathbf{v}\cdot(\mathbf{r} - \mathbf{R}) \le r_0 \mathbf{u}\cdot\mathbf{v} + v^2 t, \tag{2.10c}$$

u being any vector of the sphere of unit radius.

To any point of Δ_1, there correspond two vectors **u** and **b** and a time τ such as

$$\mathbf{b} = \mathbf{r} - \mathbf{R} - \frac{\mathbf{v}\cdot(\mathbf{r} - \mathbf{R})}{v^2}\mathbf{v}, \qquad b^2 \le r_0^2, \tag{2.11}$$

$$r_0 \mathbf{u} = \mathbf{b} + \frac{\mathbf{v}}{v}(r_0^2 - b^2)^{1/2}, \tag{2.12}$$

$$\tau = \frac{\mathbf{v}\cdot(\mathbf{r}-\mathbf{R})}{v^2} - \frac{\mathbf{u}\cdot\mathbf{v}}{v^2} r_0. \tag{2.13}$$

In $\blacktriangle_1$ the value of g_B reads:

$$g_B(\mathbf{r},\mathbf{v};\mathbf{R}\,|\,t) = f_1(\mathbf{r}-\mathbf{v}\tau, \mathbf{v}^*\,|\,t-\tau) - f_1(\mathbf{r}-\mathbf{v}\tau,\mathbf{v}\,|\,t-\tau). \tag{2.14}$$

(ii) In the domain $\blacktriangle_2$ defined by $|\mathbf{r}-\mathbf{R}| < r_0$, g is determined by the exclusion condition which yields at any order in the density

$$g(\mathbf{r},\mathbf{v};\mathbf{R}\,|\,t) = -f_1(\mathbf{r},\mathbf{v}\,|\,t). \tag{2.15}$$

(iii) In the domain $\blacktriangle_3$, which is the complement of $\blacktriangle_1 \cup \blacktriangle_2$ in phase space $(\mathbf{r},\mathbf{v};\mathbf{R})$:

$$g_B(\mathbf{r},\mathbf{v};\mathbf{R}\,|\,t) = 0. \tag{2.16}$$

To summarize, we have in the low density limit, a single Eq. (2.9) for f_1 which is both *self-consistent* and *Markovian*. The form of this equation depends on the value of f_1 and of its first derivatives at only one specified time. This equation has been derived without any recourse to a "time-scaling." Because of the simple properties of this model, we shall be able to derive, in Sec 3, the exact expressions for f_1 and g_B for both homogeneous perturbations (independent of $\mathbf{r}$) and inhomogeneous perturbations (dependent of $\mathbf{r}$).

3. HOMOGENEOUS PERTURBATIONS IN THE LORENTZ GAS OF HARD SPHERES

We have demonstrated in Sec 2 that for this model, f_1 is determined by the solution of Eq. (2.9) and that once f_1 is known, the value of g_B can be calculated from (2.14), (2.15), and (2.16).

As it is well known, the classical scattering by a hard sphere is isotropic,[10] and (2.9) may be written as

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}} + n\pi r_0^2 v\right) f_1(\mathbf{r},\mathbf{v}\,|\,t) = \tfrac{1}{4} n v r_0^2 \int d\hat{v} f_1(\mathbf{r},\mathbf{v}\,|\,t). \tag{3.1}$$

On the right-hand side of (3.1), the integral extends over the surface of the unit sphere, since

$$\hat{v} = \mathbf{v}/v.$$

To simplify (3.1), one may notice that in the course of time, the modulus of the velocity of a light particle is constant, thus one may restrict oneself to a system in which this modulus has only one value, say v_0. In this case, $f_1(\mathbf{r},\mathbf{v}\,|\,t)$ may be written as

$$f_1(\mathbf{r},\mathbf{v}\,|\,t) = (1/v_0^2)\delta(v-v_0)\hat{f}_1(\mathbf{r},\hat{v}\,|\,t). \tag{3.2}$$

Putting now $\nu = \pi n r_0^2 v_0$, Eq. (3.1) yields

$$\left(\frac{\partial}{\partial t} + v_0\hat{v}\cdot\frac{\partial}{\partial \mathbf{r}} + \nu\right)\hat{f}_1(\mathbf{r},\mathbf{v}\,|\,t) = \frac{\nu}{4\pi}\int d\hat{v}\hat{f}_1(\mathbf{r},\hat{v}\,|\,t). \tag{3.3}$$

Let us consider an homogeneous nonequilibrium state, namely, a function $\hat{f}_1$ which does not depend on $\mathbf{r}$. The solution of (3.3) is elementary for this case, and reads:

$$\hat{f}_1(\hat{v}\,|\,t) = [\hat{f}_1(\hat{v}\,|\,t=0) - (1/4\pi)\int d\hat{v}\hat{f}_1(\hat{v}\,|\,t=0)]e^{-\nu t} + (1/4\pi)\int d\hat{v}\hat{f}_1(\hat{v}\,|\,t=0). \tag{3.4}$$

The corresponding value of g_B has various forms, depending on the domain of phase space in which g_B takes its value;

$$\text{in } \blacktriangle_3, \quad g_B = 0, \tag{3.5a}$$

$$\text{in } \blacktriangle_2, \quad g_B = -(1/v_0^2)\delta(v-v_0)\hat{f}_1(\hat{v}\,|\,t). \tag{3.5b}$$

The range of the correlations is obviously r_0 in the domains $\blacktriangle_2$ and $\blacktriangle_3$.

In $\blacktriangle_1$, the value of g is obtained from (2.20) and (3.4) and reads

$$g_B = [f_1(\mathbf{v}^*\,|\,t=0) - f_1(\mathbf{v}\,|\,t=0)] \times \exp\left[\nu\left(t + \frac{(r_0^2-b^2)^{1/2}}{v_0} - \frac{\hat{v}\cdot(\mathbf{r}-\mathbf{R})}{v_0}\right)\right] \tag{3.6}$$

Let us recall that from the definition of $\blacktriangle_1$

$$0 \le t + \frac{(r_0^2-b^2)^{1/2}}{v_0} - \frac{\hat{v}\cdot(\mathbf{r}-\mathbf{R})}{v_0} \le t. \tag{3.7}$$

For given values of $\mathbf{b}$ and $\hat{v}$, the function on the right-hand side of (3.6) has an undamped peak when

$$\hat{v}\cdot(\mathbf{r}-\mathbf{R}) = v_0 t - (r_0^2-b^2)^{1/2}$$

or, equivalently, when $t=\tau$.

This maximum of g is given by

$$g_B(t=\tau) = f_1(\mathbf{v}^*\,|\,t=0) - f_1(\mathbf{v}\,|\,t=0).$$

The spatial width of this peak is $v_0\nu^{-1}$ for large values of t, as it can be checked at once from (3.6).

One recovers the behavior of g_B which has been already found: g_B has an undamped maximum, with a spatial width of the order of the mean free path, and this peak is located at a separation distance increasing as $v_0 t$.

However it is clear from (2.14) and (3.6), that the width of the maximum of g_B strongly depends on the relaxation time of f_1. This time is ν^{-1} for homogeneous perturbations, but for a perturbation which depends on $\mathbf{r}$, another relaxation time appears, which is as large as desired, and the above conclusions about the range of the correlations must be seriously revised.

4. INHOMOGENEOUS PERTURBATIONS IN THE GAS MODEL

This section is devoted to the study of f_1 and g_B in the case of a perturbation of f_1 varying in space like $e^{i\mathbf{k}\cdot\mathbf{r}}$. We shall assume again that the modulus of the velocity of the light particles takes only one value, v_0. Since the function $\hat{f}_1(\mathbf{r}, \hat{v}\,|\,t)$ defined in (3.2) will depend on $\mathbf{r}$ like $e^{i\mathbf{k}\cdot\mathbf{r}}$, one defines $f_{\mathbf{k}}(\hat{v}\,|\,t)$ by

$$\hat{f}_1(\mathbf{r}, \hat{v}\,|\,t) = f_{\mathbf{k}}(\hat{v}\,|\,t)e^{i\mathbf{k}\cdot\mathbf{r}}. \qquad (4.1)$$

Furthermore, let us put $\mu = \mathbf{k}\cdot\hat{v}/k$ and call ϕ the angle of $\hat{v}$ in the plane perpendicular to $\mathbf{k}$. The function $f_{\mathbf{k}}(\hat{v}\,|\,t)$ depends on ϕ and μ, and may be split as

$$f_{\mathbf{k}}(\hat{v}\,|\,t) = \psi(\mu; t) + \Phi(\phi, \mu; t), \qquad (4.2)$$

where

$$\psi(\mu; t) = (1/2\pi)\int_0^{2\pi} d\phi f_{\mathbf{k}}(\hat{v}\,|\,t).$$

This splitting allows us to deduce from Eq. (3.3) two uncoupled equations for Φ and ψ, the solution of the first one being straightforward. These equations read:

$$\left(\frac{\partial}{\partial t} + iK\mu + \nu\right)\Phi(\hat{v}; t) = 0, \qquad (4.3)$$

$$\left(\frac{\partial}{\partial t} + iK\mu + \nu\right)\psi(\mu; t) = \frac{\nu}{2}\int_{-1}^{+1} d\mu\,\psi(\mu; t), \qquad (4.4)$$

where $K = kv_0$, and where the integral $\int d\hat{v}\cdots$ occurring in (3.3) has been written $\int_0^{2\pi} d\phi \int_{-1}^{+1} d\mu\cdots$.

From (4.4)

$$\Phi(\hat{v}; t) = e^{-(\nu+iK\mu)t}\Phi(\hat{v}; t=0). \qquad (4.5)$$

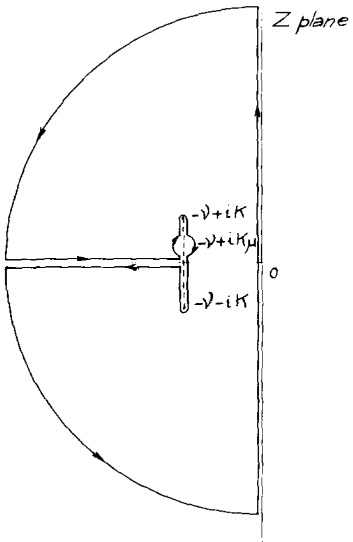

FIG. 2.

This solution has the main feature encountered in the study of homogeneous perturbations: It is damped as $e^{-\nu t}$, and the range of the corresponding correlation function is the mean free path.

But the situation is quite different for what concerns $\psi(\mu; t)$. Laplace transformed Eq. (4.4) reads

$$(z + \nu + iK\mu)\psi(\mu; z) = \tfrac{1}{2}\nu\int_{-1}^{+1} d\mu\,\psi(\mu; z) + \psi_0(\mu), \qquad (4.6)$$

where $\psi_0(\mu) = \psi(\mu; t=0)$ and

$$\psi(\mu; z) = \int_0^\infty dt\, e^{zt}\psi(\mu; t).$$

The choice of $\psi_0(\mu)$ is submitted to some restrictions, as shown in the Appendix B.

Let us define $\rho(z)$ by

$$\rho(z) = \int_{-1}^{+1} d\mu\,\psi(\mu; z). \qquad (4.7)$$

From (4.6)

$$\rho(z) = \frac{\Lambda_{\psi_0}(z)}{1 - \frac{1}{2}\nu\Lambda(z)}, \qquad (4.8)$$

where Λ_{ψ_0} is the linear functional of ψ_0 defined by

$$\Lambda_{\psi_0}(z) = \int_{-1}^{+1} \frac{d\mu'\,\psi_0(\mu')}{z + \nu + iK\mu'}, \qquad (4.9)$$

and where

$$\Lambda(z) = \Lambda_{\psi_0=1}(z) = \frac{1}{iK}\ln\left(\frac{z + \nu + iK}{z + \nu - iK}\right). \qquad (4.10)$$

Equations (4.9) and (4.10) define two functions of z, Λ, and Λ_{ψ_0}, with a cut in the z plane; this cut being the segment defined by $z = -(\nu + iK\mu_0)$, $-1 \le \mu_0$ real $\le +1$.

Inverting the Laplace transformation, we have from (4.6)

$$\psi(\mu; t) = e^{-(\nu+iK\mu)t}\psi_0(\mu) + \psi'(\mu; t), \qquad (4.11)$$

with

$$\psi'(\mu; t) = \frac{\nu}{2}\int_{-i\infty}^{+i\infty}\frac{dz}{2i\pi}e^{zt}\frac{\rho(z)}{z + \nu + iK\mu}. \qquad (4.12)$$

In order to calculate $\psi'(\mu; t)$ from (4.12), one performs the following contour integral:

$$\psi_p'(\mu; t) = \frac{\nu}{2}\int_C \frac{dz}{2i\pi}e^{zt}\frac{\rho(z)}{z + \nu + iK\mu}. \qquad (4.13)$$

The contour (C) excludes the cut of the function $\rho(z)$, and includes the imaginary axis (Fig. 2). From (4.8) the poles of $\rho(z)$ are either the poles of $\Lambda_{\psi_0}(z)$ or the roots of the equation

$$1 - \tfrac{1}{2}\nu\,\Lambda(z) = 0. \qquad (4.14)$$

It is shown in Appendix B that the poles of $\Lambda_{\psi_0}(z)$ are certainly located on the cut; thus they do not contribute to ψ_p, and the only poles of the integrant of (4.15) located inside (C) are the roots of (4.16).

From (4.10), $\Lambda(z)$ is real for real values of z, thus (4.14) may have root for z real only. From (4.10),

$$\Lambda(x) = \frac{2}{\kappa} \arctan \frac{K}{x+\nu} \text{ for x real.} \quad (4.15)$$

Thus $-\pi/K \leq \Lambda(\mathbf{x}) \leq +\pi/K$ (x real) and (4.14) has one root, and only one,

$$x_0 = -\nu + K \tan K/\nu, \quad (4.16)$$

for $K \leq \frac{1}{2}\nu\pi$; if $K > \frac{1}{2}\nu\pi$, Eq. (4.14) has no root.

Since $x_0(K = \frac{1}{2}\nu\pi) = -\nu$, at $K = -\frac{1}{2}\nu\pi$ the root x_0 is located on the cut; we shall not study this particular case and proceed from now on with $K < \frac{1}{2}\nu\pi$. In this domain of values of K

$$\psi_p'(\mu; t) = \frac{K^2}{\nu} \frac{\csc^2 K/\nu}{(x_0 + \nu + iK\mu_0)} e^{x_0 t} \Lambda_{\psi_0}(x_0). \quad (4.17)$$

Since $x_0(K=0)=0$, this contribution to ψ corresponds to a weakly damped mode in the hydrodynamic limit ($K \to 0$). This mode is simply the usual diffusion mode, and it will lead ultimately to correlations with an infinite length, as explained above.

However, before proceeding, we must deduce $\psi'(\mu; t)$ from the contour integral ψ_p'. This can be done by cutting out from ψ_p' the contribution of the cut. We shall not give the details of calculation and only furnish the result

$$\psi_p'(\mu; t) = \psi'(\mu; t) - \psi_c'(\mu; t), \quad (4.18)$$

where $\psi_c'(\mu; t)$ is the contribution of the cut to ψ_P' which is given by

$$\psi_c'(\mu; t) = -\frac{\nu}{4} e^{-(\nu + iK\mu)t}[\rho_-(\mu) + \rho_+(\mu)] - \frac{i}{4\pi} e^{-\nu t} P \int_{-1}^{+1} \frac{d\mu'}{\mu' - \mu} e^{-iK\mu' t}[\rho_-(\mu') - \rho_+(\mu')], \quad (4.19)$$

where P means "Cauchy principal part."

The two functions $\rho_\pm(\mu)$ occurring in (4.19) are two functions of a real variable $-1 \leq \mu \leq +1$ defined from $\rho(z)$ by

$$\rho_\pm(\mu) = \lim_{\epsilon \to 0_+} \rho(-(\nu + i\kappa\mu) \pm \epsilon). \quad (4.20)$$

These functions $\rho_\pm$ can be explicited without difficulty, but these expressions are unimportant for what follows.

From (4.19) it is obvious that $\psi_c'(\mu; t)$ is damped as $e^{-\nu t}$ for large values of t, so that any contribution to $f_{\mathbf{k}}(\hat{v}|t)$ is damped like $e^{-\nu t}$, except for that contribution arising from the pole x_0 which is damped as $e^{x_0 t}$[$x_0 \leq 0$ from (4.16)].

Now we are able to calculate the correlation function g which exists in this inhomogeneous perturbation. As it has been viewed in Sec. 3, the characteristic range of the correlation is the mean free path when the one-body distribution function is damped like $e^{-\nu t}$. This result remains true for the contribution to $f_{\mathbf{k}}(\hat{v}|t)$ damped like $e^{-\nu t}$, as one may ensure from Eqs. (2.14)-(2.16) which define g_B as a function of f_1. Thus the only difference in the correlation length which may exist, between the homogeneous perturbations and the inhomogeneous one, proceeds from the part of g_B linear in the contribution ψ_p' damped like $e^{x_0 t}$. Let $g_{B,p}$ be that contribution to g_B proportional to ψ_p'. From (2.15) and (2.16) the range of $g_{B,p}$ is r_0 in the domains of values of ($\mathbf{r}, \mathbf{v}; \mathbf{R}$) $\blacktriangle_2$ and $\blacktriangle_3$. In the domain $\blacktriangle_1$ of this phase space, g_B is given by (2.14) and, from (3.2) and (4.1),

$$g_B(\mathbf{r}, \mathbf{v}; \mathbf{R}|t) = v_0^{-2}\delta(v - v_0)\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}\tau)}[f_{\mathbf{k}}(\hat{v}^*|t-\tau) - f_{\mathbf{k}}(\hat{v}|t-\tau)], \quad (4.21)$$

where $\hat{v}^* = v^*/v_0$ and where τ is defined in (2.13).

The contribution to $f_{\mathbf{k}}(\hat{v}|t)$ damped like $e^{x_0 t}$ is calculated from Eqs. (4.2), (4.12), (4.17), and (4.18), and yields

$$f_{\mathbf{k}}(\hat{v}|t) = \frac{K^2 \csc^2(K/\nu) e^{x_0 t}}{2(x_0 + \nu + iK\mu)} \int_0^{2\pi} d\phi \int_{-1}^{+1} \frac{d\mu' f_{\mathbf{k}}(\hat{v}|t=0)}{x_0 + \nu + ik'} + (\text{terms damped like } e^{-\nu t}). \quad (4.22)$$

Inserting into (4.21) the first term on the right-hand side of (4.22), and taking the limit $K \to 0$, one obtains for $g_{B,p}$

$$g_{B,p}(\mathbf{r}, \mathbf{v}; \mathbf{R}|t) \underset{K\to 0}{\approx} \frac{iK}{\nu} e^{-(K^2/3\nu)(t-\tau)} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}\tau)} \times (\mu - \mu^*) v_0^{-2}\delta(v - v_0) \int d\hat{v} f_{\mathbf{k}}(\hat{v}|t=0), \quad (4.23)$$

where $\mu^* = \mathbf{k}\cdot\mathbf{v}^*/kv_0$.

Now, by inspection of (4.23) and from the definition (2.13) of τ, it can be easily seen that the correlation function $g_{B,p}$ has an undamped oscillating maximum for a separation distance along $\mathbf{v}$ such as $t = \tau$; the spatial width of this maximum being $3\nu v_0/k^2$ and its amplitude of order K near $K = 0$.

Calling again the width of the maximum of g_B the "correlation length," one concludes that in the limit $K \to 0$, correlations appear with an infinite range. That is precisely what has been announced in the introduction: In the hydrodynamical limit there exist relaxation processes with a time rate of order k^{-2}, and during these relaxation processes correlations appear with a very long range, if three-body collisions are neglected.

5. LONG-RANGE CORRELATIONS AND DIVERGENCES OF THE KINETIC THEORY

In this section we shall show that the divergences occurring in the virial expansion of the collision operator are closely connected to the correlations with an infinite range which appear at the Boltzmann order in a nonequilibrium gas. In fact, we have seen that we are allowed to suppose that f_1 takes a constant nonequilibrium value when we are dealing in a hydrodynamic nonequilibrium state for which the relaxation time and the scale of inhomogeneity are as large as desired. Considering the value of g_B given in Eq. (2.14), it is obvious from the definition of τ that if f_1 does not depend on space and time, (actually f_1 depends on $\mathbf{r}$ and t, but *as slowly as desired* in the hydrodynamic limit) then g_B has a nonzero value in the region Δ_1 which extends up to infinity in the hydrodynamic limit.

We shall now examine the consequences of the existence of this long-range correlation on the virial expansion of the two-body correlation, and of the collision term in the kinetic equation for f_1. More precisely we shall show that, if we introduce an arbitrary cut for the range of the correlation function g_B, we remove the first divergence which appear in the virial expansion of the collision term. This proof will need an explicit connection between g_B and the virial expansion of the collision operator. By means of a method which has been recently explained,[2] we are able to express the "Ring collision term" from g_B; this Ring collision term including precisely the most divergent terms which appear at each order in the virial expansion of the collision term. We shall only give a brief outline of this method with a view to its application in the present model.

First of all, the right-hand side of the second equation of the BBGKY hierarchy, written in (2.8), is replaced by a sort of collision term leading to a self-consistent system relating f_2 and f_1. In the present model, this equation for f_2 is obtained by putting into the right-hand side of (2.8) the following value for f_3:

$$f_3(\mathbf{r},\mathbf{v};\mathbf{R}_1,\mathbf{R}_2)=f_1(\mathbf{r},\mathbf{v})\phi_1(\mathbf{R}_1)\phi_1(\mathbf{R}_2) + g(\mathbf{r},\mathbf{v};\mathbf{R}_1)\,\phi(\mathbf{R}_2)+g(\mathbf{r},\mathbf{v};\mathbf{R}_2)\phi_1(\mathbf{R}_2), \tag{5.1}$$

g being the above-defined correlation function, and $\phi_1(\mathbf{R}_j)$ the one-body distribution function for hard spheres. Due to the normalizations chosen here and to the homogeneity of the array of hard spheres:

$$\phi_1(\mathbf{R})=1. \tag{5.2}$$

Dealing as in Appendix A, we may deduce the following set of differential equations and of boundary conditions relating g and f_1:

$$\left(\frac{\partial}{\partial t}+\nu\right)\hat{f}_1(\hat{v}\,|\,t)-\frac{\nu}{4\pi}\int d\hat{v}\hat{f}_1(\hat{v}\,|\,t) =\frac{\nu}{4\pi}\int d\hat{v}[\hat{g}(\hat{v}^*;r_0\mathbf{u}\,|\,t)-\hat{g}(\hat{v};\,-r_0\mathbf{u}\,|\,t)], \tag{5.3a}$$

$$\left(\frac{\partial}{\partial t}+v_0\hat{v}\cdot\frac{\partial}{\partial\boldsymbol{\beta}}+\nu\right)\hat{g}(\hat{v},\boldsymbol{\beta}\,|\,t)=\frac{\nu}{4\pi}\int d\hat{v}\hat{g}(\hat{v},\boldsymbol{\beta}\,|\,t), \tag{5.3b}$$

and

$$\hat{g}(\hat{v},r_0\mathbf{u})=\hat{f}_1(\hat{v}^*)+\hat{g}(\hat{v},{}^*r_0\mathbf{u}) \tag{5.3c}$$

for

$$|\mathbf{u}|=1 \quad\text{and}\quad \mathbf{v}\cdot\mathbf{u}\geq 0.$$

In order to write (5.3), we have supposed that the velocity of the light particle has a well-defined value v_0, so that f_1 and g depend on $\mathbf{v}$ only through $\hat{v}=\mathbf{v}/v_0$. Furthermore we have written (5.3a) and (5.3b) as if the system were homogeneous, so that $\hat{f}_1$ does not depend on $\mathbf{r}$, and $\hat{g}$ only depends on $\hat{v}$ and on the mutual distance $\boldsymbol{\beta}$ between the light particle and the center of the fixed scatterer. However, we have in mind a nonequilibrium hydrodynamic situation, in which $\hat{f}_1$ depends very slowly on $\mathbf{r}$ and t: But to simplify the formalism we have dropped this dependence of $\hat{f}_1$ on $\mathbf{r}$. Let us examine briefly the connection between this assumption and the existence of a transport theory deduced from (5.3).

By assuming that $\hat{f}_1$ takes a stationary nonequilibrium value, we shall derive from (5.3b) a synchroneous value for $\hat{g}$, which is the asymptotic solution of (5.3b), $\hat{f}_1$ being held constant.

Inserting this synchroneous value of $\hat{g}$ into (5.3a) we shall obtain a Markovian collision operator which reads

$$\frac{\partial\hat{f}_1(t)}{\partial t}=S[\hat{v}_1\,|\,\hat{f}_1(t)], \tag{5.4}$$

S being a linear function of $\hat{f}_1$ which only depends on the value of $\hat{f}_1$ at time t. When we want to study an inhomogeneous hydrodynamic state, we cannot rule out the dependence on $\mathbf{r}$ and (5.4) becomes

$$\frac{\partial\hat{f}_1}{\partial t}+v_0\hat{v}\cdot\frac{\partial\hat{f}_1}{\partial\mathbf{r}}=S[\hat{v}_1\,|\,\hat{f}_1(t,\mathbf{r})], \tag{5.5}$$

S being in (5.5) the *same functional* as in (5.4). The recourse to this synchronous functional is legitimate, since in the hydrodynamic limit the $(\mathbf{r},t)$ dependence of $\hat{f}_1$ is as slow as desired, and since the nonlocal effects which could be accounted for through a nonlocal collision operator have a finite, microscopic scale of length and time. Furthermore, the existence of this local functional is needed, if one wants to derive from the kinetic equation a transport theory in the usual sense, which would lead to local transport coefficients in the hydrodynamic limit. However, as it has been recently shown[2] there are strong indications in favor of the nonexistence of this local collision operator in two-dimensional mono-atomic gases.

We have studied in Sec. 4 the low density limit of S, namely the Boltzmann collision operator. Furthermore, even in the approximation corresponding to the system (5.3a), we are not able to derive an explicit collision operator. In fact we only need the collision operator which includes the most diverging terms of the density expansion, or Ring collision operator.

Since [from (2.16)] $\hat{g}_B$ is equal to zero in the region $\blacktriangle_3$ of phase space, and since the right-hand side of (5.3a) involves precisely the value of $\hat{g}$ in $\blacktriangle_3$, the corresponding contribution of $\hat{g}_B$ is equal to zero. But the Ring correlation function $\hat{g}_r$ is not *a priori* equal to zero in $\blacktriangle_3$ and yields a nonvanishing contribution when inserted into (5.3a).

Let us solve now (5.6). For that purpose we use the Fourier transform of $\hat{g}_B$ which reads from (2.14)-(2.16)

$$\hat{g}_B(\mathbf{k}, \hat{v}) = \int_{\boldsymbol{\beta},\mathbf{v}\in\blacktriangle_1} d\beta e^{-i\mathbf{k}\cdot\boldsymbol{\beta}}\{f_1(\hat{v}^*) - f_1(\hat{v})\} - \int_{|\boldsymbol{\beta}|\leq r_0} d\beta e^{-i\mathbf{k}\cdot\boldsymbol{\beta}}\hat{f}_1(\hat{v}). \quad (5.6)$$

The domain $\blacktriangle_1$ occurring in (5.6) depends on t: However, as we are looking for a Markovian kinetic operator, we need the value of the correlation function for $t = \infty$, $\hat{f}_1$ itself being considered as stationary. As it merges clearly from (2.13) and (2.14), this asymptotic value of $\hat{g}_B$ is constant in the infinite domain $\blacktriangle_1$ for a given value of $\hat{v}$ and $\mathbf{b}$: Hence the Fourier transform of this function must be considered in the sense of the distributions, and is singular at $k = 0$. This singularity will play a major role in the occurrence of the divergences of the virial expansion; this singularity may be artificially removed as follows: Let us assume that

$$\text{if } \tau(\boldsymbol{\beta}, \mathbf{v}) \geq \theta, \quad \text{then } \hat{g}_B(\boldsymbol{\beta}, \hat{v}) = 0, \quad (5.7)$$

θ being some fixed, positive time.

It may be easily seen from (2.11) and (2.12)(recall that $\boldsymbol{\beta} = \mathbf{r} - \mathbf{R}$) that the assumption (5.7) yields a correlation function $\hat{g}_B(\boldsymbol{\beta}, \hat{v})$ which vanishes for $|\boldsymbol{\beta}| \geq v_0\theta + r_0$. Define as $\hat{g}_{B,\theta}(\boldsymbol{\beta}, \hat{v})$ the correlation function at the Boltzmann order which is equal to the asymptotic value of $\hat{g}_B$ deduced from (2.14)-(2.16) except, that for $\hat{g}_B$ the domain $\blacktriangle_3$ is restricted by the arbitrary condition (5.7); the true asymptotic value of $\hat{g}_B$ being obviously $\hat{g}_{B,\theta=\infty}$. From (5.6) the Fourier transform of $\hat{g}_{B,\theta}$ is given by

$$\hat{g}_{B,\theta}(\mathbf{k}, \hat{v}) = -v_0 \frac{e^{-i\mathbf{k}\cdot\mathbf{v}\theta} - 1}{i\mathbf{k}\cdot\mathbf{v}} \int d\mathbf{b} e^{-i\mathbf{k}\cdot\mathbf{u}r_0}[f_1(\hat{v}^*) - f_1(\hat{v})]. \quad (5.8)$$

In order to go from (5.6) to (5.8), we have neglected the last term on the right-hand side of (5.6) which is well behaved at $k = 0$ and does not yield any trouble in the terms of order n^2 and n^3 of the density expansion of the Ring collision term; in fact, we shall deal with divergences of the term of order n^3 in this expansion.

Solving now (5.3) in Fourier transform, with the initial value $\hat{g}_R(\beta, \hat{v}\,|\,t = 0) = 0$, we obtain for the asymptotic value of $\hat{g}_{R,\theta}$, $\hat{g}_{B,\theta}$ being held constant:

$$\hat{g}_{R,\theta}(\mathbf{k}, \hat{v}) = \frac{\nu}{\nu + i\mathbf{k}\cdot\mathbf{v}} \frac{1 + \nu/2\lambda(k)}{1 - \nu/2\lambda(k)} \frac{1}{4\pi} \int d\hat{v}\hat{g}_{B,\theta}(\mathbf{k}, \hat{v}) - \frac{\nu}{\nu + i\mathbf{k}\cdot\mathbf{v}} \frac{1}{1 - \nu/2\lambda(k)} \lambda(k\,|\,\hat{g}_{B,\theta}) + \frac{\nu}{\nu + i\mathbf{k}\cdot\mathbf{v}} \hat{g}_{B,\theta}(\mathbf{k}, \hat{v}). \quad (5.9)$$

To derive (5.9) we have used the method outlined at the beginning of Sec. 4, and we have put

$$\lambda(k) \equiv \Lambda(z = 0), \quad (5.10a)$$

$\Lambda(z)$ being defined in (4.10) and

$$\lambda(k\,|\,\hat{g}_{B,\theta}) \equiv \frac{1}{2\pi} \int \frac{d\hat{v}\hat{g}_{B,\theta}(\mathbf{k}, \hat{v})}{\nu + i\mathbf{k}\cdot\hat{v}v_0}. \quad (5.10b)$$

The Ring collision term is obtained by inserting into the right-hand side of (5.2a) the value of $\hat{g}_{B,\theta}$ deduced from (5.9). Further it can be seen that, since $\hat{g}_{B,\theta}(\mathbf{k}, \hat{v})$ is the Fourier transform of a function which is null in Δ_3, then $\nu\hat{g}_{B,\theta}(\mathbf{k}, \hat{v})/(\nu + i\mathbf{k}\cdot\mathbf{v})$ is the Fourier transform of a function which is null too in $\blacktriangle_3$. Hence the last term on the right-hand side of (5.9) does not contribute to the Ring collision term, as being null in $\blacktriangle_3$, and this Ring collision term reads:

$$S_{R,\theta}(\hat{v}\,|\,\hat{f}_1) = \nu^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{1 - \frac{1}{2}\nu\lambda(k)} \left[\left(1 + \frac{\nu}{2}\lambda(k)\right)\frac{1}{4\pi} \times \int d\hat{v}\hat{g}_{B,\theta}(\mathbf{k}, \hat{v}) - \frac{\nu}{2}\lambda(k\,|\,g_{B,\theta})\right] \times \int d\hat{v} e^{i\mathbf{k}\cdot\mathbf{u}r_0}\left(\frac{1}{\nu + i\mathbf{k}\cdot\mathbf{v}^*} - \frac{1}{\nu + i\mathbf{k}\cdot\mathbf{v}}\right). \quad (5.11)$$

Starting from this expression of the Ring collision term, which accounts for the arbitrary cut limiting the range of the correlation function $g_{B,\theta}$, we shall examine the following statements: The integral over $\mathbf{k}$ defining $S_{R,\theta}$ converges at $k = 0$ for any finite value of θ, and for $\theta = \infty$ the same result holds for the term of order n^2 in the density expansions of $S_{R,\theta}$ and $S_{R,\theta=\infty}$: But the term of order n^3 in this density expansion yields a diverging integral for $S_{R,\theta=\infty}$ while this divergence does not appear when θ remains finite.

A. Definition and Density Expansion of $S_{R,\,\theta=\infty}$

The expression of $S_{R,\theta=\infty}$ is obtained by putting into (5.9) the value of $\hat{g}_{B,\theta=\infty}$ deduced from (5.6):

$$g_{B,\theta=\infty}(\mathbf{k}, \hat{v}) = 2\pi v_0 \delta(\mathbf{k}\cdot\mathbf{v}) \int d\mathbf{b} e^{-i\mathbf{k}\cdot\mathbf{b}r_0}[\hat{f}_1(\hat{v}^*) - \hat{f}_1(\hat{v})]. \quad (5.12)$$

Since near $k = 0$, $\hat{g}_{B,\theta=\infty}(\mathbf{k}, \hat{v}) \sim k^{-1}$ and since from (4.15) and (5.10a), $1 - \frac{1}{2}\nu\lambda(k) \sim k^{-2}$, as $k \to 0$, it may be readily seen that the whole integrand on the right-hand side of (5.11) is of order k^{-2} near $k = 0$, when $\theta = \infty$; and the integral converges at $k = 0$ when multiplied by the volume element expressed in spherical coordinates k^2dk.

Let us consider now the lowest-order term in the virial expansion of $S_{R,\theta=\infty}$. It is calculated by expanding the integrand in powers of n for any finite value of k (recall that $\nu \propto n$) and reads:

$$S_{R,\theta=\infty}(\hat{v}\,|\,\hat{f}_1) \underset{n\to 0}{\simeq} 2\pi\nu^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \int d\hat{v} e^{i\mathbf{k}\cdot\mathbf{n}r_0} \times \left(\frac{1}{i\mathbf{k}\cdot\mathbf{v}^*} - \frac{1}{i\mathbf{k}\cdot\mathbf{v}}\right) \frac{1}{4\pi} \int d\hat{v}\hat{g}_{B,\theta=\infty}(\mathbf{k}, \hat{v}). \quad (5.13)$$

This collision term is again defined by an integral which converges at $k = 0$, since the integrand is of order k^{-2} at $k = 0$.

There are many terms of order n^3 in the virial expansion of $S_{R,\theta}$, and we shall consider only one term among them, since our object is not an exhaustive study of the divergences of the virial expansion of $S_{R,\theta}$. For example, from the density expansion of

$$\frac{1}{\nu + i\mathbf{k}\cdot\mathbf{v}^*} - \frac{1}{\nu + i\mathbf{k}\cdot\mathbf{v}}$$

a term rather similar to the contribution of order n^2 arises, except that the factor

$$\left(\frac{1}{i\mathbf{k}\cdot\mathbf{v}^*} - \frac{1}{i\mathbf{k}\cdot\mathbf{v}}\right)$$

occurring in the right-hand side of (5.13) is to be replaced by

$$-\nu\left[\frac{1}{(i\mathbf{k}\cdot\mathbf{v}^*)^2} - \frac{1}{(i\mathbf{k}\cdot\mathbf{v})^2}\right],$$

and the corresponding integrant is of order $k = 0$ [k^{-2} due to $(\mathbf{k}\cdot\mathbf{v})^{-2}$ multiplied by k^{-1} due to $\hat{g}_{B,\theta=\infty}(\mathbf{k}, \hat{v})$], and the integral diverges logarithmically near $k = 0$.

B. Definition and Density Expansion of $S_{R,\theta}$ at Finite θ

The integrand defining $S_{R,\theta}$ depends linearly on $\hat{g}_{B,\theta}$. It may be seen further from (5.8) and (5.12) that $\hat{g}_{B,\theta=\infty}(v,\mathbf{k}) \sim k^{-1}$ as $k \to 0$, while $\hat{g}_{B,\theta}(\hat{v}, k)$ remains finite at $k = 0$. More precisely, $\hat{g}_{B,\theta}(\hat{v}, \mathbf{k} = 0) \propto \theta$. Henceforth, if the integrand of $S_{R,\theta=\infty}$ or a term in its density expansion has been found to be of order $k^{-\alpha}$ near $k = 0$, the corresponding quantity in $S_{R,\theta}$ is of order $k^{-\alpha+1}$ near $k = 0$. In this way, one merely deduces that the integrand of $S_{R,\theta}$ is of order k^{-1} near $k = 0$, that its lowest-order term in the virial expansion, of order n^2, behaves as k^{-1} near $k = 0$, and that its term of order n^3 behaves as k^{-2} near $k = 0$ yielding a convergent contribution of order n^3 in the virial expansion $S_{R,\theta}$, while the contribution of the same order in n diverges for $S_{R,\theta=\infty}$.

Now the connection between the long-range behavior of g_B and the divergences of the virial expansion of $S_{R,\theta=\infty}$ has been established.

6. CONCLUSION

We have shown that, in a nonequilibrium gas, the occurrence of long-range correlations is *not* due to some incorrect assumption about the "synchronization" between f_1 and g, and that these long-range correlations exist in the hydrodynamic perturbations ($k \to 0$). We have shown further that the divergences appearing in the virial expansion of the collision operator are closely connected with the correlation with an infinite range appearing at the Boltzmann order. The Ring collision operator [its particular form valid for this model is given in (5.11)] has been constructed in order to eliminate these divergences. In fact, it accounts for the "most dangerous divergences."

In two (and three) dimensions this renormalized virial expansion is free of divergences[2,11] for the perfect Lorentz gas, at least for the lowest orders in n. The infinite correlation length appearing in the powers virial expansion are cut at the mean free path by the introduction of these three-body effects, even when the synchronization between f_1 and g is assumed. But the situation is much more complicated for two-dimensional gases with one species of particles, and it has been shown[2,6] that by accounting for three-body events as explained above, one finds a renormalized density expansion with divergences.

Hence, in this last case the synchronization assumption between g_R and $\hat{f}_1$ must be removed. But it must be pointed out that, even in this case, the relaxation time for $\hat{f}_1$ can be taken as long as desired in the hydrodynamic limit.

APPENDIX A

We shall derive in this appendix the Boltzmann equation for f_1 and the corresponding value of the correlation function g_B. For that purpose we shall replace in (2.8), f_3 by its low density value f_3^{LD} which yields:

$$f_3^{LD}(\mathbf{r}, \mathbf{v}; \mathbf{R}_1, \mathbf{r} - r_0\mathbf{u} \,|\, t) = f_1(\mathbf{r}, \mathbf{v} \,|\, t)\phi(\mathbf{R}_1)\phi(\mathbf{r} - r_0\mathbf{u}), \tag{A1}$$

$\mathbf{u}$ being an unit vector such as $\mathbf{v}\cdot\mathbf{u} \le 0$, and $\phi(\mathbf{R}_j)$ being the one-body distribution function of the hard spheres. Due to the normalization used here, and to the homogeneity of the system of hard spheres:

$$\phi(\mathbf{R}_j) = 1. \tag{A2}$$

The condition (A1) expresses that, in the low density limit, the binary correlations arise from the *direct* interaction between particles only, and that any effect of the surrounding particles on this correlation is of a lowest order in n: in fact it may be shown[2] that, under this assumption for f_3, f_2 is correctly described in the low density limit.

Inserting the value (A1) of f_3 into (2.8) and replacing the singular term $\kappa_1 f_2$ by a boundary condition, we obtain

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right)f_2 = nv\int d\mathbf{b}\{f_1(\mathbf{r}, \mathbf{v}^* \,|\, t) - f_1(\mathbf{r}, \mathbf{v} \,|\, t) \tag{A3a}$$

for $|\mathbf{r} - \mathbf{R}| > r_0$,

$$f_2(\mathbf{r}, \mathbf{v}; \mathbf{r} + r_0\mathbf{u} \,|\, t) = f_2(\mathbf{r}, \mathbf{v}^*; \mathbf{r} + r_0\mathbf{u} \,|\, t) \tag{A3b}$$

for $|\mathbf{u}| = 1$ and $\mathbf{v}\cdot\mathbf{u} \ge 0$,

$$f_2(\mathbf{r}, \mathbf{v}; \mathbf{R}|t) = 0 \tag{A3c}$$

for $|\mathbf{r}-\mathbf{R}| < r_0$.

Condition (A3b) is obtained by integrating (2.8) over a small volume element across the surface $|\mathbf{r}-\mathbf{R}| = r_0$, and (A3c) stems from the exclusion condition (2.5). Conditions (A3b) and (A3c) are valid even outside the low density limit.

Now the problem is how to derive from (2.7) and (A3) the Boltzmann equation for f_1 and compute the corresponding value for f_2. For that purpose we shall make the stosszahlansatz. In fact, we shall only need an "initial" stosszahlansatz, taking as an initial condition for f_2,

$$f_2(\mathbf{r}, \mathbf{v}; \mathbf{R}|t=0) = 0 \quad \text{for } |\mathbf{r}-\mathbf{R}| < r_0, \tag{A4a}$$

$$f_2(\mathbf{r}, \mathbf{v}; \mathbf{R}|t=0) = f_1(\mathbf{r}, \mathbf{v}|t=0) \quad \text{for } |\mathbf{r}-\mathbf{R}| > r_0, \tag{A4b}$$

$$f_2(\mathbf{r}, \mathbf{v}; \mathbf{r}-r_0\mathbf{u}|t=0) = f_1(\mathbf{r}, \mathbf{v}|t=0) \quad \text{for } \mathbf{u}^2 = 1, \tag{A4c}$$

and $\mathbf{v}\cdot\mathbf{u} \le 0$ and

$$f_2(\mathbf{r}, \mathbf{v}; \mathbf{r}-r_0\mathbf{u}|t=0) = f_1(\mathbf{r}, \mathbf{v}^*|t=0) \quad \text{for } \mathbf{u}^2 = 1, \tag{A4d}$$

and $\mathbf{v}\cdot\mathbf{u} > 0$.

To proceed, we shall suppose that, *a priori*, (A4c) which is valid at $t=0$ remains true at any time $t > 0$. Partially solving the system relating f_1 and f_2, we shall prove *a posteriori* that this condition (A4c) remains fulfilled at any time $t > 0$.

Defining now the correlation function g by

$$g(\mathbf{r}, \mathbf{v}; \mathbf{R}|t) = f_2(\mathbf{r}, \mathbf{v}; \mathbf{R}|t) - f_1(\mathbf{r}, \mathbf{v}; \mathbf{R}|t), \tag{A5}$$

one shows at once from (A3a) and from the stosszahlansatz for f_2 that g is given at the Boltzmann order by the solution of

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right) g_B(\mathbf{r}, \mathbf{v}; \mathbf{R}|t) = 0, \tag{A6}$$

provided that $|\mathbf{r}-\mathbf{R}| > r_0$. The correlation function g_B is equally defined by an initial condition deduced from (A4a) and (A4b), plus a boundary condition deduced from the stosszahlansatz, namely, from the assumption that (A4c) is valid at any time $t \ge 0$. Integrating now (A6) by the method of the trajectories, one shows that, the stosszahlansatz (A4c) is actually true at any time $t \ge 0$, and that in the regions of phase space $(\mathbf{r}, \mathbf{v}; \mathbf{R})$ called $\blacktriangle_1, \blacktriangle_2$, and $\blacktriangle_3$, g is actually given by (2.14)–(2.16).

Further, since (A4c) is true at any time $t \ge 0$, (2.9) follows at once from (2.7).

APPENDIX B

In this appendix, it is shown that $\Lambda_{\psi_0}(z)$ is finite for any value of z located outside the cut $z = -(\nu + iK\mu)(-1 \le \mu \text{ real} \le +1)$.

For that purpose one notices that the perturbation f_1 of the one-body distribution function must check:

$$f_1(\mathbf{r}, \hat{v}|t) + \hat{f}_{1,0} \ge 0, \tag{B1}$$

$\hat{f}_{1,0}$ being the equilibrium value of the distribution function of the light particles, a constant here. The condition (B1) expresses simply the fact that the whole distribution function $\hat{f}_1 + \hat{f}_{1,0}$ must be positive definite, as usual for a probability distribution.

In Sec. 4, for simplicity, one has used a perturbation $e^{i\mathbf{k}\cdot\mathbf{r}}$ instead of $\cos\mathbf{k}\cdot\mathbf{r}$. In order to obtain from the results of this section the true physical quantities, one must add at any place the complex conjugate, an imaginary distribution function being meaningless. Thus the function $f_{\mathbf{k}}(\hat{v}|t)$ defined in (4.1) must be real, and verifies, from (4.1), by replacing $e^{i\mathbf{k}\cdot\mathbf{r}}$ by $(e^{i\mathbf{k}\cdot\mathbf{r}} + e^{-i\mathbf{k}\cdot\mathbf{r}})$:

$$+ f_{1,0} \ge f_{\mathbf{k}}(\hat{v}|t) \ge -f_{1,0}. \tag{B2}$$

Integrating (B2) over the angle ϕ and taking $t = 0$,

$$\hat{f}_{1,0} \le \psi_0(\mu) \ge -\hat{f}_{1,0}. \tag{B3}$$

And the function $\Lambda_{\psi_0}(z)$ defined by

$$\Lambda_{\psi_0}(z) = \int_{-1}^{+1} \frac{d\mu'\psi_0(\mu')}{z + \nu + iK\mu'}$$

is obviously finite for any value of z outside the cut.

---

[1] E. G. D. Cohen, *Fundamental Problems in Statistical Mechanics* (North-Holland, Amsterdam, 1968) Vol. II.

[2] Y. Pomeau, Thesis, University of Orsay; Phys. Rev. A **3**, 1174 (1971).

[3] A. H. Kritz, G. V. Ramanathan, and G. Sandri, Phys. Letters **31A**, 477 (1970); **25**, 437 (1970).

[4] Bogoliubov, *Studies in Statistical Mechanics* (North-Holland Amsterdam, 1962), Vol. I.

[5] G. V. Ramanathan and G. Sandri, J. Math. Phys. **10**, 1763 (1969).

[6] Y. Pomeau, Phys. Letters **27A**, 601 (1968).

[7] G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics* (American Mathematical Society, Providence, R. I., 1963).

[8] *Transport Theory*, 20 th Symposium in Applied Math (N.Y., 1967) (American Mathematical Society, Providence, R.I., 1969), Vol. I.

[9] J. J. Hopfield and J. F. Bastin, Phys. Rev. **168**, 193 (1968).

[10] L. Landau and E. Lifshitz, *Mécanique*, Ed. de la Paix (Moscow, 1962).

[11] J. M. J. Van Leeuwen and A. Weigland, Physica **36**, 457 (1967); **38**, 35 (1968).

Variational Field Theory*

Weston M. Stacey, Jr.
Applied Physics Division, Argonne National Laboratory, Argonne, Illinois 60439
(Received 14 June 1971)

Equations which define a "consistent" set of "boundary" conditions, and hence a field, for a given set of differential equations are derived from a variational principle. The equivalence of functionals defined over an entire domain and functionals defined over only a subdomain, but with a surface term added to account for the contribution of the excluded subdomain, is exploited. The appropriate surface term is found to satisfy the Hamilton–Jacobi equation. The formalism is specialized to neutron diffusion theory, and it is demonstrated that Stark's double sweep method follows as a natural consequence of this field theoretic formulation. The relation of this formalism to Pontryagin's Maximum Principle and Bellman's Dynamic Programming is demonstrated for problems which can be characterized by minimum variational principles.

1. INTRODUCTION

Many problems in mathematical physics are specified by a set of differential equations defined on an interval $0 \leqslant x \leqslant L$ and an associated set of boundary conditions at $x = 0$ and $x = L$. It is well known that if one is interested in the solution only over some subinterval $0 \leqslant x \leqslant z < L$, and if the "boundary" conditions can be specified at $x = z$, it suffices to solve the equations only within the interval $0 \leqslant x \leqslant z$. The use of symmetry considerations to provide "boundary" conditions at a midplane is a familiar example.

If consistent "boundary" conditions could be specified at each point in the interval $0 \leqslant x \leqslant L$, functions which satisfied these "boundary" conditions would, by definition, satisfy the original set of differential equations and the original boundary conditions at $x = 0$ and $X = L$. Such consistent "boundary" conditions may be thought of as a field for the original set of differential equations.[1]

The purposes of this paper are to derive a consistent set of "boundary" conditions (i.e., field equations) from a variational argument and to introduce a field theoretic formulation for neutron diffusion theory. It is demonstrated that Stark's[2] method for solving the neutron diffusion equations, which is widely used in one-dimensional problems, is a natural consequence of this field theoretic formulation.[3]

2. VARIATIONAL FIELD THEORY

It is well known from the calculus of variations[1] that a variational functional can be associated with a set of differential equations and associated boundary conditions. For example, the functional

$$J[y] = \int_0^L dx\, F[x, y(x), y'(x)] \tag{1}$$

defined on the set of functions $y_j(x)$ ($y \equiv \sum_{j=1}^N y_j$ in the argument), which have continuous first derivatives[4] in $0 \leqslant x \leqslant L$ and satisfy prescribed conditions at $x = 0$ and $x = L$, is stationary (i.e., $\delta J = 0$) about the functions $\bar{y}_j(x)$ which satisfy

$$\frac{\partial F}{\partial y_j} - \frac{d}{dx}\left(\frac{\partial F}{\partial y_j'}\right) = 0, \quad 0 \leqslant x \leqslant L, \quad j = 1, \ldots, N, \tag{2}$$

and the prescribed conditions at $x = 0$ and $x = L$. (Prime indicates the total derivative with respect to the independent variable, x in this case.)

If the appropriate boundary conditions can be specified at some point $x = z < L$, the same functions $\bar{y}_j(x)$ can be determined by solving Eqs. (2) on the interval $0 \leqslant x \leqslant z$, subject to the prescribed conditions at $x = 0$ and $x = z$. The determination of these boundary conditions is accomplished by seeking a functional

$$\hat{J}[y] = \int_0^z dx\, F[x, y(x), y'(x)] - G[z, y(z)], \tag{3}$$

which is equivalent to the functional J in the sense that $\hat{J}$ is also stationary about the functions $\bar{y}_j(x)$ which satisfy Eqs. (2) on the interval $0 \leqslant x \leqslant L$ and the prescribed conditions at $x = 0$ and $x = L$. Thus, we seek to replace a variational functional defined on the interval $0 \leqslant x \leqslant L$ with a functional defined on the interval $0 \leqslant x \leqslant z$, which has a surface term to account for the contribution of the complementary interval $z < x \leqslant L$.

The surface term G is determined from the requirement that $\delta\hat{J} = 0$ for the functions $\bar{y}_j(x)$ which satisfy Eqs. (2). The general formula for the variation of $\hat{J}$ is[5]

$$\delta\hat{J} = \int_0^z \sum_{j=1}^N \left[\frac{\partial F}{\partial y_j} - \frac{d}{dx}\left(\frac{\partial F}{\partial y_j'}\right)\right] \delta y_j\, dx + \sum_{j=1}^N \left(\frac{\partial F}{\partial y_j'} - \frac{\partial G}{\partial y_j}\right) \delta y_j \Big|_{x=z} + \left(F - \sum_{j=1}^N y_j' \frac{\partial F}{\partial y_j'} - \frac{\partial G}{\partial x}\right) \delta x \Big|_{x=z}. \tag{4}$$

The requirement $\delta\hat{J} = 0$ is satisfied if

$$\frac{\partial F}{\partial y_j'} = \frac{\partial G}{\partial y_j}, \quad j = 1, \ldots, N \tag{5}$$

and

$$\frac{\partial G}{\partial z} - F + \sum_{j=1}^N y_j' \frac{\partial F}{\partial y_j'} = 0. \tag{6}$$

Using Eqs. (5), Eq. (6) becomes

$$\frac{\partial G[z, y(z)]}{\partial z} - F[z, y(z), y'(z)]$$

$$+\sum_{j=1}^{N} y_j'(z)\,\frac{\partial G[z, y(z)]}{\partial y_j} = 0, \tag{7}$$

where y_j' is assumed to be given in terms of y_j and $\partial G/\partial y_j$ by Eqs. (5). Defining

$$H\left(z, y(z), \frac{\partial G[z, y(z)]}{\partial y(z)}\right) \equiv -F[z, y(z), y'(z)]$$
$$+\sum_{j=1}^{N} y_j'(z)\,\frac{\partial G[z, y(z)]}{\partial y_j}, \tag{8}$$

Eq. (7) becomes

$$\frac{\partial G}{\partial z} + H = 0, \tag{9}$$

which is the Hamilton–Jacobi equation.[6]

If Eqs. (5) and (6) are satisfied, the second and third terms in Eq. (4) vanish. It is now shown that Eqs. (5) and (7) being satisfied is sufficient to ensure that Eqs. (2) are satisfied, and hence that $\delta\hat{J} = 0$. By virtue of Eqs. (5)

$$\frac{d}{dx}\left(\frac{\partial F}{\partial y_j'}\right) = \frac{d}{dx}\left(\frac{\partial G}{\partial y_j}\right) = \frac{\partial^2 G}{\partial x \partial y_j} + \sum_{i=1}^{N} \frac{\partial^2 G}{\partial y_i \partial y_j}\, y_i'$$
$$= \frac{\partial}{\partial y_j}\left(\frac{\partial G}{\partial x} + \sum_{i=1}^{N} y_i' \frac{\partial G}{\partial y_i}\right), \qquad j = 1, \ldots, N.$$

Using Eq. (7), this reduces to

$$\frac{d}{dx}\left(\frac{\partial F}{\partial y_j'}\right) = \frac{\partial F}{\partial y_j}, \qquad j = 1, \ldots, N,$$

which are Eqs. (2).

A boundary condition for G follows from the requirement that J and $\hat{J}$ are equivalent for all z, $0 \le z \le L$, and particularly for $z = L$:

$$G[L, y(L)] = 0. \tag{10}$$

Thus, functions $\bar{y}_j$ which satisfy Eqs. (5) and (7) or (9) also satisfy Eqs. (2). In this sense, Eqs. (5) are referred to as the field equations corresponding to the variational functional of Eq. (1). Equations (5) suggest that G has the form of a field potential.

The equivalence of J and $\hat{J}$ at $z = 0$ implies

$$-G[0, y(0)] = J[y] = \int_0^L dx\; F[x, y(x), y'(x)].$$

Consequently, the stationary value of the variational functional of Eq. (1) can be obtained by solving Eqs. (5) and (7) for $G[0, y(0)]$.

3. MONOENERGETIC NEUTRON DIFFUSION THEORY

The general results of the preceeding section can readily be specialized to one-dimensional monoenergetic neutron diffusion theory. In this case, the function F, which is sometimes referred to as the Lagrangian density function, is

$$F(x, \phi, \phi') = D(\phi')^2 + (\Sigma_a - \nu\Sigma_f)\phi^2 - 2\phi S, \tag{11}$$

where D, Σ_a, ν, Σ_f, and S are the diffusion coefficient, absorption cross section, neutron yield per fission, fission cross section, and source, respectively. ϕ is the neutron flux.

For F given by Eq. (11), Eqs. (2) reduce to the familiar neutron diffusion equation

$$-(D\phi')' + (\Sigma_a - \nu\Sigma_f)\phi = S, \tag{12}$$

and the field equations, Eqs. (5), reduce to

$$2D\phi' = \frac{\partial G}{\partial \phi}. \tag{13}$$

The Hamilton–Jacobi equation, Eq. (7) or (9), becomes

$$\frac{\partial G}{\partial z} + \frac{1}{4D}\left(\frac{\partial G}{\partial \phi}\right)^2 - (\Sigma_a - \nu\Sigma_f)\phi^2 + 2\phi S = 0, \tag{14}$$

where

$$G = G(z, \phi).$$

Boundary conditions of the general form

$$b_0 D\phi'(0) = C_0\phi(0) + d_0, \tag{15}$$

$$b_1 D\phi'(L) = C_1\phi(L) + d_1 \tag{16}$$

are normally associated with the problem, and Eq. (10) becomes

$$G[L, \phi(L)] = 0. \tag{17}$$

If we seek a solution to Eq. (14) of the form

$$G(z, \phi) = -\alpha(z)\phi^2 + 2\beta(z)\phi + \gamma(z), \tag{18}$$

Stark's method[2] for solving Eq. (12) follows immediately. Substituting Eq. (18) into Eq. (14) results in

$$-\phi^2\alpha' + \frac{\alpha^2\phi^2}{D} - \frac{2\alpha\beta\phi}{D} + \frac{\beta^2}{D} - (\Sigma_a - \nu\Sigma_f)\phi^2$$
$$+ 2\phi S + 2\phi\beta' + \gamma' = 0.$$

This equation is satisfied for arbitrary ϕ if

$$\alpha'(z) - [\alpha^2(z)/D] = -(\Sigma_\alpha - \nu\Sigma_f), \tag{19}$$

$$\beta'(z) - \alpha(z)\beta(z)/D = -S, \tag{20}$$

$$\gamma'(z) + \beta^2(z)/D = 0. \tag{21}$$

Using Eq. (18), Eq. (13) becomes

$$D\phi'(z) = -\alpha(z)\phi(z) + \beta(z). \tag{22}$$

Comparing Eq. (22) with the boundary condition of

Eq. (15), for $b_0 \neq 0$, we obtain "initial" conditions for α and β:

$$\alpha(0) = -C_0/b_0, \qquad \beta(0) = d_0/b_0. \tag{23}$$

From Eq. (22) and the boundary condition of Eq. (16), we obtain a "final" condition for ϕ:

$$\phi(L) = \frac{b_1\beta(L) - d_1}{b_1\alpha(L) - C_1}, \tag{24}$$

and using Eq. (18) in the boundary condition of Eq. (17), we obtain a "final" condition for γ:

$$\gamma(L) = \alpha(L)\phi^2(L) - 2\beta(L)\phi(L). \tag{25}$$

Thus, Eqs. (19) and (20) are solved by sweeping from $z = 0$ to $z = L$, using the "initial" conditions of Eq. (23). Then Eqs. (21) and (22) are solved by sweeping from $z = L$ to $z = 0$, using the "final" conditions of Eqs. (24) and (25).

Note that if only the flux is sought, it is not necessary to solve for γ. In this case, the procedure is identical to the method attributed to Stark,[2] and usually postulated on an ad hoc basis for solving Eq. (12).[7] It is interesting that this powerful and widely used method is suggested almost immediately by the field theoretic formulation.

A simple example serves to illustrate some of the concepts which have been discussed. Consider a uniform critical slab nuclear reactor of half-thickness L with the plane of symmetry at $z = 0$. For this case, $b_0 = C_1 = 1, C_0 = d_0 = b_1 = d_1 = 0$, and the "initial" and "final" conditions of Eqs. (23)-(25) become $\alpha(0) = \beta(0) = \gamma(L) = \phi(L) = 0$. It is easy to demonstrate that Eqs. (19)-(22) are satisfied by

$$\phi(z) = \cos\frac{\pi z}{2L}, \tag{26}$$

$$\alpha(z) = \frac{\pi D}{2L}\tan\frac{\pi z}{2L}, \tag{27}$$

$$\beta(z) = \gamma(z) = 0, \tag{28}$$

and hence, from Eq. (18),

$$G(z) = -\left(\frac{\pi D}{4L}\right)\sin\frac{\pi z}{L}. \tag{29}$$

As mentioned previously, $G(z)$ is interpreted as a "surface" term which accounts for the contribution to the functional J from the interval $z < x \leq L$. Using Eqs. (26) and (11), with $S = 0$, it is readily shown that $J = 0$. On the other hand

$$\hat{J} = \int_0^z dx \left[D\left(\frac{\pi}{2L}\right)^2 \sin^2\frac{\pi x}{2L} + (\Sigma_a - \nu\Sigma_f)\cos^2\frac{\pi x}{2L}\right] + \frac{\pi D}{4L}\sin\frac{\pi z}{L}.$$

Making use of the criticality condition

$$\Sigma_a - \nu\Sigma_f = -D(\pi/2L)^2,$$

direct integration yields

$$\hat{J} = -\frac{\pi D}{4L}\sin\frac{\pi z}{D} + \frac{\pi D}{4L}\sin\frac{\pi z}{L} \equiv 0.$$

Alternatively, it is noted that

$$\int_z^L dx\left[D\left(\frac{\pi}{2L}\right)^2\sin^2\frac{\pi x}{2L} + (\Sigma_a - \nu\Sigma_f)\cos^2\frac{\pi x}{2L}\right] = \frac{\pi D}{4L}\sin\frac{\pi z}{L} = -G(z).$$

Thus, $G(z)$ is, in fact, the contribution to the functional J from the interval $z < x \leq L$.

The stationary value of the variational functional of Eq. (1), with F given by Eq. (11) and $S = 0$, is zero. From Eq. (29), it is seen that $G[0, \phi(0)] = 0$, in agreement with the conclusion of the previous section.

4. MULTIGROUP NEUTRON DIFFUSION THEORY

An appropriate bilinear variational functional for the one-dimensional multigroup neutron diffusion equations may be constructed from the Lagrangian density function

$$F = \sum_g \Big(\phi_g^{*\prime} D_g\phi_g' + \phi_g^* A_g\phi_g - \phi_g^*\chi_g\sum_{g'}F_{g'}\phi_{g'} - \phi_g^*\sum_{g'}K_{gg'}\phi_{g'} - \phi_g^* S_g - S_g^*\phi_g\Big), \tag{30}$$

where D, A, χ, F, and K are the diffusion coefficient, removal cross section, fission spectrum, fission cross section times the fission neutron yield, and the scattering transference cross section, respectively, in the multigroup representation. ϕ^* and S^* are the adjoint flux and source, respectively.

The field equations, Eqs. (5), become

$$D_g\phi_g' = \frac{\partial G}{\partial\phi_g^*}, \quad g = 1, \ldots, \text{no. of groups}, \tag{31}$$

$$D_g\phi_g^{*\prime} = \frac{\partial G}{\partial\phi_g}, \quad g = 1, \ldots, \text{no. of groups}, \tag{32}$$

and the Hamilton-Jacobi equation, Eq. (7) or (9), becomes

$$\frac{\partial G}{\partial z} + \sum_g\left[\frac{1}{D_g}\left(\frac{\partial G}{\partial\phi_g^*}\frac{\partial G}{\partial\phi_g}\right) - \phi_g^* A_g\phi_g + \phi_g^*\chi_g\sum_{g'}F_{g'}\phi_{g'} + \phi_g^*\sum_{g'}K_{gg'}\phi_{g'} + \phi_g^* S_g + S_g^*\phi_g\right] = 0, \tag{33}$$

where

$$G = G\Big(z, \sum_g\phi_g^*, \sum_g\phi_g\Big).$$

Equations (31) associate the current with the functional derivative of G with respect to the adjoint flux, while Eqs. (32) associate the adjoint current with the functional derivative of G with respect to the flux.

Analogous to the procedure of the previous section, we seek a bilinear solution to Eq. (33) of the form

$$G = \sum_g \left[-\phi_g^* \sum_{g'} \alpha_{gg'}(z)\phi_{g'} + \beta_g(z)\phi_g^* + \gamma_g(z)\phi_g + \Omega_g(z)\right]. \tag{34}$$

Substituting Eq. (34) into Eq. (33) results in a single scalar equation which is, anticipating subsequent development, written in matrix notation:

$$\begin{aligned}&[\boldsymbol{\phi}^{*T}\boldsymbol{\alpha}'\boldsymbol{\phi} + \boldsymbol{\phi}^{*T}\boldsymbol{\alpha}\mathbf{D}^{-1}\boldsymbol{\alpha}\boldsymbol{\phi} - \boldsymbol{\phi}^{*T}\mathbf{A}\boldsymbol{\phi} + \boldsymbol{\phi}^{*T}\chi\mathbf{F}^T\boldsymbol{\phi} + \boldsymbol{\phi}^{*T}\mathbf{K}\boldsymbol{\phi}]\\ &+ [\boldsymbol{\phi}^{*T}\boldsymbol{\beta}' + \boldsymbol{\phi}^{*T}\boldsymbol{\alpha}\mathbf{D}^{-1}\boldsymbol{\beta} + \boldsymbol{\phi}^{*T}\mathbf{S}]\\ &+ [\boldsymbol{\gamma}'^T\boldsymbol{\phi} + \boldsymbol{\gamma}^T\mathbf{D}^{-1}\boldsymbol{\alpha}\boldsymbol{\phi} + \mathbf{S}^{*T}\boldsymbol{\phi}] + [\mathbf{I}^T\boldsymbol{\Omega}' + \mathbf{I}^T\boldsymbol{\theta}] = 0,\end{aligned} \tag{35}$$

where $\boldsymbol{\phi}^*$, $\boldsymbol{\phi}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, χ, $\mathbf{F}$, and $\boldsymbol{\Omega}$ are column vectors whose elements are the corresponding group components, $\boldsymbol{\theta}$ is a column vector whose elements are the group components $\beta_g\gamma_g/D_g$, and $\mathbf{I}$ is a column vector with all elements unity. $\boldsymbol{\alpha}$, $\mathbf{D}$, $\mathbf{A}$, and $\mathbf{K}$ are square matrices whose elements are the corresponding group components. Equation (35) is satisfied for arbitrary $\boldsymbol{\phi}^*$ and $\boldsymbol{\phi}$ if the following matrix equations are satisfied by $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, and Ω:

$$\boldsymbol{\alpha}' - \boldsymbol{\alpha}\mathbf{D}^{-1}\boldsymbol{\alpha} = -[\mathbf{A} - \chi\mathbf{F}^T - \mathbf{K}], \tag{36}$$

$$\boldsymbol{\beta}' - \boldsymbol{\alpha}\mathbf{D}^{-1}\boldsymbol{\beta} = -\mathbf{S}, \tag{37}$$

$$\boldsymbol{\gamma}'^T - \boldsymbol{\gamma}^T\mathbf{D}^{-1}\boldsymbol{\alpha} = \mathbf{S}^*, \tag{38}$$

$$\boldsymbol{\Omega}' + \boldsymbol{\theta} = 0. \tag{39}$$

The similarity between Eqs. (36)-(39) and Eqs. (19) -(21) suggests that the former may be considered as a multigroup extension of Stark's method.[8]

Assuming that a general set of homogeneous boundary conditions

$$b_0^g D^g \phi_g'(0) = \sum_{g'} C_0^{gg'} \phi_{g'}(0), \tag{40}$$

$$b_1^g D^g \phi_g'(L) = \sum_{g'} C^{gg'} \phi_{g'}(L) \tag{41}$$

are associated with the flux, it can be demonstrated that the appropriate boundary conditions for the adjoint flux are

$$D_g\phi_g^{*\prime}(0) = \sum_{g'} \frac{C_0^{g'g}}{b_0^{g'}} \phi_{g'}^*(0), \tag{42}$$

$$D_g\phi_g^{*\prime}(L) = \sum_{g'} \frac{C_1^{g'g}}{b_1^{g'}} \phi_{g'}^*(L),$$

$$g = 1, \ldots, \text{no. of groups.} \tag{43}$$

For G given by Eq. (34), the field equations (31) and (32) become

$$D\phi_g'(z) = \sum_{g'} \alpha_{gg'}(z)\phi_{g'}(z) + \beta_g(z), \tag{44}$$

$$D\phi_g^{*\prime}(z) = \sum_{g'} \alpha_{g'g}(z)\phi_{g'}^*(z) + \gamma_g(z),$$

$$g = 1, \ldots, \text{no. of groups.} \tag{45}$$

Comparing Eqs. (44) and (45) with Eqs. (40)-(43), and using the boundary condition of Eq. (10), we obtain the "initial" conditions

$$\alpha_{g'g}(0) = C_0^{g'g}/b_0^{g'},$$

$$\beta_g(0) = \gamma_g(0) = 0, \quad g, g' = 1, \ldots, \text{no. of groups} \tag{46}$$

and the "final" conditions

$$\boldsymbol{\phi}(L) = \boldsymbol{\Lambda}^{-1}\boldsymbol{\beta}(L), \tag{47}$$

$$\boldsymbol{\phi}^*(L) = (\boldsymbol{\Lambda}^T)^{-1}\boldsymbol{\gamma}(L), \tag{48}$$

$$\begin{aligned}\Omega_g(L) = -\Big(&\phi_g^*(L)\sum_{g'}\alpha_{gg'}(L)\phi_{g'}(L) + \beta_g(L)\phi_g^*(L)\\ &+ \gamma_g(L)\phi_g(L)\Big), \quad g = 1, \ldots, \text{no. of groups.}\end{aligned} \tag{49}$$

The matrix $\boldsymbol{\Lambda}$ has elements

$$\Lambda^{gg'} \equiv C_1^{gg'}/b_1^g - \alpha_{gg'}(L),$$

$$g, g' = 1, \ldots, \text{no. of groups.} \tag{50}$$

Thus, Eqs. (36)-(38) are solved by sweeping from $z = 0$ to $z = L$, using the "initial" conditions of Eqs. (46). Then Eqs. (39), (44), and (45) are solved by sweeping from $z = L$ to $z = 0$, using the "final" conditions of Eqs. (47) and (48).

The formalism of this section was applied to a two-group reflected slab model with nuclear properties characteristic of a pressurized-water reactor. The model was subcritical, and a uniform source in the fast group was present in the core. The thermal-group fission cross section was used as a thermal-group adjoint source, so the stationary value of the functional corresponded to the thermal-group fission rate.

Neutron and adjoint fluxes for the problem are shown in Fig. 1, and G is shown in Fig. 2. ($x = 0$ corresponds to the core midplane.) The magnitude of G decreases rapidly in the reflector, consistent with the decreasing contribution of the external parts of the reflector to the functional J. The value of G at $x = 0$ agrees with the value of the thermal-group fission rate (the stationary value of the functional) to within the numerical accuracy of the calculation, in agreement with the conclusion of Sec. 2.

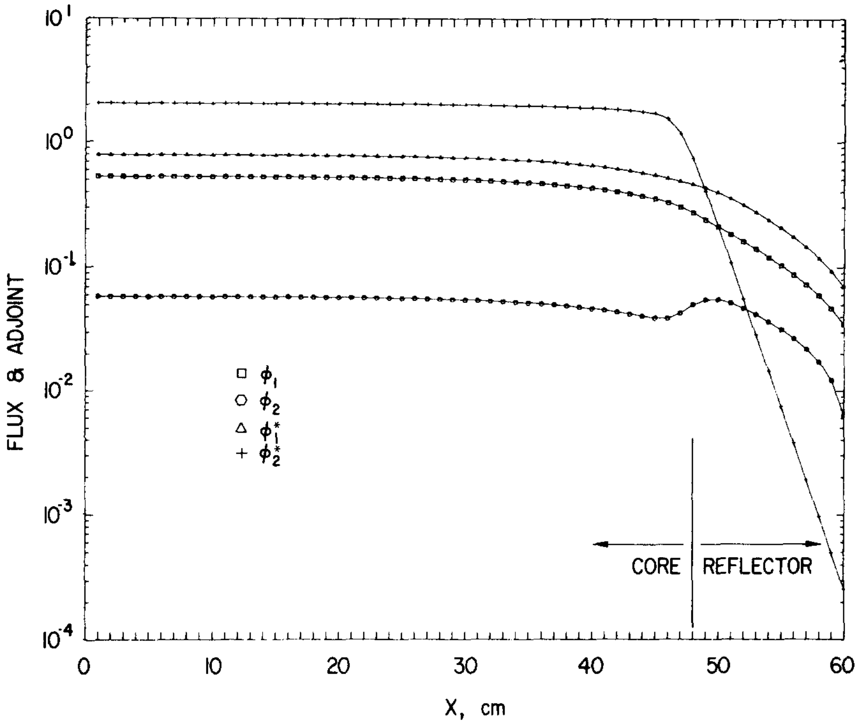

FIG. 1

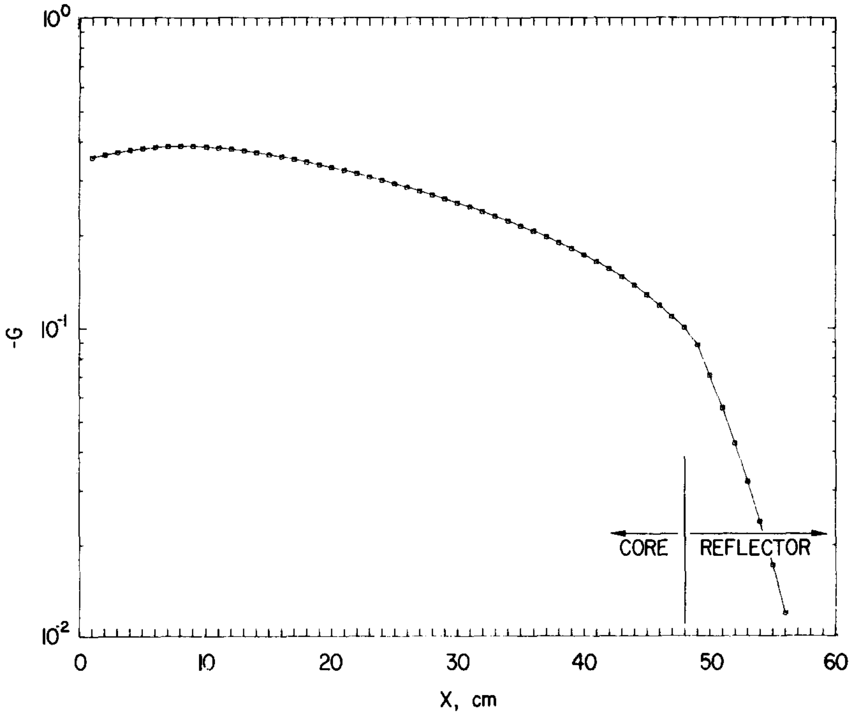

FIG. 2

5. MAXIMUM PRINCIPLE AND DYNAMIC PROGRAMMING

A slight variant of the procedure that was employed in Sec. 2 can be used to derive the Maximum Principle[9] of Pontryagin and the Dynamic Programming[10] algorithm of Bellman.[11] If the variational function of Eq. (1) represents a minimum principle, then $\delta J = 0$ when evaluated for the functions $\bar{y}_j(x)$ which satisfy Eqs. (2), and $\delta J > 0$ when evaluated for any other functions. Making the same arguments as in Sec. 1, we seek an equivalent functional

$$\tilde{J}[y] = -G[z, y(z)] + \int_z^L dx\, F[x, y(x), y'(x)]. \quad (51)$$

Because J, hence $\tilde{J}$, is a minimum principle, we have

$$\delta\tilde{J} = \int_z^L \sum_{j=1}^N \left[\frac{\partial F}{\partial y_j} - \frac{d}{dx}\left(\frac{\partial F}{\partial y_j'}\right)\right] \delta y_j\, dx - \sum_{j=1}^N \left[\frac{\partial F}{\partial y_j'} + \frac{\partial G}{\partial y_j}\right] \delta y_j \Big|_{x=z} - \left(F - \sum_{j=1}^N y_j' \frac{\partial F}{\partial y_j'} + \frac{\partial G}{\partial x}\right) \delta x \Big|_{x=z} \geqslant 0. \tag{52}$$

If we require that Eqs. (2) be satisfied, and that

$$\frac{\partial F}{\partial y_j'} + \frac{\partial G}{\partial y_j} = 0, \quad j = 1, \ldots, N, \tag{53}$$

then, because $\delta x > 0$,[12]

$$\frac{\partial G}{\partial z} + F + \sum_{j=1}^N y_j' \frac{\partial G}{\partial y_j} \leqslant 0. \tag{54}$$

An argument similar to that given in Sec. 2 leads to the conclusion that when the equality obtains in Eq. (54), functions $\bar{y}_j$, which satisfy Eqs. (53) and (54), also satisfy Eqs. (2). Thus, this development is completely equivalent to that of Sec. 2, and a field theory could equally well be based on Eqs. (53) and (54), when the equality obtains in the latter. Equation (10) would be replaced by $G[0, y(0)] = 0$ in this case, and $G[L, y(L)]$ would correspond to the stationary value of the functional.

If we define

$$\psi_j(z) \equiv -\frac{\partial G}{\partial y_j}, \quad j = 1, \ldots, N,$$

$$\psi_{N+1}(z) \equiv -\frac{\partial G}{\partial z},$$

then Eq. (54) can be written

$$0 = \max_{y'} \left(\psi_{N+1} + \sum_{j=1}^N \psi_j y_j' - F\right). \tag{55}$$

Equation (55) is the Maximum Principle of Pontryagin.

An alternate way of writing Eq. (54) is

$$-\frac{dG[z, y(z)]}{dz} \geqslant F[z, y(z), y'(z)]. \tag{56}$$

Integrating Eq. (56) over the subinterval z to $z + \Delta z$, and approximating F in this subinterval by its value at z, we obtain

$$G[z, y(z)] \geqslant G[z + \Delta z, y(z + \Delta z)] + \Delta z F[z, y(z), y'(z)].$$

Because the equality obtains for the functions $\bar{y}_j$ which satisfy Eqs. (2), this may be written

$$G[z, \bar{y}(z)] = \min_{y'} \{G[z + \Delta z, \bar{y}(z + \Delta z)] + \Delta z F[z, \bar{y}(z), y'(z)]\}. \tag{57}$$

Equation (57) is the Dynamic Programming algorithm.

---

* Work performed under the auspices of the U.S. Atomic Energy Commission.

1 I. M. Gel'fand and S. V. Fomin, *Calculus of Variations* (Prentice-Hall, Englewood Cliffs, N.J., 1963).

2 M. K. Butler and J. M. Cook, "One-Dimensional Diffusion Theory," in *Computing Methods in Reactor Physics*, edited by H. Greenspan, C. Kelber, and D. Okrent (Gordon and Breach, New York, 1968); also R. Ehrlich and H. Hurwitz, Jr., Nucleonics **12**, 23 (1954).

3 S. Kaplan and E. M. Gelbard [J. Math. Anal. Appl. 11, 538 (1965)] have shown that Stark's method may be related to invariant imbedding techniques, which suggests that field theory may provide a link between conventional diffusion (or transport) theory and invariant imbedding.

4 The same results obtain when $y_j(x)$ have discontinuous first derivatives at a finite number of points x_i, providing that $\partial F/\partial y_j'$ is continuous at these points. (See Ref. 1.) This is the case for material interfaces in neutron diffusion theory, where the latter quantity turns out to be the current.

5 This is the general formula for the variation of a functional with a variable end point at $x = z$. The point $x = 0$ is considered fixed, and only functions which satisfy the prescribed conditions at $x = 0$ are considered.

6 H. Rund [the Hamilton–Jacobi theory in the Calculus of Variations (Van Nostrand, London, 1966)] has discussed the role of the Hamilton–Jacobi equation in the calculus of variations in terms of hypersurfaces $G[z, y(z)]$ which are geodesically equidistant with respect to the function $F[z, y(z), y'(z)]$. Gel'fand and Fomin (Ref. 1) also concluded that Eqs. (5) define a "consistent" field if and only if G satisfies the Hamilton–Jacobi equation, but arrived at their result by requiring that the field equations be consistent and self-adjoint for each point in the domain $0 \leqslant x \leqslant L$. The above development introduces the Hamilton–Jacobi equation from a different point of view.

7 At first glance it may seem that nothing has been gained by converting a single linear second-order differential equation to a coupled set of nonlinear first-order differential equations. However, the nonlinearity is of no consequence when the solution is obtained on a digital computer, and the round-off errors associated with a straightforward numerical solution of Eq. (12) are generally greater than those associated with a numerical solution of Eqs. (19)–(22). (See Refs. 2 and 3.)

8 Stark's method is routinely applied to multigroup problems.

9 L. S. Pontryagin *et al.*, *The Mathematical Theory of Optimum Processes* (Wiley, New York, 1962).

10 R. Bellman, *Dynamic Programming* (Princeton U.P., Princeton N.J., 1957).

11 A relation among the calculus of variations, the maximum principle, and dynamic programming has been discussed by many authors. However, the derivation given in this section, which is based on the introduction of a surface term in a variational functional to represent the contribution from a subinterval, represents a new point of view which provides a consistent relation among these theories and the Hamilton–Jacobi theory.

12 If variations $\delta x < 0$ were considered, the sign on the last term in Eq. (51) would be reversed, and the same conclusion would result.

T-Matrix Analyticity Using Fredholm Theory

Gedaliah R. Shaffer
Joseph Henry Laboratories, Princeton University, Princeton, New Jersey 08540
(Received 12 May 1971)

The behavior of the Regge pole residues for the T matrix analyzed into partial waves is studied as a function of E for scattering from a Yukawa potential. Using a variational formulation of Fredholm theory, we explicitly show that the residues on the energy shell have no branch cuts in the left-hand E plane.

We consider nonrelativistic scattering from a Yukawa potential. Using Fredholm theory, we contemplate solving the Lippmann–Schwinger equation for the T matrix expanded into partial waves. If we go onto the energy shell and consider the behavior of the partial wave projections as a function of energy, we find branch cuts appearing in the left-hand E plane. Superficially, these cuts seem to be present as well in the residue of the T matrix at a Regge pole. It is a well-known consequence of dispersion theory however, that at a Regge pole, the residue has a right-hand cut only.[1] In this paper an explicit demonstration of the extinction of these left-hand cuts is presented. We use a formulation of Fredholm theory in which the Fredholm resolvent kernel is expressed as a functional derivative of the Fredholm denominator. Since this denominator is determined by the traces of the iterated kernels, with the energy appearing only in the propagator, it clearly has no left-hand E-plane branch cuts. This provides the motivation for anticipating that the functional derivative of this denominator at a Regge pole has no left-hand cuts also.

We start from the Lippmann–Schwinger equation for the T matrix[2] for scattering from a potential V, which we choose to be central:

$$T = V + V\frac{1}{E - H_0 + i\epsilon}T.$$

In the momentum representation this becomes (for incoming momentum $\mathbf{k}$, outgoing momentum $\mathbf{k}'$)

$$T_{\mathbf{k},\mathbf{k}'}(E) = V(\mathbf{k}-\mathbf{k}') + \int\frac{d^2q}{(2\pi)^3}V(\mathbf{q}-\mathbf{k})\frac{1}{E - q^2/2m + i\epsilon}T_{\mathbf{q},\mathbf{k}'}(E).$$

For a Yukawa potential

$$V(\mathbf{k}-\mathbf{q}) = g^2/(\mu^2 + |\mathbf{k}-\mathbf{q}|^2).$$

We make a partial wave expansion

$$T_{\mathbf{k},\mathbf{k}'}(E) = 4\pi\textstyle\sum_{lm}Y_l^{m*}(\hat{k}')Y_l^m(\hat{k})T_l(E,k,k')$$

$$V(\mathbf{k}'-\mathbf{q}) = \frac{g^2}{(\mu^2 + q^2 + k'^2 - 2\mathbf{k}\cdot\mathbf{q})}$$

$$= \frac{4\pi g^2}{2k'q}\textstyle\sum_{lm}Q_l\left(\frac{\mu^2 + q^2 + k'^2}{2qk'}\right)Y_l^{m*}(\hat{k}')Y_l^m(\hat{q}),$$

where we have used the addition theorems for Legendre functions and spherical harmonics. This yields

$$T_l^\lambda(E,k,k') = \frac{g^2}{2k'k}Q_l\left(\frac{\mu^2 + k^2 + k'^2}{2kk'}\right) + \frac{4\pi g^2}{(2\pi)^3}\lambda\int_0^\infty dq\frac{q^2}{2kq}\frac{Q_l((\mu^2 + q^2 + k^2)/2qk)}{(E - q^2/2m + i\epsilon)} \times T_l^\lambda(E,q,k'), \tag{1}$$

where we have inserted a parameter λ, such that $\lambda = 1$ gives us the correct equation, i.e.,

$$T_l(E,k,k') = T_l^1(E,k,k').$$

For any nonhomogeneous equation of the form

$$\psi(k) = \varphi(k) + \lambda\int dqN(k,q)\psi(q), \tag{2}$$

where the kernel satisfies certain well-known properties, the solution[3] given by Fredholm theory may be written

$$\psi(k) = \varphi(k) + \lambda\int dq\frac{D(k,q,\lambda)}{D(\lambda)}\varphi(q), \tag{3}$$

where

$$D(\lambda) = 1 + \sum_{i=1}^\infty \lambda^i\mathfrak{D}^{(i)},\quad \mathfrak{D}^{(i)} = \frac{(-1)^i}{i!}\int ds_1\cdots\int ds_i\begin{vmatrix}N(s_1,s_1) & \cdots & N(s_1,s_i)\\ \vdots & & \vdots\\ N(s_i,s_1) & \cdots & N(s_i,s_i)\end{vmatrix} \tag{4}$$

is the Fredholm denominator, and $D(k,q,\lambda)$ is the Fredholm numerator which satisfies

$$D(k,k',\lambda) = N(k,k')D(\lambda) + \lambda\int dqD(k,q,\lambda)N(q,k'). \tag{5}$$

For the special class of nonhomogeneous equations for which

$$\varphi(k) = N(k,k')/h(k'),$$

we find by comparing Eq. (2) with Eq. (5),

$$\psi(k) = D(k,k',\lambda)/[h(k')D(\lambda)]. \tag{6}$$

Hence if we identify

$$N(k,q) = \frac{4\pi g^2}{(2\pi)^3}\frac{q^2}{2kq}\frac{Q_l\ ((\mu^2 + q^2 + k^2)/2qk)}{E - q^2/2m + i\epsilon}$$

and

$$h(q) = (4\pi q^2/(2\pi)^3)(E - q^2/2m + i\epsilon),$$

we find

$$T_l^\lambda(E,k,k') = D(k,k',\lambda)/[h(k')D(\lambda)].$$

The Regge poles are located at those values of l

(call one l_0) for which $D(\lambda)$ has a zero at $\lambda = 1$. For if $D(l, \lambda_0) = 0$ (where we explicitly write the l dependence), and[4]

$$\frac{\partial D}{\partial l} \neq 0\,, \quad \frac{\partial D}{\partial \lambda} \neq 0$$

in some neighborhood of (λ_0, l_0), we implicitly determine a function $\lambda_0(l)$ such that near l_0

$$\lambda_0(l) = \lambda_0(l_0) + \frac{d\lambda_0}{dl}\bigg|_{l=l_0} (l - l_0) = \lambda_0(l_0) - \left[\frac{\partial D}{\partial l}\bigg/\frac{\partial D}{\partial \lambda_0}\right]\bigg|_{l=l_0} (l - l_0)$$

and [near a simple zero of $D(\lambda)$]

$$D(\lambda) = (\lambda - \lambda_0)d(\lambda_0) = d(\lambda_0)\left[\lambda - \lambda_0(l_0) + \left(\frac{\partial D}{\partial l}\bigg/\frac{\partial D}{\partial \lambda_0}\right)\bigg|_{l=l_0} (l - l_0)\right].$$

If $\lambda_0(l_0) = 1$, we have

$$D(1) = d(1)\left[\left(\frac{\partial D}{\partial l}\bigg/\frac{\partial D}{\partial \lambda_0}\right)\bigg|_{l=l_0}\right](l - l_0),$$

i.e , a Regge pole at $l = l_0$. The residues of the Regge poles [for a simple zero of $D(\lambda)$, $\lambda = 1$] are seen to be proportional to

$$D(k, k', \lambda)/[h(k')], \quad \text{for } \lambda = 1.$$

Using the standard expansion of the Fredholm numerator we have

$$\frac{D(k, k', \lambda)}{[h(k')]} = \frac{g^2}{2kk'} Q_l\left(\frac{\mu^2 + k^2 + k'^2}{2kk'}\right) + \lambda \int \cdots .$$

If we go onto the energy shell this becomes (with $k^2 = k'^2 = 2mE$)

$$\frac{D(k, k', \lambda)}{[h(k')]}\bigg|_{\text{on shell}} = \frac{g^2}{4mE} Q_l\left(1 + \frac{\mu^2}{4mE}\right) + \lambda \int \cdots ,$$

the first term of which has a branch point at $E = -\mu^2/8m$, which superficially seems to remain even at a Regge pole. To see explicitly how this branch cut is extinguished, we utilize a variational form of the Fredholm theory.[5]

The Fredholm resolvent kernel of Eq. (2) may also be expressed in the form

$$\psi(k) = -\frac{1}{\lambda} \int dq \frac{\delta D(\lambda)}{\delta N(q, k)} \frac{\varphi(q)}{D(\lambda)}, \tag{7}$$

where

$\delta D(\lambda)/\delta N(q, k)$

is a functional derivative of the Fredholm denominator $D(\lambda)$, with respect to the adjoint kernel $N(q, k)$. As usual, this functional derivative may be found by replacing $N(q', k')$ by

$$N(q', k') + \eta\delta(q' - q)\,\delta(k' - k)$$

and then evaluating the first derivative with respect to the parameter η at $\eta = 0$. By comparing Eqs. (7) and (3), we can relate this kernel to the usual Fredholm numerator:

$$D(k, q, \lambda) = -\frac{D(\lambda)}{\lambda}\delta(k - q) + \frac{1}{\lambda^2}\frac{\delta D(\lambda)}{\delta N(q, k)}. \tag{8}$$

Near a simple zero of the Fredholm denominator

$$D(\lambda) = (\lambda - \lambda_0)d(\lambda_0),$$

where λ_0 depends implicitly on the kernel $N(k, q)$. Hence

$$\frac{\delta D(\lambda)}{\delta N(q, k)} = -\frac{\delta\lambda_0}{\delta N(q, k)} d(\lambda_0) + (\lambda - \lambda_0)\frac{\delta d(\lambda_0)}{\delta N(q, k)}. \tag{9}$$

At $\lambda = \lambda_0$ the second term in (9) vanishes and by (8) we find

$$\frac{D(k, q, \lambda_0)}{[h(q)]} = -\frac{d(\lambda_0)}{\lambda_0^2 h(q)}\frac{\delta\lambda_0}{\delta N(q, k)}. \tag{10}$$

If we approximate $D(\lambda)$ to the nth order in λ,

$$D(\lambda) \approx D_n(\lambda) = \sum_{i=1}^{n} (\lambda)^i \mathfrak{D}^{(i)}, \tag{11}$$

evaluate it at a zero of $D(\lambda)$, $D_n(\lambda_0) \approx 0$, and apply $\delta/\delta N(q, k)$ to this finite sum, we find (collecting terms)

$$\begin{aligned}\frac{1}{h(q)}\frac{\delta\lambda_0}{\delta N(q, k)}d(\lambda_0) = &-\lambda_0\frac{\delta(q - k)}{h(q)}\sum_{i=0}^{n-1}\lambda_0^i\mathfrak{D}^{(i)} \\ &-\lambda_0^2\frac{N(k, q)}{h(q)}\sum_{i=0}^{n-2}\lambda_0^i\mathfrak{D}^{(i)} \\ &\vdots \\ &-\lambda_0^n\frac{N_{n-1}(k, q)}{h(q)}1,\end{aligned} \tag{12}$$

where

$$N_n(k, q) = \int_0^\infty ds_1 N(k, s_1)\int_0^\infty ds_2 N(s_1, s_2)\cdots \times \int_0^\infty ds_{n-1}N(s_{n-2}, s_{n-1})N(s_{n-1}, q) \tag{13}$$

is the nth iterated kernel.

Since the series

$$\sum_{i=0}^{n} \lambda_0^i \mathfrak{D}^{(i)}$$

converges to $D(\lambda_0) = 0$, by taking enough terms we can make the coefficients of any given $N_j(k, q)$ as small as desired. We will show that on the energy shell, N_j has no branch cuts in the left-hand E plane in the region

$-(j)^2\mu^2/8 < E < 0.$

Hence the sum of the iterated kernels has only a finite number of branch points located in the region $(E, 0)$ for any finite $E < 0$. Since the coefficients of each of them may be made vanishingly small by taking enough terms in the expansion of $D(\lambda_0)$, we find that in the limit all the branch cuts in the left-hand E plane are extinguished for the function

$$\frac{1}{h(q)}\frac{\delta\lambda_0}{\delta N(q,k)}d(\lambda_0) = -\lambda_0^2\frac{D(k,q,\lambda_0)}{h(q)}.$$

Hence if l is such that $\lambda_0 = 1$, we have shown that the residue of

$$T_l(E,k,k') = D(k,k',\lambda_0 = 1)/h(k')D(\lambda_0 = 1)$$

has no left-hand cuts on the energy shell.

It remains only to show that the region of analyticity of the successive iterated kernels expands successively to the left. Let

$$Q(x,y) = Q_l\left(\frac{\mu^2 + x^2 + y^2}{2xy}\right).$$

Then from Eq. (13) we have

$$\frac{N_n(k,k')}{h(k')} = \left(\frac{4\pi g^2}{(2\pi)^3}\right)^{n-1} g^2\int_0^\infty dy_1\,\frac{Q(k,y_1)}{E - y_1^2/2m + i\epsilon}\,\frac{y_1^2}{2ky_1}\cdots\int_0^\infty dy_{n-1}\,\frac{Q(y_{n-1},y_{n-2})}{E - y_{n-1}^2/2m + i\epsilon}\,\frac{y_{n-1}^2}{2y_{n-1}y_{n-2}}\,Q(y_{n-1},k')$$
$$\times\frac{k'^2}{2y_{n-1}k'}\,\frac{1}{k'^2}.$$

We introduce the following representation for the Legendre functions[6]:

$$Q_l\left(\frac{\mu^2 + x^2 + y^2}{2xy}\right) = \pi(xy')^{1/2}\int_0^\infty dt e^{-\mu t}J_{l+1/2}(xt)J_{l+1/2}(yt)$$

and hence find

$$\frac{N_n(k,k')}{h(k')} = \frac{(2m)^{n-1}\pi^n}{2^n}\left(\frac{4\pi g^2}{(2\pi)^3}\right)^{n-1} g^2\int_0^\infty dt_1\int_0^\infty dt_n e^{-\mu(t_1+t_2+\cdots+t_n)}(kk')^{-1/2}J_{l+1/2}(kt_1)J_{l+1/2}(k't_n)$$
$$\times f(t_1,t_2)f(t_2,t_3)\cdots f(t_{n-1},t_n),$$

where[7]

$$f(t_i,t_{i+1}) = \lim_{\epsilon\to\infty}\int_0^\infty\frac{dy_i y_i J_{l+1/2}(y_i t_i)J_{l+1/2}(y_i t_{i+1})}{2mE - y_i^2 + i\epsilon'}$$
$$= -\frac{\pi i}{2}\begin{bmatrix}J_{l+1/2}(t_i(2mE)^{1/2})H^{(1)}_{l+1/2}(t_{i+1}(2mE)^{1/2})\theta(t_{i+1}-t_i)\\ + J_{l+1/2}(t_{i+1}(2mE)^{1/2})H^{(1)}_{l+1/2}(t_i(2mE)^{1/2})\theta(t_i - t_{i+1})\end{bmatrix}.$$

Since we want to evaluate the iterated kernel on the energy shell for $E < 0$, we set $k = k' = (2mE)^{1/2} = ic, c > 0$. We can then change all the variables of integration $ct_i = s_i$ and find

$$\frac{N_n(k,k')}{h(k')} = \beta\int_0^\infty ds_1\cdots\int_0^\infty ds_n e^{-(\mu/c)(s_1+s_2+\cdots s_n)}I_{l+1/2}(s_1)$$
$$\times I_{l+1/2}(s_n)\prod_{i=1}^{n-1}\begin{Bmatrix}I_{l+1/2}(s_i)K_{l+1/2}(s_{i+1})\theta(s_{i+1}-s_i)\\ + I_{l+1/2}(s_{i+1})K_{l+1/2}(s_i)\theta(s_i - s_{i+1})\end{Bmatrix},$$

$$\beta = (-1)^{n-1}\left(\frac{4\pi g^2}{(2\pi)^3}\right)^{n-1} g^2 e^{\pi i l}\,\frac{(2m)^{n-1}\pi^n}{2^n c^{n+1}}.$$

Clearly, the only role the factor of μ/c can play is in damping out the integrals for large s_i. Hence we may substitute into this expression the asymptotic forms

$$I_{l+1/2}(z) \sim e^z, K_{l+1/2}(z) \sim e^{-z}.$$

By judicious manipulation of the theta functions, all the regions of integration may be made finite except for the outermost say for s_1. Since in each of the steps of the integration the growing exponential is dominated by the decreasing one, at worst each term contributes as much as

$$I_{l+1/2}(s_i)K_{l+1/2}(s_{i+1})\theta(s_{i+1} - s_i) \to \sim 1,$$
$$I_{l+1/2}(s_1)I_{l+1/2}(s_n) \to \sim e^{2s_1},$$
$$e^{-(\mu/c)s_i} \to e^{-(\mu/c)s_1},$$

after all but one of the integrations are done. Hence the existence of the integral is assured if at least

$$\int_0^\infty ds_1 e^{-(n\mu/c-2)s_1}$$

is finite, i.e., when $n\mu/c - 2 > 0$ or alternatively when

$$0 > E = -c^2/2m > -n^2\mu^2/8m.$$

Clearly, any finite number of derivatives may be taken with respect to the parameter μ/c without affecting the existence of the integral (since the exponential factor dominates the powers of s_1 which appear). Hence the nth iterated kernel on the energy shell is analytic on the negative real axis for $0 > E > -n^2\mu^2/8m$.

This argument can be extended to show that the iterated kernel is analytic for $0 > ReE > -n^2\mu^2/8m$ (a strip in the left-hand E plane).

ACKNOWLEDGMENTS

The author is deeply indebted to Professor Marvin L. Goldberger for suggesting the problem, and many stimulating discussions. A useful conversation with Professor George Tiktopoulos is also gratefully acknowledged.

Research sponsored by Air Force Office of Scientific Research under Contract AF 49(638)-1545.

1 See article by G. F. Chew in the 1965 Les Houches Lecture Volume, *High Energy Physics*, edited by C. Dewitt and M. Jacob (Gordon and Breach, New York, 1965), pp. 231–2.

2 M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

3 E. T. Whittaker and K. M. Watson, *A Course in Modern Analysis* (Cambridge U.P., Cambridge, 1965), Chap. 11.

4 That these conditions are in fact satisfied may be seen by looking at the weak coupling limit for example, where $l = -1 + \lambda_0 \alpha, \alpha \neq 0$ and

$$\left.\frac{d\lambda_0}{dl}\right|_{l=l_0} = \frac{1}{\alpha}.$$

5 For previous use of this variational approach to Fredholm theory in scattering theory see article by R. Blankenbecler in *Strong Interactions and High Energy Physics* (Plenum, New York, 1964).

6 *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. 1, p. 183.

7 K. M. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge U.P., Cambridge, 1966), p. 429.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Exact Equilibration of Harmonically Bound Oscillator Chains

M. A. Huerta, H. S. Robertson, and J. C. Nearing
Department of Physics, University of Miami, Coral Gables, Florida 33124
(Received 26 April 1971)

The approach to equilibrium of a finite segment of an infinite chain of harmonically coupled, harmonically bound oscillators is treated exactly, both when the initial description of the rest of the chain is canonical and when it is Gaussian. The necessary mathematical properties of the bound oscillator functions are developed and used to demonstrate exact equipartition of energy. The entropy of the finite segment, or system, is shown to evolve to a time-independent equilibrium state that is, in the limit of weak coupling, the correct one for a system of noninteracting harmonic oscillators.

1. INTRODUCTION

A finite segment of an infinite chain of coupled oscillators can be treated as a model of a system interacting with a heat bath. One of the most easily treated models of a thermodynamic system is one composed of weakly interacting individual elements, with the system interacting weakly with the heat bath. The usual chain of alternate springs and masses is inconvenient as such a model because we are unable to speak of individual-oscillator energies, but must instead assign energies to masses and to springs, or else to normal modes.

A model more compatible with the thermodynamic idea of a system of weakly interacting particles, each with nearly its own energy, interacting through its boundaries with a weakly coupled heat bath may be formed as follows: Each mass m is strongly bound to its home position by a harmonic spring of constant K. The oscillators thus formed are set in a linear array, and the nearest neighbors are weakly coupled with harmonic springs of constant k. We consider an infinite linear chain of these weakly coupled, harmonically bound oscillators, with a finite segment of N oscillators regarded as

Clearly, the only role the factor of μ/c can play is in damping out the integrals for large s_i. Hence we may substitute into this expression the asymptotic forms

$$I_{l+1/2}(z) \sim e^{z}, K_{l+1/2}(z) \sim e^{-z}.$$

By judicious manipulation of the theta functions, all the regions of integration may be made finite except for the outermost say for s_1. Since in each of the steps of the integration the growing exponential is dominated by the decreasing one, at worst each term contributes as much as

$$I_{l+1/2}(s_i)K_{l+1/2}(s_{i+1})\theta(s_{i+1}-s_i) \to \sim 1,$$
$$I_{l+1/2}(s_1)I_{l+1/2}(s_n) \to \sim e^{2s_1},$$
$$e^{-(\mu/c)s_i} \to e^{-(\mu/c)s_1},$$

after all but one of the integrations are done. Hence the existence of the integral is assured if at least

$$\int_0^\infty ds_1 e^{-(n\mu/c-2)s_1}$$

is finite, i.e., when $n\mu/c - 2 > 0$ or alternatively when

$$0 > E = -c^2/2m > -n^2\mu^2/8m.$$

Clearly, any finite number of derivatives may be taken with respect to the parameter μ/c without affecting the existence of the integral (since the exponential factor dominates the powers of s_1 which appear). Hence the nth iterated kernel on the energy shell is analytic on the negative real axis for $0 > E > -n^2\mu^2/8m$.

This argument can be extended to show that the iterated kernel is analytic for $0 > ReE > -n^2\mu^2/8m$ (a strip in the left-hand E plane).

ACKNOWLEDGMENTS

The author is deeply indebted to Professor Marvin L. Goldberger for suggesting the problem, and many stimulating discussions. A useful conversation with Professor George Tiktopoulos is also gratefully acknowledged.

Research sponsored by Air Force Office of Scientific Research under Contract AF 49(638)-1545.

1 See article by G. F. Chew in the 1965 Les Houches Lecture Volume, *High Energy Physics*, edited by C. Dewitt and M. Jacob (Gordon and Breach, New York, 1965), pp. 231–2.

2 M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

3 E. T. Whittaker and K. M. Watson, *A Course in Modern Analysis* (Cambridge U.P., Cambridge, 1965), Chap. 11.

4 That these conditions are in fact satisfied may be seen by looking at the weak coupling limit for example, where $l = -1 + \lambda_0 \alpha, \alpha \neq 0$ and

$$\left.\frac{d\lambda_0}{dl}\right|_{l=l_0} = \frac{1}{\alpha}.$$

5 For previous use of this variational approach to Fredholm theory in scattering theory see article by R. Blankenbecler in *Strong Interactions and High Energy Physics* (Plenum, New York, 1964).

6 *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. 1, p. 183.

7 K. M. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge U.P., Cambridge, 1966), p. 429.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Exact Equilibration of Harmonically Bound Oscillator Chains

M. A. Huerta, H. S. Robertson, and J. C. Nearing
Department of Physics, University of Miami, Coral Gables, Florida 33124
(Received 26 April 1971)

The approach to equilibrium of a finite segment of an infinite chain of harmonically coupled, harmonically bound oscillators is treated exactly, both when the initial description of the rest of the chain is canonical and when it is Gaussian. The necessary mathematical properties of the bound oscillator functions are developed and used to demonstrate exact equipartition of energy. The entropy of the finite segment, or system, is shown to evolve to a time-independent equilibrium state that is, in the limit of weak coupling, the correct one for a system of noninteracting harmonic oscillators.

1. INTRODUCTION

A finite segment of an infinite chain of coupled oscillators can be treated as a model of a system interacting with a heat bath. One of the most easily treated models of a thermodynamic system is one composed of weakly interacting individual elements, with the system interacting weakly with the heat bath. The usual chain of alternate springs and masses is inconvenient as such a model because we are unable to speak of individual-oscillator energies, but must instead assign energies to masses and to springs, or else to normal modes.

A model more compatible with the thermodynamic idea of a system of weakly interacting particles, each with nearly its own energy, interacting through its boundaries with a weakly coupled heat bath may be formed as follows: Each mass m is strongly bound to its home position by a harmonic spring of constant K. The oscillators thus formed are set in a linear array, and the nearest neighbors are weakly coupled with harmonic springs of constant k. We consider an infinite linear chain of these weakly coupled, harmonically bound oscillators, with a finite segment of N oscillators regarded as the system, and the rest of the chain as the heat bath.

The Hamiltonian of the system is

$$H = \sum_{n=-\infty}^{\infty} \left(\frac{p_n^2}{2m} + \frac{K}{2} x_n^2 + \frac{k}{2} (x_{n+1} - x_n)^2 \right), \quad (1)$$

and the solutions to the equations of motion have already been reported [1-3] to be

$$x_n(t) = \sum_{r=-\infty}^{\infty} [x_{n+r}(0) f_r(t) + P_{n+r}(0) g_r(t)/m\Omega] \quad (2a)$$

and

$$p_n(t) = m \dot{x}_n(t), \quad (2b)$$

where these "bound-oscillator functions" are given by

$$f_r(t) = \pi^{-1} \int_0^{\pi} d\psi \cos r\psi \cos[\Omega t (1 - 2\gamma \cos\psi)^{1/2}] \quad (3)$$

$$g_r(t)/\Omega = \int_0^t f_r(t') dt', \quad (4)$$

$$\Omega^2 = (K + 2k)/m, \quad (5)$$

$$\omega^2 = k/m, \quad (6)$$

and

$$\gamma = (\omega/\Omega)^2 = k/(K + 2k). \quad (7)$$

In the weak-coupling limit, with $\gamma << 1$, we have used the approximate solutions[1-3]

$$f_r(t) \approx J_r(\gamma\Omega t) \cos(\Omega t - r\pi/2) \quad (8a)$$

and

$$g_r(t) \approx J_r(\gamma\Omega t) \sin(\Omega t - r\pi/2), \quad (8b)$$

with J_r the ordinary Bessel function.

Statistical mechanics is introduced via our assumed knowledge of the initial conditions appearing in Eqs. (2). As already shown,[2] we can define an entropy

$$S_N(t) = -k_B \int \rho_N \, ln(h^N \rho_N) \prod_{i=1}^{N} dx_i dp_i, \quad (9)$$

where k_B = Boltmann's constant, $\rho_N(t)$ is the reduced Liouville function, or probability density in the $2N$-dimensional system-variable space, and h is a constant with the units of action, introduced for dimensional purposes but evidently equal to Plank's constant in a quantum-mechanical treatment of the problem. We have been able to write $\rho_N(t)$ as

$$\rho_N(t) = (2\pi)^{-N} (\det W)^{-1/2} \exp[-\tilde{X}' W^{-1} X'/2], \quad (10)$$

where X' is a $2N$-component column vector, the transpose of which is $\tilde{X}' = (x_1' x_2' \cdots x_N' p_1' \cdots p_N')$, with $x_n' = x_n'(t) = x_n(t) - \langle x_n(t) \rangle$, etc., and the covariance matrix W is given by

$$W = \begin{pmatrix} M & G \\ \tilde{G} & Q \end{pmatrix}, \quad (11)$$

where $M = (M_{ij})$, etc., and

$$M_{ij} = \langle x_i'(t) x_j'(t) \rangle, \quad (12a)$$

$$Q_{ij} = \langle p_i'(t) p_j'(t) \rangle, \quad (12b)$$

and

$$G_{ij} = \langle x_i'(t) p_j'(t) \rangle. \quad (12c)$$

When ρ_N from Eq. (10) is used in Eq. (9), we obtain the simple expression for the entropy

$$S_N(t) = N k_B + k_B \ln[\hbar^{-N} (\det W)^{1/2}], \quad (13)$$

where $\hbar = h/2\pi$. Thus the entropy is given entirely by the covariance matrix, the elements of which can be calculated directly from the initial probability density of the entire chain, by use of Eqs. (2). We have, for example,

$$\langle x_i(t) \rangle = \int \rho_0 x_i(t) \prod_{n=-\infty}^{\infty} dx_n(0) dp_n(0), \quad (14)$$

where Eq. (2a) is used for $x_i(t)$, and ρ_0 is the initial probability density, or Liouville function, for the entire chain. Then, since $x_i'(t) = x_i(t) - \langle x_i(t) \rangle$, we can write

$$M_{ij} = \int \rho_0 x_i'(t) x_j'(t) \prod_{n=-\infty}^{\infty} dx_n(0) dp_n(0), \quad (15)$$

and similarly for the other matrix elements of W.

We may know the initial values of the system variables as accurately as measuring techniques permit, but typically the heat-bath initial conditions are much less well known. As the system evolves, our knowledge of its variables deteriorates, not because the dynamical calculations are imprecise, but because the values of the variables become increasingly determined by heat-bath initial conditions. Our statistical description of the system, $\rho_N(t)$ of Eq. (10), evolves to a time-independent one that can only be described as equilibrium. As we have already shown,[1-3] energy is equipartitioned, entropy evolves to its correct classical value, and the behavior of the system is generally in accord with expectations.

In this paper we treat the problem exactly, using the functions defined by Eqs. (3) and (4), rather than the weak-coupling approximations of Eqs. (8). In Sec. 2 we develop the necessary mathematical properties of the exact function, in Sec. 3 we treat the evolution of the system to equilibrium with a canonical initial distribution of heat-bath variables, and in Sec. 4 we treat a similar problem with a noncanonical initial heat bath.

2. MATHEMATICAL PROPERTIES

The function of Eq. (3) is rewritten as

$$\begin{aligned} f_n(z, \gamma) &= f_n \\ &= \pi^{-1} \int_0^{\pi} d\theta \cos n\theta \cos[z(1 - 2\gamma \cos\theta)^{1/2}] \\ &= (2\pi)^{-1} \int_{-\pi}^{\pi} d\theta \exp(in\theta) \cos[z(1 - 2\gamma \cos\theta)^{1/2}], \end{aligned} \quad (16)$$

where we have used z in place of Ωt and $0 < \gamma < \frac{1}{2}$.

In the development of mathematical properties of these functions, reference will frequently be made to convenient standard sources of material on transcendental functions.[4,5] In this way, for example (Ref. 5, Eq. 10.1.40, with $t = z\gamma\cos\theta$), we obtain the result

$$\cos[z(1-2\gamma\cos\theta)^{1/2}] = z\sum_{n=0}^{\infty}[(\gamma z\cos\theta)^n/n!]j_{n-1}(z), \quad (17)$$

where $j_n(z) = (\pi/2z)^{1/2}J_{n+1/2}(z)$ is the spherical Bessel function of the first kind. The use of Eq. (17) and the identity

$$\cos^n\theta\cos r\theta = 2^{-n}\sum_{k=0}^{n}\binom{n}{k}\cos(r+n-2k)\theta \quad (18)$$

in Eq. (16) leads to the expression

$$f_r(z,\gamma) = z\sum_{k=0}^{\infty}\frac{(\frac{1}{2}\gamma z)^{r+2k}}{k!(r+k)!}j_{r+2k-1}(z). \quad (19)$$

Equation (8a) may be obtained, for $\gamma<<1$, by expanding the square root in Eq. (16) and carrying out the resultant integration, or for large z, by using the first term of the asymptotic expansion of $j_n(z)$ (Ref. 4, Eq. 9.451; Ref. 5, Eq. 10.1.8, which is exact, or Eq. 9.2.1, or 9.2.5, which is equivalent to 10.1.8).

The Fourier inverse of Eq. (16) is

$$\cos[z(1-2\gamma\cos\theta)^{1/2}] = \sum_{n=-\infty}^{\infty}f_n(z,\gamma)\exp(-in\theta) = f_0 + 2\sum_{n=1}^{\infty}f_n(z,\gamma)\cos n\theta, \quad (20)$$

since $f_n = f_{-n}$. A power series expression, obtained from Eq. (19) and the expansion of the j's, is

$$f_r(z,\gamma) = \sqrt{\pi}\sum_{k,n=0}^{\infty}\frac{(-)^n\gamma^{2k+r}(\frac{1}{2}z)^{2r+2n+4k}}{k!n!(r+k)!\Gamma(r+n+2k+\frac{1}{2})}. \quad (21)$$

From either Eq. (19) or Eq. (21), we obtain the recursion relations, with $f' = df/dz$;

$$f_r' = f_r/z + (\gamma z/2r)(f_{r-1} - f_{r+1}) \quad (22)$$

and

$$f_r'' = -f_r + \gamma(f_{r-1} + f_{r+1}), \quad (23)$$

where Eq. (23) is equivalent to the equation of motion of the rth oscillator. Elimination of all terms except those in f_r from the recursion relations yields the fourth-order differential equation

$$\{[(zf_r')' + (2z^2 - 4r^2)(f_r/z)]'/z\}' + (1-4\gamma^2)f_r = 0. \quad (24)$$

For each r, four independent solutions should exist. These are (*i*) $f_r(z,\tau)$, as defined by Eq. (16); (*ii*) the functions obtained by replacing $\cos[z(1-2\gamma\cos\phi)^{1/2}]$ in Eq. (16) by $\sin[z(1-2\gamma\cos\phi)^{1/2}]$; (*iii*) those obtained by replacing $\cos r\phi$ by $\sin r\phi$; and (*iv*) those obtained by making both of these substitutions. Other related functions can be obtained by changing γ to $-\gamma$, $\cos\phi$ to $\sin\phi$, and combining these changes with the other variations. Only the set numbered (i–iv) obey the recursion relations, Eqs. (22) and (23), and satisfy Eq. (24). Of these functions, $f_r(z,\gamma)$ alone is even in z and r; the functions (ii) are odd in z, functions (iii) are odd in r, and functions (iv) are odd in both.

The Laplace transform of Eq. (16) is

$$\bar{f}_r(p,\gamma) = \int_0^\infty e^{-pz}f_n(z,\gamma)dz = \frac{p[(p^2+b^2)^{1/2} - (p^2+a^2)^{1/2}]^{2r}}{[(p^2+a^2)(p^2+b^2)]^{1/2}(4\gamma)^r}, \quad (25)$$

where $a = (1-2\gamma)^{1/2}$ and $b = (1+2\gamma)^{1/2}$. This result is obtained most easily by first integrating with respect to z, and then using Ref. 4, No. 3.613-1 in slightly modified form. From Eq. (25) and a well-known theorem on Laplace transforms, we obtain

$$\lim_{z\to\infty}f_r(z,\gamma) = \lim_{p\to 0}p\bar{f}_r(p,\gamma) = 0, \quad (26)$$

for all $\gamma \le \frac{1}{2}$. The function $g_r(z,\gamma)$, from Eq. (4), is

$$g_r(z,\gamma) = \int_0^z f_r(z',\gamma)dz'; \quad (27)$$

its Laplace transform is $\bar{g}_r(p,\gamma) = \bar{f}_r(p,\gamma)/p$, from which we find

$$\lim_{z\to\infty}g_r(z,\gamma) = \lim_{p\to 0}p\bar{g}_r(p,\gamma) = 0, \qquad \gamma < \tfrac{1}{2}. \quad (28)$$

But when $\gamma = \frac{1}{2}$, the same technique yields

$$\lim_{z\to\infty}g_r(z,\tfrac{1}{2}) = 1/\sqrt{2}, \quad (29)$$

a result that is to be expected from the behavior of $f_r(z,\frac{1}{2})$. As may be seen from Eq. (16) or Eq. (25), $f_r(z,\frac{1}{2}) = J_{2r}(z\sqrt{2})$, from which it follows immediately that $g_r(z,\frac{1}{2}) \to 1/\sqrt{2}$ as $z\to\infty$. It is evident, both physically and mathematically, that the system with $\gamma < \frac{1}{2}$ (i.e., $K \ne 0$) is intrinsically different from the simple chain with $\gamma = \frac{1}{2}$ or $K = 0$. Since the simple chain has been treated in detail by us elsewhere,[2,6] we shall assume in this paper that the inequality $\gamma < \frac{1}{2}$ is strictly valid.

The inverse Laplace transform, which may be used to obtain an asymptotic expression for $f_r(z,\gamma)$, is given by

$$f_r(z,\gamma) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dp\,e^{zp}\bar{f}_r(p,\gamma), \quad (30)$$

where the path of integration is to the right of all singularities of $\bar{f}_r(p,\gamma)$. Since these singularities are all square roots, at $p = \pm ia, \pm ib$, the contour can be shifted infinitely far to the left except for the path around the four branch cuts, which extend infinitely to the left of the imaginary p axis, parallel to the real p axis, starting at the singular points. The only contributions to the integral of Eq. (30) come from the sections of path along the branch cuts. For large z, the only significant parts of the path correspond to Re $p \approx 0$. Therefore the small-Re p expansion of the integrand along each of the branch cuts leads to an asymptotic expression for $f_r(z, \gamma)$, as

$$f_r(z,\gamma) \sim (2\pi\gamma z)^{-1/2}[(-)^r\sqrt{b}\,\cos(bz - \tfrac{1}{4}\pi) + \sqrt{a}\,\cos(az + \tfrac{1}{4}\pi)], \tag{31}$$

where $a = (1 - 2\gamma)^{1/2}$ and $b = (1 + 2\gamma)^{1/2}$. The asymptotic expression (31) is somewhat more accurate than that of Eq. (8a), although for small γ the expressions are essentially in agreement. The principal fault with Eq. (8a) lies in its failure to represent the phase accurately for large z, and not in its amplitude behavior. A recent paper by Agarwal[7] treats the small-γ approximation quantum mechanically.

In Sec. 3, we shall need certain infinite sums of products of the functions f_r and g_r; these will be calculated here. The first of these is given by

$$\sum_{n=-\infty}^{\infty} f_n(z,\gamma) f_{n+m}(z',\gamma) = (2\pi)^{-2}\int_{-\pi}^{\pi}d\theta\int_{-\pi}^{\pi}d\phi\ \cos[z(1-2\gamma\cos\theta)^{1/2}] \times \cos[z'(1-2\gamma\cos\phi)^{1/2}]\ \exp(im\phi) \times \sum_{n=-\infty}^{\infty}\exp[in(\theta+\phi)]. \tag{32}$$

We simplify Eq. (32) by the use of the equivalence

$$\sum_{n=-\infty}^{\infty}\exp(inx) = 2\pi\delta(x), \tag{33}$$

to obtain

$$\sum_{n=-\infty}^{\infty} f_n(z,\gamma) f_{n+m}(z',\gamma) = (2\pi)^{-1}\int_{-\pi}^{\pi}d\phi\,\exp(im\phi) \times \cos[z(1-2\gamma\cos\phi)^{1/2}]\cos[z'(1-2\gamma\cos\phi)^{1/2}], \tag{34}$$

which may be rewritten by the use of trigonometric identities as

$$\sum_{n=-\infty}^{\infty} f_n(z,\gamma) f_{n+m}(z',\gamma) = \frac{1}{2}\,[f_m(z+z',\gamma) + f_m(z-z',\gamma)]. \tag{35}$$

Similarly, we can show that

$$\sum_{n=-\infty}^{\infty} f_n(z,\gamma)\,df_{n+m}(z,\gamma)/dz = \frac{1}{4}\,df_m(2z,\gamma)/dz, \tag{36}$$

$$\sum_{n=-\infty}^{\infty} f_n(z,\gamma) g_{n+m}(z,\gamma) = \frac{1}{2} g_m(2z,\gamma), \tag{37}$$

and

$$\sum_{n=-\infty}^{\infty} g_n(z,\gamma) g_{n+m}(z,\gamma) = [(\eta/\gamma)^{|m|}/2(1-2\eta)] - F_m(2z,\gamma), \tag{38}$$

where $\gamma^2 = \eta(1-\eta)$, $0 < \eta < \frac{1}{2}$, and F_m is defined as

$$F_m(z,\gamma) = (2\pi)^{-1}\int_0^{\pi}\frac{d\theta\,\cos m\theta}{1-2\gamma\cos\theta} \times\cos[z(1-2\gamma\cos\theta)^{1/2}]. \tag{39}$$

For present purposes, the function $F_m(z,\gamma)$ is needed only for $z \to \infty$, at which limit $F_m(z,\gamma) \to 0$, and at $z = 0$, for which we have

$$F_m(0,\gamma) = \frac{(\eta/\gamma)^{|m|}}{2(1-2\eta)}. \tag{40}$$

Another type of useful sum is, for $|x| < 1$,

$$\sum_{n=1}^{\infty} x^n f_{n+m}(z,\gamma) = \left(\frac{x}{2\pi}\right)\int_{-\pi}^{\pi}\frac{d\theta\,\exp(im\theta)\cos[z(1-2\gamma\cos\theta)^{1/2}][\exp(i\theta)-x]}{1-2x\cos\theta+x^2}, \tag{41}$$

which, for $x = \gamma/(1-\eta)$, can be written as

$$\sum_{n=1}^{\infty}\left(\frac{\gamma}{1-\eta}\right)^n f_{n+m}(z,\gamma) = 2\gamma F_{m+1}(z,\gamma) - 2\eta F_m(z,\gamma). \tag{42}$$

Other similar or more complicated sums can be developed directly from the definitions of the functions involved by the techniques already shown. Some of these are available, upon request, as long as the supply lasts.[8]

3. EQUILIBRATION WITH CANONICAL INITIAL CONDITIONS

The entropy of Eq. (13) is obtained from the covariance matrix W of Eq. (11) by the use of Eq. (15) and its counterparts. Since our original treatment of the problem[2,3] with non-zero-centered initial distributions of the system variables has shown that only the variances of these variables enter the calculation of W, we simplify the notational difficulties in this paper by choosing zero-centered probability densities, both for system variables and for the heat bath. In this section, our choice of the initial probability density for the heat-bath variables is a slight generalization of the canonical one, in that we allow for different kinetic and potential temperatures, in the sense that the kinetic and potential energies of the heat bath are given different Boltzmann factors. We write for $\rho(\{x\}, \{p\}, t)$ at $t = 0$

$$\rho_0(\{x\},\{p\}) = \prod_{n=1}^{N} \frac{\exp(-x_n^2/2\alpha^2)}{\alpha(2\pi)^{1/2}} \prod_{n=1}^{N} \frac{\exp(-p_n^2/2\delta^2)}{\delta(2\pi)^{1/2}} \Pi' \frac{\exp(-p_n^2/2\zeta^2)}{\zeta(2\pi)^{1/2}}$$

$$\times \Pi' \frac{\exp[-(m\beta\Omega^2/2)\{x_n^2(1-2\gamma)+\gamma(x_{n+\nu}-x_n)^2\}]}{A_n}, \quad (43)$$

where Π' denotes the product over all except the variables numbered $1-N$, ν in the last factor is $+1$ for $n > N$, -1 for $n < 1$, and the normalization denominator A_n is given by

$$A_{N+r} = A_{1-r} = (2\pi/m\beta\Omega^2 a_r)^{1/2}, r > 0, \quad (44)$$

where

$$a_1 = 1-\gamma, \quad (45)$$

and the higher a_r's are given by the continued fraction

$$a_{r+1} = 1-\gamma^2 a_r^{-1}. \quad (46)$$

In all integrations involving the last factor of Eq. (43), we have started with the x coordinate just outside the system (x_0 or x_{N+1}) and proceeded, through successive coordinates, away from the system variables. By the use of standard definite integrals, we establish the result, for $r > 0$ and $s \geq 0$, that

$$\langle x_{N+r}(0)x_{N+r+s}(0)\rangle = (\gamma m\beta\Omega^2)^{-1} \prod_{n=r}^{r+s} \frac{\gamma}{a_n} Q_{r+s}, \quad (47)$$

where Q_r is a series, resulting from successive integrations, defined by

$$Q_r = 1 + (\gamma^2/a_r a_{r+1}) + (\gamma^4/a_r a_{r+1}^2 a_{r+2}) + (\gamma^6/a_r a_{r+1}^2 a_{r+2}^2 a_{r+3}) + \cdots, \quad (48)$$

which satisfies the recursion relation

$$Q_r = 1 + (\gamma^2/a_r a_{r+1})Q_{r+1}. \quad (49)$$

An identical result is found for $\langle x_{1-r}(0)x_{1-r-s}(0)\rangle$, $r > 0, s \geq 0$.

Although the potential energy of an oscillator is somewhat ambiguous for these coupled systems, we write the total potential energy of the heat bath (say $r > N$) as

$$\mathrm{PE} = \frac{K}{2}\sum_{r=N+1}^{\infty} x_r^2 + \frac{K}{2}\sum_{r=n}^{\infty}(x_{r+1}-x_r)^2 = (\tfrac{1}{2}m\Omega^2)[(1-\gamma)x_{N+1}^2 - 2\gamma x_{N+1}x_{N+2} + x_{N+2}^2 - 2\gamma x_{N+2}x_{N+3} + \cdots]; \quad (50)$$

from this expression, we define the expectation value of the initial potential energy of the rth oscillator, $r > N+1$, as

$$\langle \mathrm{PE}_r\rangle_0 = (m\Omega^2/2)[\langle x_r^2\rangle_0 - \gamma(\langle x_{r-1}x_r\rangle_0 + \langle x_r x_{r+1}\rangle_0)]. \quad (51)$$

By use of Eq. (47) and the recursion relations, Eqs. (46) and (49), we directly obtain the result

$$\langle \mathrm{PE}_r\rangle_0 = \frac{1}{2}\beta, \quad (52)$$

as should be expected.

Also from Eq. (46) we derive an explicit expression for a_r as

$$a_r = \frac{\gamma[\eta^r-(1-\eta)^r]-[\eta^{r+1}-(1-\eta)^{r+1}]}{\gamma[\eta^{r-1}-(1-\eta)^{r-1}]-[\eta^r-(1-\eta)^r]}, \quad (53)$$

where η appears in Eq. (38). Similarly, from Eq. (49) we obtain

$$Q_r = [\gamma^2/(a_r-a_{r+1})][a_\infty^{-1}-a_{r-1}^{-1}], \quad (54)$$

where $a_\infty = \lim_{r\to\infty} a_r = 1-\eta$.

By combining Eqs. (47), (53), and (54) we obtain after some manipulation a closed form for expression (47)

$$\langle x_{N+r}(0)x_{N+r+s}(0)\rangle = \frac{\gamma^s(1-\eta)^{-s}[U+\eta^{r-1}(1-\eta)^{1-r}]}{\beta m\Omega^2 U(1-2\eta)}, \quad (55)$$

where $U = (1-\gamma-\eta)/(\gamma-\eta)$. Correlation functions and expectation values other than this one can be found at $t = 0$ by inspection from Eq. (43).

We can now use Eq. (2) to find the covariance matrix at a later time. Using the evident consequence of Eq. (43) that $\langle x_m(0)p_m(0)\rangle = 0$, we find

$$\langle x_n(t)x_{n+m}(t)\rangle = \sum_{k,r}\langle x_k(0)x_r(0)\rangle f_{n-k}(t)f_{n+m-r}(t) + \sum_{k,r}\langle p_k(0)p_r(0)\rangle g_{n-k}(t)g_{n+m-r}(t)/m^2\Omega^2. \quad (56)$$

By a complicated though elementary series of computations this can be expressed in a more readily manipulated form.[8] The result is of specialized interest only and is not written out here.

The limiting case of large times is fairly simple, however,

$$\langle x_n(t)x_{n+r}(t)\rangle_\infty = \frac{\zeta^2}{m^2\Omega^2}\left(\frac{1}{2(1-2\eta)}\left(\frac{\eta}{\gamma}\right)^r\right) + \frac{1}{2\beta m\Omega^2(1-2\eta)}\left(\frac{\gamma}{1-\eta}\right)^r. \quad (57)$$

Similarly,

$$\langle x_n(t)p_m(t)\rangle_\infty = 0, \tag{58}$$

$$\langle p_n(t)p_{n+r}(t)\rangle_\infty = \delta_{r,0}[\zeta^2 + (m/\beta)]/2. \tag{59}$$

The average potential energy and average kinetic energy are readily found and satisfy equipartition with a temperature given by

$$k_B T = (\zeta^2/2m) + 1/2\beta. \tag{60}$$

The entropy of the N-particle system can be computed from Eq. (13). As a function of time the entropy approaches its equilibrium value, but it also exhibits oscillations.[9] These oscillations occur because the heat bath is affected by the system for a finite time and this in turn alters the way that the heat bath affects the system.

As $t\to\infty$, the entropy S_N approaches a simple expression. We find by a straightforward calculation that

$$S_N(\infty) = Nk_B + Nk_B \ln[k_B T/\hbar\Omega(1-\eta)^{1/2}] + (k_B/2)\ln(1-\eta)/(1-2\eta). \tag{61}$$

For large N, this approximately satisfies $S_N = NS_1$, and if $\gamma = 0$ (uncoupled oscillators), this property is exact.

4. EQUILIBRATION WITH NONCANONICAL INITIAL CONDITIONS

Instead of starting from a set of initial conditions as in Eq. (43), where the masses and springs of the heat bath are assigned definite temperatures, we shall now assume an initial distribution that eliminates the awkward cross terms in the final exponent of that equation. We write

$$\rho_0(\{x\},\{p\}) = \prod_{n=1}^{N} \frac{\exp(-x_n^2/2\alpha^2)}{\alpha(2\pi)^{1/2}} \prod_{n=1}^{N} \frac{\exp(-p_n^2/2\delta^2)}{\delta(2\pi)^{1/2}} \times \Pi' \frac{\exp(-p_n^2/2\zeta^2)}{\zeta(2\pi)^{1/2}} \Pi' \frac{\exp(-x_n/2\epsilon^2)}{\epsilon(2\pi)^{1/2}}. \tag{62}$$

The factors for the heat bath no longer have the form $\exp(-\beta H)$, and they are now sufficiently simple that all of the initial conditions for the covariance matrix can be read off easily.

When these are time-developed we obtain, for example,

$$\langle x_n(t)x_{n+r}(t)\rangle = (\alpha^2-\epsilon^2)\sum_{k=1}^{N} f_{n-k}f_{n+r-k} + \epsilon^2 \sum_{-\infty}^{\infty} f_{n-k}f_{n+r-k} + (\delta^2-\zeta^2)\sum_{k=1}^{N} g_{n-k}g_{n+r-k}/m^2\Omega^2 + \zeta^2\sum_{-\infty}^{\infty} g_{n-k}g_{n+r-k}/m^2\Omega^2. \tag{63}$$

The infinite sums in this expression have been calculated in Eqs. (35) and (38).

In the limit as $t\to\infty$, the finite sums vanish and the rest leaves us with

$$\langle x_n(t)x_{n+r}(t)\rangle_\infty = \frac{\epsilon^2}{2}\delta_{r,0} + \frac{\zeta^2}{2m^2\Omega^2(1-2\eta)}\left(\frac{\eta}{\gamma}\right)^r. \tag{64}$$

A similar calculation, using the second derivative of Eq. (35) with respect to z and z' (at $z = z'$), together with Eq. (23) yields

$$\langle p_n(t)p_{n+r}(t)\rangle_\infty = \tfrac{1}{2}(m^2\Omega^2\epsilon^2 + \zeta^2)\delta_{r,0} - \tfrac{1}{2}\gamma m^2\Omega^2\epsilon^2(\delta_{r,1}+\delta_{r,-}). \tag{65}$$

Again, using Eqs. (36) and (37) we find for $t\to\infty$,

$$\langle x_n(t)p_{n+m}(t)\rangle_\infty = 0. \tag{66}$$

As in previous calculations using a noncanonical distribution[2,3,6], we see a nearest-neighbor correlation in momentum.

The expression for the entropy of the N-particle system Eq. (13) does not yield a simple expression in this case. We can however find an approximate result for the case of weak coupling ($\gamma \ll 1$). With

$$k_B T = \tfrac{1}{2}(\zeta^2/m) + \tfrac{1}{2}(m\Omega^2\epsilon^2) \tag{67}$$

we have

$$S_N \approx Nk_B + Nk_B\ln(k_B T/\hbar\Omega). \tag{68}$$

For definite, small values of N, the entropy has been calculated as a function of time[9] with the result that $S_N(t)$ has the expected increasing tendency with damped oscillations superimposed. The oscillations are less important as N is increased.

5. CONCLUSION

The harmonically bound chain of coupled oscillators is of interest principally as model of a system of weakly interacting particles approaching equilibrium. Even in the case when coupling is not weak, however, the approach of a finite segment of the infinite chain to equilibrium can be treated exactly, with results that agree in most cases with our expectations. Potential and kinetic energies are exactly equipartitioned, when the infinite-time analog of Eq. (51) is used for the potential energy, even when the initial description of the heat bath is not canonical.

Residual nearest-neighbor momentum correlations are found, as in Eq. (65), when the initial description of the heat bath is not canonical, and nonextensive terms appear in the equilibrium entropy. Both of these phenomena have been discussed, especially in Ref. 6, and the discussion need not be repeated here.

The quantum-mechanical treatment of Agarwal[7] can be transcribed with little change when the exact functions of Eqs. (3) and (4) are used instead of the approximations of Eqs. (8).

ACKNOWLEDGMENT

This work was supported in part by the United States Atomic Energy Commission.

1 H. S. Robertson and M. A. Huerta, Phys. Rev. Letters 23, 825 (1969).
2 M. A. Huerta and H. S. Robertson, J. Stat. Phys. 1, 393 (1969).
3 H. S. Robertson and M. A. Huerta, Am. J. Phys. 38, 619 (1970).
4 I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1965)
5 M. Abramowitz and I. A. Stegun, Editors, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (U.S. GPO, Washington, D.C., 1964).
6 M. A. Huerta and H. S. Robertson, J. Stat. Phys. 3, 171 (1971).
7 G. S. Agarwal, Phys. Rev. A 3, 828 (1971).
8 M. A. Huerta, thesis, University of Miami, 1969.
9 H. S. Robertson and M. A. Huerta, Pure Appl. Chem. 22, 409 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Excited State Reduced Coulomb Green's Function and f-Dimensional Coulomb Green's Function in Momentum Space

Levere Hostler
Physics Department, Wilkes College, Wilkes-Barre, Pennsylvania 18703
(Received 14 May 1971)

An integral representation for the f-dimensional nonrelativistic Coulomb Green's function in momentum space and an expansion of this function in a series of Gegenbauer polynomials are obtained. It is shown that the momentum space representatives of the f-dimensional Coulomb Green's function and the related reduced Green's functions can be obtained by differentiation with respect to the momentum transfer of the corresponding functions in the one-dimensional (f odd) or two-dimensional (f even) case. Expressions in closed form are then obtained for the momentum space representatives in the one-dimensional case of the full Coulomb Green's function and of the general nth excited state reduced Coulomb Green's function.

I. INTRODUCTION

Previous work[1,2] on the f-dimensional nonrelativistic Coulomb Green's function and related functions has been concerned with their coordinate space representatives. Momentum space representatives were treated in the three-dimensional case[3,4] and only for the full Green's function.[5] We will here investigate the momentum space representatives of the Coulomb Green's function and related structures in the general f-dimensional case.

We begin by indicating briefly the derivation of an integral representation [Eq. (8)] of the full f-dimensional Coulomb Green's function in momentum space, along the lines of the previous work of Hostler.[4] By the use of this new integral representation we show that a relation derived earlier,[6] connecting the coordinate space Coulomb Green's functions and reduced Green's functions in spaces of different dimensionality, has a momentum space counterpart [Eq. (10)] in which differentiation with respect to the momentum transfer raises the dimensionality of the momentum space structure from f to $f+2$.

The integral representation Eq. (8) is converted into an expansion of the f-dimensional momentum space Coulomb Green's function in a series of Gegenbauer polynomials ($f = 2, 3, 4, \ldots$) or Tchebichef polynomials ($f = 1$) [See Eqs. (16) and (25), respectively], by expanding the integrand and integrating term by term. This generalizes to the f-dimensional case a previous three-dimensional result due to Schwinger.[7] In the two-dimensional case the Gegenbauer expansion becomes a Legendre series expansion [Eq. (27)].

In the one-dimensional case, the Tchebichef expansion is found to lead to a closed-form expression for the general nth excited state momentum space reduced Coulomb Green's function [Eq. (71)]. This structure is remarkable in that it is without hypergeometric functions. By successive differentiation with respect to the momentum transfer, one can now generate all corresponding structures in a space of any higher odd dimensionality.

II. INTEGRAL REPRESENTATION AND RECURSION RELATION IN f-DIMENSIONAL SPACE

The f-dimensional Coulomb Green's function in momentum space will be defined as the Fourier transform

$$G_f(\mathbf{k}_2, \mathbf{k}_1, E) = \int d^f r_2 d^f r_1 e^{i\mathbf{k}_1\cdot\mathbf{r}_1 - i\mathbf{k}_2\cdot\mathbf{r}_2} G_f(\mathbf{r}_2, \mathbf{r}_1, E) \quad (1)$$

of the coordinate space Green's function, defined as the solution of the differential equation

$$[\nabla_2^2 + (2k\nu/r_2) + k^2] G_f(\mathbf{r}_2, \mathbf{r}_1, E) = \delta^f(\mathbf{r}_2 - \mathbf{r}_1),$$
$$k = (2mE/\hbar^2)^{1/2}, \quad \mathrm{Im}(k) > 0 \quad (2)$$

subject to suitable regularity conditions at the origin and at infinity. Here ∇^2 denotes the Laplacian

The quantum-mechanical treatment of Agarwal[7] can be transcribed with little change when the exact functions of Eqs. (3) and (4) are used instead of the approximations of Eqs. (8).

ACKNOWLEDGMENT

This work was supported in part by the United States Atomic Energy Commission.

1 H. S. Robertson and M. A. Huerta, Phys. Rev. Letters **23**, 825 (1969).
2 M. A. Huerta and H. S. Robertson, J. Stat. Phys. **1**, 393 (1969).
3 H. S. Robertson and M. A. Huerta, Am. J. Phys. **38**, 619 (1970).
4 I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1965)
5 M. Abramowitz and I. A. Stegun, Editors, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (U.S. GPO, Washington, D.C., 1964).
6 M. A. Huerta and H. S. Robertson, J. Stat. Phys. **3**, 171 (1971).
7 G. S. Agarwal, Phys. Rev. A **3**, 828 (1971).
8 M. A. Huerta, thesis, University of Miami, 1969.
9 H. S. Robertson and M. A. Huerta, Pure Appl. Chem. 22, 409 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Excited State Reduced Coulomb Green's Function and f-Dimensional Coulomb Green's Function in Momentum Space

Levere Hostler
Physics Department, Wilkes College, Wilkes-Barre, Pennsylvania 18703
(Received 14 May 1971)

An integral representation for the f-dimensional nonrelativistic Coulomb Green's function in momentum space and an expansion of this function in a series of Gegenbauer polynomials are obtained. It is shown that the momentum space representatives of the f-dimensional Coulomb Green's function and the related reduced Green's functions can be obtained by differentiation with respect to the momentum transfer of the corresponding functions in the one-dimensional (f odd) or two-dimensional (f even) case. Expressions in closed form are then obtained for the momentum space representatives in the one-dimensional case of the full Coulomb Green's function and of the general nth excited state reduced Coulomb Green's function.

I. INTRODUCTION

Previous work[1,2] on the f-dimensional nonrelativistic Coulomb Green's function and related functions has been concerned with their coordinate space representatives. Momentum space representatives were treated in the three-dimensional case[3,4] and only for the full Green's function.[5] We will here investigate the momentum space representatives of the Coulomb Green's function and related structures in the general f-dimensional case.

We begin by indicating briefly the derivation of an integral representation [Eq. (8)] of the full f-dimensional Coulomb Green's function in momentum space, along the lines of the previous work of Hostler.[4] By the use of this new integral representation we show that a relation derived earlier,[6] connecting the coordinate space Coulomb Green's functions and reduced Green's functions in spaces of different dimensionality, has a momentum space counterpart [Eq. (10)] in which differentiation with respect to the momentum transfer raises the dimensionality of the momentum space structure from f to $f + 2$.

The integral representation Eq. (8) is converted into an expansion of the f-dimensional momentum space Coulomb Green's function in a series of Gegenbauer polynomials ($f = 2, 3, 4, \ldots$) or Tchebichef polynomials ($f = 1$) [See Eqs. (16) and (25), respectively], by expanding the integrand and integrating term by term. This generalizes to the f-dimensional case a previous three-dimensional result due to Schwinger.[7] In the two-dimensional case the Gegenbauer expansion becomes a Legendre series expansion [Eq. (27)].

In the one-dimensional case, the Tchebichef expansion is found to lead to a closed-form expression for the general nth excited state momentum space reduced Coulomb Green's function [Eq. (71)]. This structure is remarkable in that it is without hypergeometric functions. By successive differentiation with respect to the momentum transfer, one can now generate all corresponding structures in a space of any higher odd dimensionality.

II. INTEGRAL REPRESENTATION AND RECURSION RELATION IN f-DIMENSIONAL SPACE

The f-dimensional Coulomb Green's function in momentum space will be defined as the Fourier transform

$$G_f(\mathbf{k}_2, \mathbf{k}_1, E) = \int d^f r_2 d^f r_1 e^{i\mathbf{k}_1\cdot\mathbf{r}_1 - i\mathbf{k}_2\cdot\mathbf{r}_2} G_f(\mathbf{r}_2, \mathbf{r}_1, E) \quad (1)$$

of the coordinate space Green's function, defined as the solution of the differential equation

$$[\nabla_2^2 + (2k\nu/r_2) + k^2] G_f(\mathbf{r}_2, \mathbf{r}_1, E) = \delta^f(\mathbf{r}_2 - \mathbf{r}_1),$$
$$k = (2mE/\hbar^2)^{1/2}, \quad \mathrm{Im}(k) > 0 \quad (2)$$

subject to suitable regularity conditions at the origin and at infinity. Here ∇^2 denotes the Laplacian operator of the f-dimensional space. The parameters k and ν are regarded as independent complex parameters, arbitrary except for the condition $\mathrm{Im}(k) > 0$. An integral representation of the f-dimensional Coulomb Green's function in momentum space will be obtained here from the integral representation[8]

$$G_f(\mathbf{r}_2,\mathbf{r}_1,E) = \frac{(-ik)^{f-2}}{(4\pi)^{(f-1)/2}} e^{\pi i[i\nu-(f-1)/2]} \times \frac{\pi}{\sin\pi[i\nu - \frac{1}{2}(f-1)]} \times \frac{1}{2\pi i}\int_{+\infty;\,\mathrm{arc}(\zeta+1)=0}^{(1+)} d\zeta(\zeta+1)^{i\nu+(f-3)/2} \times (\zeta-1)^{-i\nu+(f-3)/2} D_f(\mathbf{r}_2,\mathbf{r}_1,E), \tag{3a}$$

$$D_f(\mathbf{r}_2,\mathbf{r}_1,E) = \frac{I_{(f-3)/2}(-ik(x^2-y^2)^{1/2}(\zeta^2-1)^{1/2})}{(-\frac{1}{2}ik(x^2-y^2)^{1/2}(\zeta^2-1)^{1/2})^{1/2(f-3)}} \times e^{ikx\zeta},$$
$$x = r_2 + r_1, \quad y = |\mathbf{r}_2 - \mathbf{r}_1|,$$
$$f = 1,2,3,4,\ldots \tag{3b}$$

of the f-dimensional coordinate space Green's function, by Fourier transforming the integrand, $D_f(\mathbf{r}_2,\mathbf{r}_1,E)$. This calculation parallels closely that of earlier work on the three-dimensional case and will be reported here only briefly, to point out the new features that enter when one considers the general case of arbitrary dimensionality.

We give details only for $f = 2,3,4,\ldots$. The one-dimensional problem requires special attention (see remarks at the end of this section), but a separate calculation verifies that our final result [Eq. (8)] holds also in the one-dimensional case.

As in the three-dimensional case, one begins with the integral representation[9]

$$\frac{I_{(f-3)/2}(z)}{(z/2)^{(f-3)/2}} = \frac{1}{2\pi i}\int_{c-i\infty;\,c>0}^{c+i\infty} t^{-(f-1)/2} e^{t+(z^2/4t)}dt, \qquad f = 2,3,4,\ldots, \tag{4}$$

of the Bessel function. One proceeds as in Ref. 4, but with the use of the new integral (assumed convergent)[10]

$$\int d^f r e^{-Ar-\mathbf{B}\cdot\mathbf{r}} = (4\pi)^{(f-1)/2}\Gamma(\tfrac{1}{2}(f+1))\frac{2A}{(A^2-\mathbf{B}\cdot\mathbf{B})^{(f+1)/2}} \tag{5}$$

and the integrals obtained from Eq. (5) by differentiation with respect to A or $\mathbf{B}$, respectively. After performing the $\mathbf{r}_1$ integration, one obtains a t integral of the form

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dt\, e^t(t-a)^{-\lambda} = \frac{e^a}{\Gamma(\lambda)},$$
$$|\mathrm{arc}(t-a)| < \pi/2, \quad c > \mathrm{Re}(a), \quad \mathrm{Re}(\lambda) > 0. \tag{6}$$

A point of difference with the previous three-dimensional calculation is encountered here. In the previous three-dimensional calculation, Eq. (6) was needed only for positive integral λ and was readily established by means of the Cauchy residue theorem. This method is still adequate in the general case of a space of any odd dimensionality; but if the dimensionality of the space is even, then Eq. (6) is needed for half-integral λ and the method fails. However, Eq. (6) can be established quite generally in terms of a standard representation of the reciprocal gamma function by translating the origin of the integration variable and deforming the integration contour.[11] The final integration over $\mathbf{r}_2$ can be performed using the same integrals, based on Eq. (5), as the first $\mathbf{r}_1$ integral. The result of this calculation is

$$D_f(\mathbf{k}_2,\mathbf{k}_1,E) = -(4\pi)^{f-1}\Gamma(\tfrac{1}{2}(f+1))2k^2 \times \frac{(k_2^2-k^2)(k_1^2-k^2)(f\zeta^2-1)+k^2|\mathbf{k}_2-\mathbf{k}_1|^2(\zeta^4-1)}{[(k_2^2-k^2)(k_1^2-k^2)-k^2|\mathbf{k}_2-\mathbf{k}_1|^2(\zeta^2-1)]^{(f+3)/2}},$$
$$f = 1,2,3,\ldots, \tag{7}$$

where $D_f(\mathbf{k}_2,\mathbf{k}_1,E)$ is the Fourier transform of $D_f(\mathbf{r}_2,\mathbf{r}_1,E)$, Eq. (3b). A separate treatment of the one-dimensional case leads to the result that Eq. (7) holds also for $f = 1$. Thus as pointed out above, the following result obtained by using Eq. (7) in conjunction with Eq. (3a), holds also in the one-dimensional case. This result is

$$G_f(k_2,k_1,q,E) = (-ik)^f(4\pi)^{(f-1)/2}\Gamma(\tfrac{1}{2}(f+1)) \times e^{\pi i(i\nu-(f-1)/2)}\frac{\pi}{\sin\pi[i\nu-\frac{1}{2}(f-1)]} \cdot \frac{1}{2\pi i}\int_{+\infty;\,\mathrm{arc}(\zeta+1)=0}^{(1+)} d\zeta(\zeta+1)^{i\nu+(f-3)/2} \times (\zeta-1)^{-i\nu+(f-3)/2}\cdot 2\frac{[p^2(f\zeta^2-1)+q^2k^2(\zeta^4-1)]}{[p^2-q^2k^2(\zeta^2-1)]^{(f+3)/2}},$$
$$f = 1,2,3,4,\ldots, \tag{8}$$

in which

$$q \equiv |\mathbf{k}_2 - \mathbf{k}_1| \text{ and } p^2 \equiv (k_2^2-k^2)(k_1^2-k^2). \tag{9}$$

This is the desired integral representation of the f-dimensional nonrelativistic Coulomb Green's function in momentum space. It generalizes to f-dimensional space the earlier three-dimensional result obtained in Ref. 4. It shares with this previous three-dimensional result the property of extracting the Z dependence of the Green's function.[12] It is this property of extracting the Z dependence which makes the integral representation (8) attractive from the point of view of applications. Although the momentum space Green's function depends upon $\mathbf{k}_1$ and $\mathbf{k}_2$ only through the two variables q and p^2 and not three as allowed by f-dimensional rotational invariance, we prefer to write the functional dependence in the form $G_f(k_2,k_1,q,E)$, in which the entire energy dependence is explicit. This will be helpful in the subsequent calculations in which differentiations with respect to energy occur. Also, differentiation with respect to the energy will spoil the functional dependence upon only the two combinations q and p^2, which for us will undo an apparent advantage in writing the Green's function as a function of only these two variables.

It is now a straightforward matter to obtain the relationship

$$-2\pi\frac{\partial G_f(k_2,k_1,q,E)}{q\partial q}=G_{f+2}(k_2,k_1,q,E), \qquad (10)$$

which exists between the momentum space Coulomb Green's functions in spaces of different dimensionality. One merely applies the operation $-2\pi\partial/q\partial q$ to both sides of Eq. (8). On the right-hand side, one takes the derivative under the integral sign, whereby the integrand for G_f is converted into the integrand for G_{f+2}. That the result (10) also applies to the momentum space reduced Coulomb Green's functions, follows as in the previous work on the coordinate space representatives.[13] We have here a prescription for obtaining all momentum space Coulomb Green's functions and reduced Green's functions in f-dimensional space by differentiating successively the corresponding functions in the one-dimensional (f odd) or two-dimensional (f even) case. Among the results to be obtained in the following will be the derivation of closed-form expressions for these structures in the one-dimensional case.

Before proceeding, however, the one-dimensional problem will be considered in more detail. The one-dimensional Green's function of Meixner, obtained by substituting $f=1$ in Eq. (3a), is defined only on the semiinfinite line $0<r<+\infty$. In order to define a momentum space representative, we must in some way continue the domain of the function into the negative half-line and zero.

We adopt the following prescription for this: Introduce Cartesian position coordinates $x_{1,2}$ in the one-dimension space, where $-\infty<x_{1,2}<+\infty$, and interpret the variables x and y of Eq. (3b) in the natural way as $x\equiv r_2+r_1$ and $y\equiv|x_2-x_1|$, where $r_{1,2}\equiv|x_{1,2}|$. One can now Fourier transform and will find that the momentum space representative is correctly given by Eq. (8) with $f=1$. The mechanics of obtaining the Fourier transform are basically the same as in the case $f=2,3,4,\ldots$ considered above. [The integral representation for $I_{-1}(z)/(\frac{1}{2}z)^{-1}$ obtained by substituting $f=1$ in Eq. (4) does not converge, but by use of the relation[14] $I_{-1}(z)=I_1(z)$, one can express $D_1(\mathbf{r}_2,\mathbf{r}_1,E)$ of Eq. (3b) in terms of $I_1(z)/(\frac{1}{2}z)$ for which we do have a convergent integral representation, Eq. (4) with $f=5$.]

A final remark about the one-dimensional Green's function will be made here for future reference. The free-particle limit of Meixner's Green's function takes the form

$$G_1^{(0)}(x_2,x_1,E)=(2ik)^{-1}(e^{ik|x_2-x_1|}-e^{ik(r_2+r_1)}), \qquad (11)$$

when the domain of his function is continued to encompass the whole real line, as described above. This Green's function is the difference of two ordinary Green's functions over the whole real line, one corresponding to a delta function source term at $x_2=x_1$ of strength unity, and one corresponding to a delta function source term at $x_2=0$ of strength $-\exp ikr_1$.

The full one-dimensional Coulomb Green's function, as defined above on the whole real line, likewise has two source terms as evidenced by the fact that it satisfies the Green's function equation[15]

$$\left[\frac{\partial^2}{\partial x_2}+\frac{2k\nu}{r_2}+k^2\right]G_1(x_2,x_1,E)=\delta(x_2-x_1)$$
$$-\delta(x_2)\,\Gamma(1-i\nu)\,W_{i\nu;\,1/2}(-2ikr_1), \qquad (12)$$

in which there are two delta functions instead of only one. However, no decomposition analogous to Eq. (11) of the full Coulomb Green's function $G_1(x_2,x_1,E)$ into two Green's functions corresponding, respectively, to the two source terms of Eq. (12) is known. One can check that $G_1^{(0)}(x_2,x_1,E)$ of Eq. (11) satisfies the free-particle limit of Eq. (12).[16] Also the extraneous delta function source term at the origin in Eq. (12) vanishes in the domain $x_{1,2}>0$, where $G_1(x_2,x_1,E)$ reduces to Meixner's original Green's function.

III. EXPANSION IN GEGENBAUER/TCHEBICHEF POLYNOMIALS

By means of the change of variables

$$t=(\zeta-1)(\zeta+1)^{-1}, \qquad (13)$$

the integral representation (8) can be brought to the form

$$G_f(k_2,k_1,q,E)=-\tfrac{1}{2}(4\pi)^{(f-1)/2}\,\frac{(-2ik)^f}{p^{f+1}}$$
$$\times\,\Gamma(\tfrac{1}{2}(f+1))\,e^{\pi i(i\nu-(f-1)/2)}\,\frac{\pi}{\sin\pi[i\nu-\frac{1}{2}(f-1)]}$$
$$\times\frac{1}{2\pi i}\int_{1;\,\mathrm{arc}\,(t)=0}^{(0+)}dt\,t^{-i\nu+(f-3)/2}$$
$$\times\frac{[-(f-1)+2t^2(f+3)-(f-1)t^4-4xt(1+t^2)]}{(1-2tx+t^2)^{(f+3)/2}},$$
$$x\equiv 1+2k^2q^2p^{-2},\quad f=1,2,3,4,\ldots, \qquad (14)$$

in which the generating function[17]

$$(1-2tx+t^2)^{-\nu}=\sum_{n=0}^{\infty}t^nC_n^\nu(x),\ \nu\neq 0 \qquad (15)$$

of the Gegenbauer polynomials appears. One can expand the integrand of Eq. (14) in a series of Gegenbauer polynomials and integrate term by term. One then obtains the infinite series expansion

$$G_f(k_2,k_1,q,E)=\sum_{n=1}^{\infty}-(4\pi)^{(f-1)/2}\frac{(-2ik)^f}{p^{f+1}}\times\Gamma(\tfrac{1}{2}(f-1))\frac{[n+\frac{1}{2}(f-3)]^2C_{n-1}^{(f-1)/2}(x)}{-i\nu+n+\frac{1}{2}(f-3)},\quad f=2,3,4,5,\ldots. \tag{16}$$

As pointed out before, this result generalizes a previous three-dimensional result due to Schwinger.[7] The functional dependence upon the nuclear charge Z occurs in the expansion (16) only in the denominator $[-i\nu+n+\frac{1}{2}(f-3)]^{-1}$, the other factors being the same as in the free-particle limit $i\nu=0$. We have here in another form the property of extracting the Z dependence of the Green's function. In order to obtain Eq. (16), a number of reductions were necessary using the recurrence relations of the Gegenbauer polynomials. Since these reductions are rather lengthy, we indicate here some of the intermediate steps. After expanding and integrating term by term, one finds the following combination of Gegenbauer polynomials:

$$-(f-1)C_{n-1}^{(f+3)/2}+2(f+3)C_{n-3}^{(f+3)/2}-(f-1)C_{n-5}^{(f+3)/2}-4xC_{n-2}^{(f+3)/2}-4xC_{n-4}^{(f+3)/2}. \tag{17}$$

This is reduced to

$$\frac{-4(n-1)}{f+1}C_{n-1}^{(f+1)/2}+\frac{4(n+f-2)}{f+1}C_{n-3}^{(f+1)/2}-(f-1)(C_{n-1}^{(f+3)/2}-2C_{n-3}^{(f+3)/2}+C_{n-5}^{(f+3)/2}) \tag{18}$$

by applying the two identities[18]

$$2\nu[xC_n^{\nu+1}(x)-C_{n-1}^{\nu+1}(x)]=(n+1)C_{n+1}^{\nu}(x),\quad \nu\neq 0,-1,\quad n=0,\pm1,\pm2,\ldots. \tag{19a}$$

and

$$2\nu[C_n^{\nu+1}(x)-xC_{n-1}^{\nu+1}(x)]=(n+2\nu)C_n^{\nu}(x),\quad \nu\neq 0,-1,\quad n=0,\pm1,\pm2,\ldots, \tag{19b}$$

to eliminate the two functions $xC_{n-2}^{(f+3)/2}$ and $xC_{n-4}^{(f+3)/2}$, respectively. One now uses the identity[19]

$$\nu[C_{n+1}^{\nu+1}(x)-C_{n-1}^{\nu+1}(x)]=(n+1+\nu)C_{n+1}^{\nu}(x),\quad \nu\neq 0,-1,\quad n=0,\pm1,\pm2,\ldots, \tag{19c}$$

to reduce the differences $C_{n-1}^{(f+3)/2}-C_{n-3}^{(f+3)/2}$ and $C_{n-3}^{(f+3)/2}-C_{n-5}^{(f+3)/2}$ occurring in (18). The expression (18) reduces then to simply

$$-2[n+\tfrac{1}{2}(f-3)](C_{n-1}^{(f+1)/2}-C_{n-3}^{(f+1)/2}), \tag{20}$$

which can be further reduced to

$$-4\frac{[n+\frac{1}{2}(f-3)]^2}{f-1}C_{n-1}^{(f-1)/2} \tag{21}$$

by another application of Eq. (19c). We have here the basic structure occurring in the series expansion (16). The last reduction leading to the expression (21) clearly breaks down if $f=1$, hence the restriction of Eq. (16) to $f=2,3,4,\ldots$. In case $f=1$, the expression (20) can be reduced to

$$-4(n-1)T_{n-1} \tag{22}$$

by means of the relation[20]

$$T_{n+1}(x)=\tfrac{1}{2}[C_{n+1}^1(x)-C_{n-1}^1(x)],\quad n=0,1,2,\ldots, \tag{23}$$

between the Gegenbauer polynomials and the Tchebichef polynomials, defined by the expansion[21]

$$-\tfrac{1}{2}\ln(1-2tx+t^2)=\sum_{n=1}^{\infty}\frac{t^n}{n}T_n(x). \tag{24}$$

The resulting expansion of the one-dimensional momentum space Coulomb Green's function is[22]

$$G_1(k_2,k_1,q,E)=\frac{4ik}{p^2}\sum_{n=1}^{\infty}\frac{nT_n(x)}{-i\nu+n} \tag{25}$$

This expansion is the momentum space form of the result

$$G_1(x_2,x_1,E)=\sum_{n=1}^{\infty}(2n)^{-1}ik(x^2-y^2)\times\frac{e^{ikx}L_{n-1}^1(-ik(x+y))L_{n-1}^1(-ik(x-y))}{-i\nu+n} \tag{26}$$

obtained earlier.[23] It is of interest to write out the two-dimensional special case of Eq. (16) since in this case the series reduces to an expansion in Legendre polynomials[24]

$$G_2(k_2,k_1,q,E)=\sum_{n=1}^{\infty}\frac{8\pi k^2}{p^3}\frac{(n-\frac{1}{2})^2P_{n-1}(x)}{-i\nu+n-\frac{1}{2}}. \tag{27}$$

Born terms can be separated out of these expansions by repeated use of the identity[25]

$$\frac{1}{-i\nu+\alpha}=\frac{1}{\alpha}+\frac{i\nu}{\alpha}\frac{1}{-i\nu+\alpha}. \tag{28}$$

Thus

$$G_f(k_2,k_1,q,E)=G_f^{(0)}+\mathcal{G}_f^{(1)}, \tag{29}$$

where the free-particle limits are given by

$$G_f^{(0)}=-\frac{(4\pi)^{f/2}}{k_2^2-k^2}\Gamma(\tfrac{1}{2}f)\frac{\delta(q)}{q^{f-1}},\quad f=2,3,4,5,\ldots \tag{30}$$

and

$$G_1^{(0)}=\frac{-2\pi\delta(q)}{k_2^2-k^2}-\frac{2ik}{(k_2^2-k^2)(k_1^2-k^2)}, \tag{31}$$

Eq. (31) being the Fourier transform of Eq. (11).[26] The remainder terms $\mathcal{G}_f^{(1)}$ are given by

$$\mathcal{G}_f^{(1)}=\sum_{n=1}^{\infty}\frac{-i\nu(-2ik)^f}{p^{f+1}}(4\pi)^{(f-1)/2}\Gamma(\tfrac{1}{2}(f-1))\times\frac{[n+\frac{1}{2}(f-3)]C_{n-1}^{(f-1)/2}(x)}{-i\nu+n+\frac{1}{2}(f-3)},\quad f=2,3,4,5,\ldots \tag{32}$$

and

$$\mathcal{G}_1^{(1)} = \sum_{n=1}^{\infty} \frac{4i\nu ik}{p^2} \frac{T_n(x)}{-i\nu + n}. \quad (33)$$

Expressions (32) and (33) are proportional to $i\nu$ and contain exactly the first- and all higher-order Born terms. By applying Eq. (28) to the expansions (32) and (33) one can isolate the first Born term, obtaining a decomposition of the form

$$G_f = G_f^{(0)} + G_f^{(1)} + \mathcal{G}_f^{(2)}, \quad (34)$$

in which $G_f^{(1)}$ is the first Born term, and the remainder $\mathcal{G}_f^{(2)}$ now contains exactly the second- and all higher-order Born terms. The remainders $\mathcal{G}_f^{(2)}$ are easily computed and will not be written down here. However, we record here for reference the first Born terms (a derivation of these Born terms will be indicated below):

$$G_f^{(1)} = \frac{i\nu 2ik}{(k_2^2 - k^2)(k_1^2 - k^2)} \frac{(4\pi)^{(f-1)/2}\Gamma(\frac{1}{2}(f-1))}{q^{f-1}},$$
$$f = 2, 3, 4, \ldots, \quad (35)$$

$$G_1^{(1)} = i\nu \frac{(-2ik)}{(k_2^2 - k^2)(k_1^2 - k^2)} \ln \frac{q^2(-2ik)^2}{(k_2^2 - k^2)(k_1^2 - k^2)},$$
$$|\operatorname{arc}(k_{1,2}^2 - k^2)| < \pi, \quad |\operatorname{arc}(-ik)| < \tfrac{1}{2}\pi. \quad (36)$$

This same separation of the Born terms expressed in Eqs. (29) and (34) can be achieved also by using the original integral representation (14).[27] If we substitute the form

$$\frac{d}{dt}\left(t^{(f-3)/2} \frac{2t(t^2-1)}{(1-2tx+t^2)^{(f+1)/2}}\right) = t^{(f-3)/2} \frac{-(f-1) + 2t^2(f+3) - (f-1)t^4 - 4xt(1+t^2)}{(1-2tx+t^2)^{(f+3)/2}} \quad (37)$$

in Eq. (14) with $f = 2, 3, 4, \ldots$ and integrate by parts, we find directly an expansion of the form (29) in which the surface term can be identified with the free-particle Green's function.[28] The other term, which is proportional to $i\nu$, is therefore $\mathcal{G}_f^{(1)}$. This approach gives us directly the integral representation

$$\mathcal{G}_f^{(1)} = i\nu \frac{(-2ik)^f}{p^{f+1}} (4\pi)^{(f-1)/2} \Gamma(\tfrac{1}{2}(f+1))$$
$$\times e^{\pi i [i\nu - (f-1)/2]} \frac{\pi}{\sin\pi[i\nu - \frac{1}{2}(f-1)]}$$
$$\times \frac{1}{2\pi i} \int_{1;\operatorname{arc}(t)=0}^{(0+)} dt\, t^{-i\nu + (f-3)/2} \frac{1-t^2}{(1-2tx+t^2)^{(f+1)/2}},$$
$$f = 2, 3, 4, 5, \ldots, \quad (38)$$

of the remainder term $\mathcal{G}_f^{(1)}$. It should be stressed that Eq. (38) will not give the correct answer for the remainder term in the one-dimensional case. The identity (37) remains valid for $f = 1$, and so does the integration by parts, but this integration by parts does not separate out the one-dimensional free-particle Green's function Eq. (31). This is reflected in the fact that if we substitute $f = 1$ in Eq. (38), we obtain an expression which is still zero-order small in the parameter $i\nu$. The method can be applied also to the one-dimentional Green's function, but one must begin with the identity

$$\frac{d}{dt}\left(t \frac{t-x}{1-2tx+t^2}\right) = \frac{2t - x(1+t^2)}{(1-2tx+t^2)^2}, \quad (39)$$

instead of Eq. (37). Using the same method as before (Ref. 28), the surface term from the integration by parts can be identified with the free-particle Green's function, now equal to the function of Eq. (31). The remaining integral is then

$$\mathcal{G}_1^{(1)} = \frac{4i\nu ik}{p^2} e^{\pi i i\nu} \frac{\pi}{\sin\pi i\nu} \frac{1}{2\pi i} \int_{1;\operatorname{arc}(t)=0}^{(0+)} dt\, t^{-i\nu} \frac{t-x}{1-2tx+t^2}. \quad (40)$$

Due to the vanishing of the contour integral at $i\nu = 0$, this expression is indeed first-order small in $i\nu$.[29] This process of separating out the Born terms by means of an integration by parts can be repeated. The identities needed for the last transformation are

$$\frac{d}{dt}\left(\frac{2}{f-1} \frac{t^{(f-1)/2}}{(1-2tx+t^2)^{(f-1)/2}}\right)$$
$$= \frac{t^{(f-3)/2}(1-t^2)}{(1-2tx+t^2)^{(f+1)/2}}, \quad f = 2, 3, 4, 5, \ldots, \quad (41)$$

and (for the one-dimensional problem)

$$\frac{d}{dt} \ln(1 - 2tx + t^2) = 2 \frac{t-x}{1-2tx+t^2}. \quad (42)$$

We have here the promised explanation of the from of Eqs. (35) or (36) for the first Born term. This Born term is the surface term which arises when one substitutes Eq. (41) or (42), respectively, into Eq. (38) or (40), and integrates by parts. The final integral obtained after this integration by parts provides an integral representation of the remainder term $\mathcal{G}_f^{(2)}$ of Eq. (34). This remainder term is

$$\mathcal{G}_f^{(2)} = (i\nu)^2 \frac{(-2ik)^f}{p^{f+1}} (4\pi)^{(f-1)/2} \Gamma(\tfrac{1}{2}(f-1)) \times e^{\pi i (i\nu-(f-1)/2)} \frac{\pi}{\sin\pi[i\nu - \frac{1}{2}(f-1)]} \times \frac{1}{2\pi i} \int_{1;\operatorname{arc}(t)=0}^{(0+)} dt\, t^{-i\nu+(f-3)/2} \times (1-2tx+t^2)^{-(f-1)/2}, \quad f = 2,3,4,5,\ldots, \tag{43}$$

or in the one-dimensional case

$$\mathcal{G}_1^{(2)} = \frac{(i\nu)^2 2ik}{p^2} e^{\pi i i\nu} \frac{\pi}{\sin\pi i\nu} \frac{1}{2\pi i} \times \int_{1;\operatorname{arc}(t)=0}^{(0+)} dt\, t^{-i\nu-1} \ln(1-2tx+t^2). \tag{44}$$

The Gegenbauer or Tchebichef expansions of $\mathcal{G}_f^{(2)}$ can be obtained directly from Eqs. (43) or (44) with no need of recurrence relations. The lengthy calculations with recurrence relations performed above are needed, however, to obtain the Gegenbauer or Tchebichef expansions (16) or (25) of the full Green's function including the zero-order and first-order Born terms.

The closed-form expression

$$\mathcal{G}_1^{(1)} = \frac{2i\nu ik}{p^2} \Gamma(1-i\nu) \{\rho\, {}_2\mathfrak{F}_1(1, 1-i\nu, 2-i\nu; \rho) + \rho^{-1}\, {}_2\mathfrak{F}_1(1, 1-i\nu, 2-i\nu; \rho^{-1})\}, \tag{45}$$

in which

$${}_2\mathfrak{F}_1(1, 1-i\nu, 2-i\nu; z) \equiv [1/\Gamma(2-i\nu)]\, {}_2F_1(1, 1-i\nu, 2-i\nu; z), \tag{46}$$

is easily derived from the integral representation (40) using the method of Ref. 4. Here ρ is defined as a root of the quadratic equation

$$x = \tfrac{1}{2}(\rho + \rho^{-1}), \tag{47}$$

and ${}_2F_1(1, 1-i\nu, 2-i\nu; z)$ denotes the ordinary Gaussian hypergeometric function.[30] This function is divided by $\Gamma(2-i\nu)$ in Eq. (46) in order to exhibit the pole structure of the momentum space Green's function when regarded as a function of $i\nu$. This pole structure of the Green's function is contained in the gamma function factor $\Gamma(1-i\nu)$ in Eq. (45), the other factors being analytic functions of $i\nu$.

IV. ONE-DIMENSIONAL EXCITED STATE GREEN'S FUNCTION IN MOMENTUM SPACE

The one-dimensional ground state reduced Coulomb Green's function in coordinate space has been treated elsewhere.[31] We will here obtain a closed-form expression [Eq. (71)] which expresses this function in momentum space and which applies more generally to an arbitrary excited state. In view of the remarks following Eq. (10), the corresponding three-dimensional functions can be obtained from this one-dimensional result by differentiation with respect to the momentum transfer. This investigation is based on the Tchebichef expansion (33) of $\mathcal{G}_1^{(1)}$. Since the theory of the reduced Green's function has been developed in the references cited above, the derivation of the new result will be brief. We here assume the relation

$$i\nu = i/ka_1, \quad a_1 = \text{the first Bohr radius}, \tag{48}$$

between the parameters k and $i\nu$. The calculation begins with the formula[32]

$$K_1(k_2, k_1, q; E_n) = \frac{d}{dE}[(E-E_n)G_1(k_2, k_1, q; E)]\Big|_{E=E_n}, \tag{49}$$

relating the reduced Green's function K_1 and the full Green's function G_1. The parameter $i\nu$ is a function of the energy through Eq. (48) and the relation $k = (2mE/\hbar^2)^{1/2}$, $0 < \operatorname{arc}(k) < \pi$ [Cf. Eq. (2)]. It is convenient to rewrite Eq. (49) using $i\nu$ as independent variable instead of E:

$$K_1(k_2, k_1, q; E_n) = \tfrac{1}{2}n^3 \frac{d}{di\nu}\left((i\nu - n)\frac{i\nu + n}{(i\nu)^2 n^2} G_1(k_2, k_1, q; E)\right)_{i\nu=n}, \quad n = 1,2,3,\ldots. \tag{50}$$

(The energy eigenvalues E_n correspond to the values $i\nu = n = 1, 2, 3, \ldots$ of the Coulomb parameter $i\nu$.) We now substitute for $G_1(k_2, k_1, q; E)$ in Eq. (50) the sum of Eqs. (31) and (33), and apply the operation

$$OF(i\nu) \equiv \frac{d}{di\nu}[(i\nu - n)F(i\nu)]\Big|_{i\nu=n} \tag{51}$$

term by term. It is easy to see that the operation O leaves unaltered any function $F(i\nu)$ which is analytic in the neighborhood of $i\nu = n$ and simply evaluates it at $i\nu = n$: $OF(i\nu) = F(n)$. This applies to the expression (31) and also to all except the nth term of Eq. (33). This nth term of Eq. (33) contains the factor $(i\nu - n)^{-1}$ which removes the factor $(i\nu - n)^{+1}$ of O and leaves one with a simple derivative of a function which is now regular, evaluated at $i\nu = n$. Thus

$$K_1(E_n) = \frac{-2\pi\delta(\mathfrak{q})n^3 a_1^3}{1+\mathfrak{k}_2^2} + \frac{2n^3 a_1^3}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)} + \sum_{l=1,\, l\neq n}^{\infty} -\frac{4n^3 a_1^3}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)} \frac{nT_l(\mathfrak{x})}{-n+l} + \frac{n^3 a_1^3}{\mathfrak{q}^2} \frac{d}{di\nu}[(i\nu + n)(1-x)T_n(x)]\big|_{i\nu=n},$$

$$\mathfrak{k}_1 \equiv n a_1 \mathbf{k}_1, \quad \mathfrak{k}_2 \equiv n a_1 \mathbf{k}_2, \quad \mathfrak{q} \equiv \mathfrak{k}_2 - \mathfrak{k}_1, \tag{52}$$

$$x = 1 - \frac{2a_1^2(i\nu)^2 q^2}{(1 + a_1^2(i\nu)^2 k_2^2)(1 + a_1^2(i\nu)^2 k_1^2)}, \tag{53}$$

$$\mathfrak{x} \equiv 1 - \frac{2\mathfrak{q}^2}{(1 + \mathfrak{k}_2^2)(1 + \mathfrak{k}_1^2)}. \tag{54}$$

In the following we will derive an expression in closed form for the infinite part of the series in Eq. (52) (for the sum from $l = n + 1$ to infinity) and will work out the derivative indicated in the last term. The derivative is evaluated by use of the identities

$$\left.\frac{dx}{di\nu}\right|_{i\nu = n} = \frac{2(1 - \mathfrak{x})}{n} \frac{\mathfrak{k}_1^2 \mathfrak{k}_2^2 - 1}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} \tag{55}$$

and[33]

$$\left(\frac{d}{dx}\right) T_n(x) = n C_{n-1}^1(x), \quad n = 1, 2, 3, \ldots. \tag{56}$$

Thus

$$\frac{n^3 a_1^3}{\mathfrak{q}^2} \frac{d}{di\nu} [(i\nu + n)(1 - x) T_n(x)]|_{i\nu = n}$$

$$= 2n^3 a_1^3 T_n(\mathfrak{x}) \frac{5 + \mathfrak{k}_1^2 + \mathfrak{k}_2^2 - 3\mathfrak{k}_1^2 \mathfrak{k}_2^2}{(1 + \mathfrak{k}_1^2)^2 (1 + \mathfrak{k}_2^2)^2}$$

$$+ 16 n^3 a_1^3 n C_{n-1}^1(\mathfrak{x}) \frac{\mathfrak{q}^2(\mathfrak{k}_1^2 \mathfrak{k}_2^2 - 1)}{(1 + \mathfrak{k}_1^2)^3 (1 + \mathfrak{k}_2^2)^3}. \tag{57}$$

The key to obtaining the infinite part of the series in Eq. (52) in closed form is the identity[34]

$$T_n(x) = \tfrac{1}{2}(\rho^n + \rho^{-n}), \quad n = 1, 2, 3, \cdots, \tag{58}$$

in which ρ is defined by

$$\mathfrak{x} = \tfrac{1}{2}(\rho + \rho^{-1}). \tag{59}$$

{This is the same ρ as before [Eq. (47)], but is now evaluated for $i\nu = n$.} We note the inequality

$$\frac{\mathfrak{q}^2}{(1 + \mathfrak{k}_2^2)(1 + \mathfrak{k}_1^2)} \le 1, \tag{60}$$

which follows from $1 + 2\,\mathfrak{k}_1 \mathfrak{k}_2 \cos\theta + \mathfrak{k}_2^2 \mathfrak{k}_1^2 \ge 0$, θ being the angle between $\mathfrak{k}_1$ and $\mathfrak{k}_2$. As a consequence of (60) we have

$$-1 \le \mathfrak{x} \le 1, \tag{61}$$

and can therefore write ρ in the form

$$\rho \equiv \mathfrak{x} + i(1 - \mathfrak{x}^2)^{1/2} \equiv -e^{-2i\psi}, \tag{62}$$

with

$$0 \le \psi \le \pi/2.$$

If we substitute the expansion (58) of the Tchebichef polynomial into the infinite part of the series in Eq. (52), this series becomes

$$I(1^-) \equiv \sum_{l=n+1}^{\infty} - \frac{2n^3 a_1^3}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} \frac{n(\rho^l + \rho^{-l})}{-n + l} \tag{63}$$

in which ρ has modulous unity. This series is visualized as the limit as $h \to 1^-$ of the series

$$I(h) \equiv \sum_{l=n+1}^{\infty} - \frac{2n^3 a_1^3}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} \frac{n(h^l \rho^l + h^l \rho^{-l})}{-n + l}, \quad |h| < 1, \tag{64}$$

which one is permitted to split up into a sum of two series. These individual series are just logarithmic series of the type

$$\ln(1 - z) = -\sum_{l=1}^{\infty} \frac{z^l}{l}, \quad |z| < 1.] \tag{65}$$

Thus,

$$I(h) = \frac{2n^3 a_1^3}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} n(-h)^n [e^{-2ni\psi} \ln(1 + he^{-2i\psi}) + e^{2ni\psi} \ln(1 + he^{2i\psi})] \tag{66}$$

and

$$I(1^-) = \frac{4n^3 a_1^3 (-1)^n n}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} [-\psi \sin(n2\psi) + \cos(n2\psi) \times \ln(2\cos\psi)]. \tag{67}$$

The calculations are completed by noting the following relations:

$$\cos 2\psi = -\mathfrak{x}, \quad \sin 2\psi = (1 - \mathfrak{x}^2)^{1/2}, \tag{68}$$

$$(-1)^n \cos(n2\psi) = T_n(\mathfrak{x}),$$
$$(-1)^n \sin(n2\psi) = -(1 - \mathfrak{x}^2)^{1/2} C_{n-1}^1(\mathfrak{x}), \tag{69}$$

$$\psi = \cos^{-1}\left(\frac{\mathfrak{q}}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)}\right)^{1/2}. \tag{70}$$

Equations (68) are just a rephrasing of Eq. (62). The second of relations (69) can be obtained by differentiation of the first, with the use of Eq. (56). In Eq. (70) the acute angle must be taken, in conformity with Eq. (62). When these results and Eq. (57) are inserted in Eq. (52) we find

$$K_1(E_n) = \frac{-2\pi\delta(\mathfrak{q}) n^3 a_1^3}{(1 + \mathfrak{k}_2^2)} + \frac{2n^3 a_1^3}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} + \sum_{l<n} \frac{4n^3 a_1^3}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} \frac{n T_l(\mathfrak{x})}{n - l} + 2n^3 a_1^3 T_n(\mathfrak{x}) \frac{5 + \mathfrak{k}_1^2 + \mathfrak{k}_2^2 - 3\mathfrak{k}_1^2 \mathfrak{k}_2^2}{(1 + \mathfrak{k}_1^2)^2 (1 + \mathfrak{k}_2^2)^2}$$
$$+ 16 n^3 a_1^3 n C_{n-1}^1(\mathfrak{x}) \frac{\mathfrak{q}^2(\mathfrak{k}_1^2 \mathfrak{k}_2^2 - 1)}{(1 + \mathfrak{k}_1^2)^3 (1 + \mathfrak{k}_2^2)^3} + \frac{4n^3 a_1^3}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)} (1 - \mathfrak{x}^2)^{1/2} n C_{n-1}^1(\mathfrak{x}) \cos^{-1}\left(\frac{\mathfrak{q}^2}{(1 + \mathfrak{k}_1^2)(1 + \mathfrak{k}_2^2)}\right)^{1/2}$$

$$+\frac{4n^3a_1^3}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)}nT_n(\mathfrak{x})\tfrac{1}{2}\ln\left(\frac{4\mathfrak{q}^2}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)}\right),\quad n=1,2,3,\ldots,\tag{71}$$

in which the sum $l < n$ is interpreted to mean zero if $n = 1$, otherwise to mean $\sum_{l=1}^{n-1}$. The notations in Eq. (71) have been defined above [Eqs. (52) and (54)]. We have here the desired closed-form expression for the general excited state reduced Coulomb Green's function in momentum space. This expression is without hypergeometric functions and may be useful for applications. For the momentum space representative of the ground state reduced Coulomb Green's function, studied earlier in coordinate space, Eq. (71) gives

$$K_1(E_1)=\frac{-2\pi\delta(\mathfrak{q})a_1^3}{(1+\mathfrak{k}_2^2)}+4a_1^3\frac{3+\mathfrak{k}_1^2+\mathfrak{k}_2^2-\mathfrak{k}_1^2\mathfrak{k}_2^2}{(1+\mathfrak{k}_1^2)^2(1+\mathfrak{k}_2^2)^2}$$

$$+4a_1^3\mathfrak{q}^2\frac{-9-\mathfrak{k}_1^2-\mathfrak{k}_2^2+7\mathfrak{k}_1^2\mathfrak{k}_2^2}{(1+\mathfrak{k}_1^2)^3(1+\mathfrak{k}_2^2)^3}+\frac{4a_1^3}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)}\times(1-\mathfrak{x}^2)^{1/2}\cos^{-1}\left(\frac{\mathfrak{q}^2}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)}\right)^{1/2}$$

$$+\frac{4a_1^3}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)}\frac{\mathfrak{x}}{2}\ln\left(\frac{4\mathfrak{q}^2}{(1+\mathfrak{k}_1^2)(1+\mathfrak{k}_2^2)}\right).\tag{72}$$

---

1 R. J. White and F. H. Stillinger, Jr., J. Chem. Phys. **52**, 5800 (1970).

2 L. Hostler, J. Math. Phys. **11**, 2966 (1970).

3 J. Schwinger, J. Math. Phys. **5**, 1606 (1964).

4 L. Hostler, J. Math. Phys. **5**, 1235 (1964).

5 The term "full Green's function" refers to the ordinary Green's function as defined here in Eq. (2). This term is used when necessary to avoid ambiguity in order to distinguish between the Green's function of Eq. (2) and the "reduced Green's function," defined by

$$K(\mathbf{r}_2,\mathbf{r}_1,E_n)=-\frac{\hbar^2}{2m}\sum_{l\neq n}\sum_{\alpha}\frac{\varphi_{l\alpha}(\mathbf{r}_2)\varphi_{l\alpha}^*(\mathbf{r}_1)}{E_l-E_n}.$$

This function, which plays an important role in Rayleigh–Schrödinger bound state perturbation theory, has been studied in the Coulomb case for $n = 1$ (ground state) by H. F. Hameka, J. Chem. Phys. **47**, 2728 (1967); **48**, 4810 (E) (1968); L. Hostler, Phys. Rev. **178**, 126 (1969) and in Ref. 2.

6 Reference 2, Eq. (8).

7 Reference 3. The corresponding coordinate space result was obtained by Hostler [Ref. 2, Eq. (21)].

8 Reference 2, Eq. (5).

9 G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge U.P., London, 1962), 2nd ed., p. 177, Eq. (8), and the relation on p. 77

$$I_\nu(z)=e^{-\pi i\nu/2}J_\nu(ze^{\pi i/2}),\qquad -\pi<\arg(z)\le\tfrac{1}{2}\pi.$$

10 This integral may be evaluated by first assuming $A > 0$ and B real, and then extending the result by analytic continuation. One introduces polar spherical coordinates in the f-dimensional space, with the polar axis in the direction of **B**. Integration over the polar angle is evaluated using Watson's Eq. (9) (the fourth form), p. 79. The final integration over the radial coordinate uses Watson's Eq. (6), p. 386, and the connection between I_ν and J_ν (cf. Ref. 9).

11 E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U.P., Cambridge, England, 1927), 4th ed., p. 245. The condition $\mathrm{Re}(\lambda) > 0$ is needed to permit one to deform the integration contour (cf. Jordan's lemma, p. 115).

12 The term "extracting the Z dependence" of the Green's function refers to the property of Eq. (8) of expressing the Coulomb Green's function as an integral whose integrand is the same function of $\mathbf{k}_2$ and $\mathbf{k}_1$ as in the free-particle limit (cf. Ref. 4).

13 Reference 2, Eq. (16).

14 Reference 9, Eq. (8), p. 79.

15 Equation (12) is obtained by explicitly differentiating the closed-form expression [Eq. (6), Ref. 2] for the one-dimensional Green's function. The function $W_{i\nu;1/2}$ is the Whittaker function as defined in H. Buchholz, *The Confluent Hypergeometric Function*, translated by H. Lichtblau and K. Wetzel (Springer, New York, 1969), Sec. 2. 5.

16 For this we need the relation

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

[Buchholz, Ref. 15, p. 24] Eq. (29a).

17 Bateman, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. II, p. 235 Eq. (16).

18 Reference 17, Vol. I, p. 178 Eqs. (27) and (28). A great deal of labor is saved by defining $C_n^\nu(x) = 0$, $\nu \neq 0$, $n = -1, -2, -3, \ldots$, whereupon all the identities (19) hold for unrestricted positive or negative integral n or zero.

19 Reference 17, p. 178, Eq. (36).

20 Reference 17, p. 184 Eqs. (3) and (6), can be combined to give

$$T_{n+1}=C_{n+1}^1-xC_n^1,\ n=0,1,2,3,\ldots.$$

Equation (23) now results by use of the identity

$$0=C_{n+1}^1-2xC_n^1+C_{n-1}^1,\qquad n\neq-1.$$

This last identity results if one multiplies Eq. (15) (with $\nu=1$) through on both sides with the factor $(1-2tx+t^2)$, and compares coefficients of like powers of t on both sides of the resulting equation.

21 Reference 17, p. 236, Eq. (23).

22 If the calculation for the one-dimensional case and for the higher-dimensional cases are carried along together up to the point indicated by Eq. (20), one obtains directly the expansion

$$G_1=\sum_{n=1}^{\infty}\frac{2ik}{p^2}\frac{(n-1)(C_{n-1}^1-C_{n-3}^1)}{-i\nu+n-1},$$

in which the $n = 1$ term evidently drops out. If one looks at the free-particle limit, however, one obtains the indeterminant form 0/0 for this term. By treating the one-dimensional problem from the beginning as a separate case, one can arrive at Eq. (25) without encountering this ambiguity.

23 Reference 2, Eq. (19).

24 Reference 17, p. 179, Eq. (3).

25 Cf. Ref. 3.

26 It may be of interest to point out that Eq. (31) can also be obtained by summing Eq. (25) in the free-particle limit $i\nu=0$ if we interpret the resulting series as the limit as $h \to 1^-$ of the series

$$\frac{4ik}{p^2}\sum_{n=1}^{\infty}h^nT_n(x)=\frac{4ikh}{p^2}\frac{x-h}{1-2hx+h^2}$$

[obtained by differentiating Eq. (24) with respect to the expansion parameter]. This sum can be rewritten as

$$\frac{-2ik}{p^2}+\frac{2ik}{p^2}\frac{1-h^2}{(1-h)^2-2h2k^2q^2p^{-2}},$$

in which the last term gives the $\delta(q)$ part of Eq. (31), in the limit $h \to 1^-$.

[27] This generalizes a calculation of Ref. 4.

[28] This is done by retaining an upper limit $t < 1$ in the surface term, and identifying the distribution obtained in the limit as $t \to 1^-$, along the lines of Ref. 26.

[29] The contour integral is an analytic function of $i\nu$, vanishing at $i\nu = 0$ [if $i\nu = 0$, there is no singularity of the integrand within the contour (see Appendix to Ref. 4)], and therefore has the general form $i\nu\phi(i\nu)$, where $\phi(i\nu)$ is likewise analytic in $i\nu$. One sees that Eq. (40) has the form

$$i\nu\cdot(1/\sin\pi i\nu)\cdot i\nu\phi(i\nu),$$

which is first-order small in $i\nu$.

[30] Reference 11, Chap. XIV.

[31] Reference 2. For the treatment of the three-dimensional problem, see the work cited in Ref. 5. Also, see Ref. 5 for the definition of "reduced Green's function."

[32] Reference 2, Eq. (15).

[33] Reference 17, p. 186, Eq. (26).

[34] Reference 17, p. 235, Eq. (20).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Motion and Structure of Singularities in General Relativity. II*

Ezra T. Newman† and Roger Posadas‡
Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania 15213
(Received 23 November 1970)

This, the second paper in a series on the motion and structure of a class of (elementary) singularities, extends the earlier work on "free" singularities to the interaction of these singularities with "background" gravitational and electromagnetic fields. The principle result is an unusual derivation of the Lorentz–Dirac equations of motion for a charged particle. The results do not depend on any ad hoc assumptions nor upon any renormalization, but follow uniquely from the Einstein–Maxwell equations applied to the elementary singularities. A concomitant result is the time evolution of the structure of the singularity.

1. INTRODUCTION

This is the second part of a series of papers on a new approach to equations of motion in general relativity. As shown in the first paper,[1] this new approach is based on the structure and behavior of the family of null cones emanating from a singular world line in space-time, where the singularity is a suitably defined singularity in the Weyl tensor. The advantage of this approach over other approaches to the problem of motion is that it gives an intrinsic description of the motion of a singularity in its own space-time and does not depend on the assumption of a regular background space. By applying Einstein's field equations in spin-coefficient formalism to the singular world line, we are able to derive equations of motion for the singularity in terms of the time dependence of the null cones. In addition, we obtain the concomitant result that the singularity has an internal structure whose time development is also governed by the field equations.

In the first paper we applied our approach to the Robinson-Trautman (RT) type II metrics and their charged counterparts, namely the Robinson-Trautman-Maxwell (RTM) metrics. It was shown that these two special classes of solutions lead to equations of motion for "free singularities", i.e. singularities not interacting with incoming background fields. From the RTM solutions, in particular, we were able to obtain the Abraham radiation reaction force[2] in a rigorous fashion, with no ad hoc assumptions or mass renormalization.

Here we shall consider the more general case in which both incoming gravitational and electromagnetic fields are allowed to interact with the singularity. In Sec. 2, we give a brief review of the formalism. Sec. 3 will deal with the motion and structure of a singularity in the presence of an incoming gravitational field in a general empty space ($R_{\mu\nu} = 0$). Then, in Sec. 4, we analyze the motion of a charged singularity in the Einstein-Maxwell theory. It is here where we obtain our major result, namely, the derivation of the Lorentz-Dirac equations of motion for a charged particle.[2]

2. REVIEW OF THE FORMALISM

A brief review of the formalism and of the basic assumptions will now be given. It will be assumed that the reader is familiar with the spin-coefficient formalism.[3]

Since our approach to motion is based on the properties of the null cones emanating from a singular world line, we begin by introducing null coordinates $x^0 = u, x^1 = r$, and $x^A, A = 2, 3$, such that $\sqrt{2}u$ is a "retarded time" parameter labeling a family of outgoing null hypersurfaces; $r/\sqrt{2}$ is a standard affine parameter measuring "distance" along the null geodesics lying in each u = const hypersurface, and x^A are "angular coordinates" labeling the null geodesics. We then introduce a standard null tetrad system $(l^\mu, n^\mu, m^\mu, \overline{m}^\mu)$ where l^μ and n^μ are real null vectors, m^μ and its complex conjugate $\overline{m}^\mu$ are complex null vectors, and

$$l_\mu n^\mu = -m_\mu \overline{m}^\mu = 1,$$

with all other scalar products vanishing. In the [obtained by differentiating Eq. (24) with respect to the expansion parameter]. This sum can be rewritten as

$$\frac{-2ik}{p^2}+\frac{2ik}{p^2}\frac{1-h^2}{(1-h)^2-2h2k^2q^2p^{-2}},$$

in which the last term gives the $\delta(q)$ part of Eq. (31), in the limit $h \to 1^-$.

27 This generalizes a calculation of Ref. 4.

28 This is done by retaining an upper limit $t < 1$ in the surface term, and identifying the distribution obtained in the limit as $t \to 1^-$, along the lines of Ref. 26.

29 The contour integral is an analytic function of $i\nu$, vanishing at $i\nu = 0$ [if $i\nu = 0$, there is no singularity of the integrand within the contour (see Appendix to Ref. 4)], and therefore has the general form $i\nu\phi(i\nu)$, where $\phi(i\nu)$ is likewise analytic in $i\nu$. One sees that Eq. (40) has the form

$$i\nu\cdot(1/\sin\pi i\nu)\cdot i\nu\phi(i\nu),$$

which is first-order small in $i\nu$.

30 Reference 11, Chap. XIV.

31 Reference 2. For the treatment of the three-dimensional problem, see the work cited in Ref. 5. Also, see Ref. 5 for the definition of "reduced Green's function."

32 Reference 2, Eq. (15).

33 Reference 17, p. 186, Eq. (26).

34 Reference 17, p. 235, Eq. (20).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Motion and Structure of Singularities in General Relativity. II*

Ezra T. Newman† and Roger Posadas‡

Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania 15213

(Received 23 November 1970)

This, the second paper in a series on the motion and structure of a class of (elementary) singularities, extends the earlier work on "free" singularities to the interaction of these singularities with "background" gravitational and electromagnetic fields. The principle result is an unusual derivation of the Lorentz–Dirac equations of motion for a charged particle. The results do not depend on any ad hoc assumptions nor upon any renormalization, but follow uniquely from the Einstein–Maxwell equations applied to the elementary singularities. A concomitant result is the time evolution of the structure of the singularity.

1. INTRODUCTION

This is the second part of a series of papers on a new approach to equations of motion in general relativity. As shown in the first paper,[1] this new approach is based on the structure and behavior of the family of null cones emanating from a singular world line in space-time, where the singularity is a suitably defined singularity in the Weyl tensor. The advantage of this approach over other approaches to the problem of motion is that it gives an intrinsic description of the motion of a singularity in its own space-time and does not depend on the assumption of a regular background space. By applying Einstein's field equations in spin-coefficient formalism to the singular world line, we are able to derive equations of motion for the singularity in terms of the time dependence of the null cones. In addition, we obtain the concomitant result that the singularity has an internal structure whose time development is also governed by the field equations.

In the first paper we applied our approach to the Robinson-Trautman (RT) type II metrics and their charged counterparts, namely the Robinson-Trautman-Maxwell (RTM) metrics. It was shown that these two special classes of solutions lead to equations of motion for "free singularities", i.e. singularities not interacting with incoming background fields. From the RTM solutions, in particular, we were able to obtain the Abraham radiation reaction force[2] in a rigorous fashion, with no ad hoc assumptions or mass renormalization.

Here we shall consider the more general case in which both incoming gravitational and electromagnetic fields are allowed to interact with the singularity. In Sec. 2, we give a brief review of the formalism. Sec. 3 will deal with the motion and structure of a singularity in the presence of an incoming gravitational field in a general empty space ($R_{\mu\nu} = 0$). Then, in Sec. 4, we analyze the motion of a charged singularity in the Einstein-Maxwell theory. It is here where we obtain our major result, namely, the derivation of the Lorentz-Dirac equations of motion for a charged particle.[2]

2. REVIEW OF THE FORMALISM

A brief review of the formalism and of the basic assumptions will now be given. It will be assumed that the reader is familiar with the spin-coefficient formalism.[3]

Since our approach to motion is based on the properties of the null cones emanating from a singular world line, we begin by introducing null coordinates $x^0 = u, x^1 = r$, and $x^A, A = 2, 3$, such that $\sqrt{2}u$ is a "retarded time" parameter labeling a family of outgoing null hypersurfaces; $r/\sqrt{2}$ is a standard affine parameter measuring "distance" along the null geodesics lying in each $u =$ const hypersurface, and x^A are "angular coordinates" labeling the null geodesics. We then introduce a standard null tetrad system $(l^\mu, n^\mu, m^\mu, \overline{m}^\mu)$ where l^μ and n^μ are real null vectors, m^μ and its complex conjugate $\overline{m}^\mu$ are complex null vectors, and

$$l_\mu n^\mu = -m_\mu \overline{m}^\mu = 1,$$

with all other scalar products vanishing. In the null coordinate system which we have adopted, we take l^μ to be tangent to the null geodesics and parallelly propagate the rest of the tetrad along l^μ. This leads to the following form for the tetrad vectors:

$$l_\mu = \delta^0_\mu, \quad l^\mu = \delta^\mu_1, \quad m^\mu = \omega\delta^\mu_1 + \xi^A\delta^\mu_A,$$
$$n^\mu = \delta^\mu_0 + U\delta^\mu_1 + X^A\delta^\mu_A, \quad A = 2, 3. \tag{2.1}$$

This also leads to the following form for the contravariant metric tensor:

$$g^{\mu 0} = \delta^\mu_1, \quad g^{11} = 2(U - \omega\overline{\omega}),$$
$$g^{A1} = X^A - (\xi^A\overline{\omega} + \omega\overline{\xi}^A), \tag{2.2}$$
$$g^{AB} = -(\xi^A\overline{\xi}^B + \overline{\xi}^A\xi^B), \quad A, B = 2, 3.$$

Now, the properties of each null hypersurface can be characterized by the two spin coefficients ρ and σ defined by

$$\rho = l_{\mu;\nu}m^\mu\overline{m}^\nu = -\tfrac{1}{2}\, l^\mu{}_{;\mu},$$
$$\sigma = l_{\mu;\nu}m^\mu m^\nu = \text{(complex shear)}.$$

The basic condition which we impose on this family of null hypersurfaces is that ρ and σ have the following behavior:[4]

$$\rho = -r^{-1} + O(r), \quad \sigma = O(r) \tag{2.3}$$

near $r = 0$. Geometrically, this restriction means that in the neighborhood of the origin $r = 0$, the null hypersurfaces behave like cones. When condition (2.3) is satisfied, and the Weyl tensor is singular at $r = 0$ (i.e., it becomes infinite at $r = 0$), we call the singularity an elementary singularity. It is this type of singularity which we choose to represent matter.

It can be shown easily from (2.3) that the 2-surfaces, u and r constant (i.e., the cross sections of the "cones"), possess a metric given by

$$g_{AB} = -\tfrac{1}{2}r^2\, g^0_{AB} + O(r^3), \quad g^0_{AB} = g^0_{AB}(u, x^C). \tag{2.4}$$

The limiting metric given by

$$g^0_{AB} = \lim_{r\to 0}\left(-\frac{2}{r^2}\, g_{AB}\right) \tag{2.5}$$

defines the limiting 2-surface, which we call the *fundamental 2-surface* (F2S). By using conformally-flat coordinates, the F2S line element can be written most conveniently as

$$dl^2 = g^0_{AB}\, dx^A\, dx^B = P^{-2}\, d\zeta\, d\overline{\zeta}, \tag{2.6}$$

where $\zeta = x^2 + ix^3$ and $P = P(u, \zeta, \overline{\zeta})$. The quantity P plays a fundamental role in our approach to motion. When there is an elementary singularity at $r = 0$, Einstein's field equations yield differential equations for the determination of P from which one can, in principle, derive all information about the motion and internal structure of the singularity.

In flat space, where a similar null coordinate system attached to an arbitrary timelike world line can be constructed, the F2S reduces to a unit sphere and P becomes[1]

$$P = P_0 = \dot{\xi}_\mu b^\mu, \tag{2.7}$$

where $\dot{\xi}^\mu$ is the velocity of the timelike world line and

$$b^\mu = (1/2\sqrt{2})\,(1 + \zeta\overline{\zeta}, \zeta + \overline{\zeta}, (\zeta - \overline{\zeta})/i, \zeta\overline{\zeta} - 1). \tag{2.8}$$

It is shown in Ref. 1 that there is a unique equivalence between the acceleration vector $\ddot{\xi}^\mu$ and the quantity $\dot{P}_0/P_0$ and between $(\dddot{\xi}^\mu + \tfrac{1}{2}\ddot{\xi}^2\dot{\xi}^\mu)$ and $(\ddot{P}_0/P_0 + \tfrac{1}{2}\ddot{\xi}^2)$, where $\ddot{\xi}^2 \equiv \ddot{\xi}^\alpha\ddot{\xi}_\alpha$. It is also shown in that paper that $\dot{P}_0/P_0$ and $(\ddot{P}_0/P_0 + \tfrac{1}{2}\ddot{\xi}^2)$ are both expandable in $l = 1$ spherical harmonics. This can therefore be used to give alternative expressions for equations of motion in flat space. For example, for motion with the Abraham radiation reaction force, we have the equivalent expression

$$\sqrt{2}\, m\, \dot{P}_0/P_0 = \tfrac{2}{3}e^2\,(\ddot{P}_0/P_0 + \tfrac{1}{2}\ddot{\xi}^2), \tag{2.9}$$

where the $\sqrt{2}$ is due to the fact that u is not the proper time.

In the case of a general curved space with an elementary singularity at $r = 0$, we make the assumption that the F2S is a distorted sphere, that is, we impose the regularity condition that

$$P = P_0\,(1 + I), \tag{2.10}$$

where P_0 is the quantity defined by (2.7) and (2.8) and I is a regular function on the sphere, expandable in $l > 2$ spherical harmonics, with the additional property $I > -1$. We define $\dot{P}_0/P_0$ to be the "acceleration" of the singularity, in analogy with the flat-space case, and take I to represent its internal degrees of freedom.

In general, when space-time has an elementary singularity at $r = 0$, the field equations will yield an equation for $\dot{P}/P$. Then by imposing the regularity condition (2.10), we can, in principle, decompose this equation into spherical harmonics such that the $l = 1$ part gives the equation of motion in terms of the "acceleration" $\dot{P}_0/P_0$ and the $l \geqslant 2$ parts give the time dependence of the internal structure I.

3. MOTION IN A GENERAL EMPTY SPACE

In this section we will discuss the motion and structure of an elementary singularity in a general empty space ($R_{\mu\nu}=0$). The integration of the field equations is done asymptotically in the neighborhood of $r=0$, in a manner analogous to that used in the far field ($r\to\infty$) analysis.[5] We start by considering the two coupled spin-coefficient equations

$$\frac{\partial\rho}{\partial r}=\rho^2+\sigma\bar{\sigma},\quad \frac{\partial\sigma}{\partial r}=2\rho\sigma+\psi_0, \tag{3.1}$$

where ψ_0, which represents the incoming gravitational background field, is defined by $\psi_0=-C_{\mu\nu\rho\sigma}l^\mu m^\nu l^\rho m^\sigma$, $C_{\mu\nu\rho\sigma}$ being the Weyl tensor. If condition (2.3), namely, $\rho=-r^{-1}+O(r)$ and $\sigma=O(r)$, is now imposed on Eq. (3.1), it can be easily checked that ψ_0 must necessarily have the form $\psi_0=0(1)$, i.e., ψ_0 must be a regular function of r around $r=0$. Thus, condition (2.3) excludes, for example, r^{-5} and higher-order singularities whose presence in ψ_0, in linear theory, corresponds to the presence of intrinsic quadrupole and higher multipole moments. It can also be shown that condition (2.3) leads to the vanishing of the coefficient of the r^{-4} term in $\psi_1=-C_{\mu\nu\rho\sigma}l^\mu n^\nu l^\rho m^\sigma$, which means that the elementary singularity cannot have an intrinsic mass dipole moment and angular momentum.[5] In other words, only elementary singularities of the nonrotating, mass-monopole type are allowed by condition (2.3).

If we now assume an explicit form for ψ_0, namely

$$\psi_0=\psi_0^0+\psi_0^1 r+O(r^2), \tag{3.2}$$

the "radial" spin-coefficient equations can be integrated asymptotically around $r=0$ to find the r-dependence of the spin coefficients, metric variables, and tetrad components of the Weyl tensor, up to the orders allowed by (3.2). Each step of the integration will yield a "constant" independent of r, which will be denoted by a superscript 0. Then, by substituting the results of the "radial" integration into the nonradial spin-coefficient equations and comparing powers of r, we can obtain relationships among these "constants." The calculations, which are extremely tedious, are given elsewhere.[6] We shall merely give a summary of the results here.

A. Tetrad components of the Weyl tensor:

$$\psi_0=\psi_0^0+\psi_0^1 r+O(r^2), \tag{3.3a}$$

$$\psi_1=-\tfrac{1}{4}\bar{\eth}\psi_0^0-\tfrac{1}{5}\bar{\eth}\psi_0^1 r+O(r^2), \tag{3.3b}$$

$$\psi_2=\psi_2^0 r^{-3}+\tfrac{1}{12}\bar{\eth}^2\psi_0^0+\tfrac{1}{20}(\bar{\eth}^2\psi_0^1+2\psi_2^0|\psi_0^0|^2)r+O(r^2), \tag{3.3c}$$

$$\psi_3=\psi_3^0 r^{-2}-\tfrac{1}{8}\psi_2^0\eth\bar{\psi}_0^0 r^{-1}-(\tfrac{1}{24}\bar{\eth}^3\psi_0^0+\tfrac{1}{40}\psi_2^0\eth\bar{\psi}_0^1)+O(r), \tag{3.3d}$$

$$\psi_4=[\bar{\eth}\psi_3^0-(\psi_2^0)^2\bar{\psi}_0^0]r^{-2}+\psi_4^0 r^{-1}+O(1). \tag{3.3e}$$

B. Spin coefficients:

$$\rho=-r^{-1}+\tfrac{1}{45}|\psi_0^0|^2 r^3+\tfrac{1}{36}\operatorname{Re}(\psi_0^0\bar{\psi}_0^1)r^4+O(r^5), \tag{3.4a}$$

$$\sigma=\tfrac{1}{3}\psi_0^0 r+\tfrac{1}{4}\psi_0^1 r^2+O(r^3), \tag{3.4b}$$

$$\alpha=\alpha^0 r^{-1}-\tfrac{1}{6}\bar{\alpha}^0\bar{\psi}_0^0 r-\tfrac{1}{12}\bar{\alpha}^0\bar{\psi}_0^1 r^2+O(r^3), \tag{3.4c}$$

$$\beta=-\bar{\alpha}^0 r^{-1}+(\tfrac{1}{6}\alpha^0\psi_0^0-\tfrac{1}{8}\bar{\eth}\psi_0^0)r+(\tfrac{1}{12}\alpha^0\psi_0^1-\tfrac{1}{15}\bar{\eth}\psi_0^1)r^2+O(r^3), \tag{3.4d}$$

$$\tau=-\tfrac{1}{8}\bar{\eth}\psi_0^0 r-\tfrac{1}{15}\bar{\eth}\psi_0^1 r^2+O(r^3), \tag{3.4e}$$

$$\lambda=-\tfrac{1}{3}\psi_2^0\bar{\psi}_0^0+(\tfrac{1}{6}\mu^0\psi_0^0-\tfrac{1}{8}\psi_2^0\bar{\psi}_0^1)r+O(r^2), \tag{3.4f}$$

$$\mu=-\psi_2^0 r^{-2}+\mu^0 r^{-1}+\tfrac{1}{24}\bar{\eth}^2\psi_0^0 r+(\tfrac{1}{60}\bar{\eth}^2\psi_0^1-\tfrac{1}{90}\psi_2^0|\psi_0^0|^2)r^2+O(r^3), \tag{3.4g}$$

$$\gamma=-\tfrac{1}{2}\psi_2^0 r^{-2}+\gamma^0+[\tfrac{1}{12}\bar{\eth}^2\psi_0^0-\tfrac{1}{4}\operatorname{Im}(\alpha^0\bar{\eth}\psi_0^0)]r+[\tfrac{1}{40}\bar{\eth}^2\psi_0^1+\tfrac{1}{20}\psi_2^0|\psi_0^0|^2-\tfrac{1}{15}\operatorname{Im}(\alpha^0\bar{\eth}\psi_0^1)]r^2+O(r^3), \tag{3.4h}$$

$$\nu=-\psi_3^0 r^{-1}+\nu^0+\tfrac{1}{24}(\psi_2^0\eth\bar{\psi}_0^1-\bar{\eth}^3\psi_0^0-3\mu^0\eth\bar{\psi}_0^0)r+O(r^2), \tag{3.4i}$$

$$\kappa=\epsilon=\pi=0. \tag{3.4j}$$

C. Metric variables:

$$\omega=\tfrac{1}{24}\bar{\eth}\psi_0^0 r^2+\tfrac{1}{60}\bar{\eth}\psi_0^1 r^3+O(r^4), \tag{3.5a}$$

$$U=-\psi_2^0 r^{-1}+U^0-(\gamma^0+\bar{\gamma}^0)r-\tfrac{1}{12}\operatorname{Re}(\eth^2\bar{\psi}_0^0)r^2-\tfrac{1}{60}\operatorname{Re}(\eth^2\bar{\psi}_0^1+2\psi_2^0|\psi_0^0|^2)r^3+O(r^4), \tag{3.5b}$$

$$\xi^A=\xi^{0A}r^{-1}+\tfrac{1}{6}\psi_0^0\bar{\xi}^{0A}r+\tfrac{1}{12}\psi_0^1\bar{\xi}^{0A}r^2+O(r^3), \tag{3.5c}$$

$$X^A=X^{0A}-\tfrac{1}{4}\operatorname{Re}(\xi^{0A}\eth\bar{\psi}_0^0)r-\tfrac{1}{15}\operatorname{Re}(\xi^{0A}\eth\bar{\psi}_0^1)r^2+O(r^3). \tag{3.5d}$$

D. Line element:

$$ds^2=2[\psi_2^0 r^{-1}-U^0+(\gamma^0+\bar{\gamma}^0)r+0(r^2)]du^2+2du\,dr+0(r^2)(du\,d\zeta+du\,d\bar{\zeta})-\left[\frac{r^2}{2P^2}+0(r^4)\right]d\zeta d\bar{\zeta}. \tag{3.6}$$

E. Relationships among the "constants":

$$\omega^0 = \lambda^0 = \psi_1^0 = 0, \quad \tau^0 = \bar{\alpha}^0 + \beta^0 = 0, \tag{3.7a}$$

$$\xi^{02} = i\xi^{03} = -P(u, \zeta, \bar{\zeta}), \quad P = \bar{P}, \tag{3.7b}$$

$$\alpha^0 = -\frac{\partial P}{\partial \bar{\zeta}}, \quad \beta^0 = -\bar{\alpha}^0, \tag{3.7c}$$

$$U^0 = \mu^0 = \bar{\mu}^0 = -K, \quad K \equiv ð\bar{ð} \log P, \tag{3.7d}$$

$$Z^0 \equiv P^{-1}(X^{02} + iX^{03}), \quad ð Z^0 = -\tfrac{4}{3}\psi_2^0\psi_0^0, \tag{3.7e}$$

$$\gamma^0 = -\tfrac{1}{2}\dot{P}/P + \tfrac{1}{4}\bar{ð}Z^0 - \mathrm{Im}(\alpha^0 Z^0), \tag{3.7f}$$

$$\nu^0 = -\bar{ð}(\gamma^0 + \bar{\gamma}^0) - \tfrac{1}{6}\psi_2^0 ð\bar{\psi}_0^0, \tag{3.7g}$$

$$\bar{ð}ð\psi_0^0 = -3\psi_2^0\psi_0^1, \tag{3.7h}$$

$$\psi_3^0 = -\bar{ð}U^0 = \bar{ð}K, \tag{3.7i}$$

$$\psi_4^0 = -\bar{ð}\nu^0 + \tfrac{1}{6}\psi_2^0(\bar{ð}ð\bar{\psi}_0^0 - 4K\bar{\psi}_0^0), \tag{3.7j}$$

$$ð\psi_2^0 = 0, \quad \psi_2^0 = \bar{\psi}_2^0, \tag{3.7k}$$

$$\dot{\psi}_2^0 + 3(\gamma^0 + \bar{\gamma}^0)\psi_2^0 = -ð\psi_3^0. \tag{3.7l}$$

To analyze these results, we shall impose the regularity condition $P = P_0(1 + I)$ and use the properties of the operator $ð$ (edth), which is defined as

$$ð\eta = 2P^{1-s}\frac{\partial}{\partial \zeta}(P^s \eta) \tag{3.8}$$

for any function η of spin weight s. It will again be assumed that the reader is familiar with this operator and the related class of spin-weighted functions.[7]

First, we note that (3.7k) implies

$$ð_0\psi_2^0 = 0, \tag{3.9}$$

where $ð_0$ is defined with respect to P_0. This in turn implies that ψ_2^0 is an $l = 0$ spherical harmonic, i.e.,

$$\psi_2^0 = -M(u), \tag{3.10}$$

where $M(u)$ is related to the "mass" of the singularity. (For the Schwarzschild solution, $\psi_2^0 = -\sqrt{2}\, km$, where k is twice the gravitational constant and m is the Schwarzschild mass.) Now, consider Eq. (3.7e). Since Z^0 and ψ_0^0 are, respectively, $s = 1$ and $s = 2$ quantities, we can write

$$Z^0 = ðV, \quad \psi_0^0 = ð^2 R, \tag{3.11}$$

where V and R are both $s = 0$ quantities. Substituting (3.10) and (3.11) into (3.7e), we obtain

$$ð^2(V - \tfrac{4}{3}MR) = 0, \tag{3.12}$$

which implies that

$$V = \tfrac{4}{3}MR + J,$$

where J is an $s = 0$ quantity satisfying $ð^2 J = 0$. By means of the coordinate freedom $\zeta' = g(u, \zeta)$, it can be shown that J can be transformed away. Therefore, we have

$$V = \tfrac{4}{3}MR. \tag{3.13}$$

If we now substitute (3.7f), (3.7i), (3.10), and (3.13) into (3.7l), we get

$$\dot{M} - 3M\dot{P}/P = ð\bar{ð}[K - M(R + \bar{R})]. \tag{3.14}$$

With the use of the regularity condition $P = P_0(1 + I)$ and the expression (3.7d) for K, Eq. (3.14) becomes

$$\dot{M} - 3M\dot{P}_0/P_0 - 3M\dot{I}/(1+I)^2 ð_0\bar{ð}_0[(1+I)^2 + (1+I)ð_0\bar{ð}_0 I - ð_0 I\cdot\bar{ð}_0 I - M^2(R + \bar{R})].$$

By carrying out the differentiation of the terms inside the bracket, we can write this equation further as

$$\dot{M} - 3M\dot{P}_0/P_0 - 3M\dot{I}/(1+I)^3(ð_0\bar{ð}_0ð_0\bar{ð}_0 I + 2ð_0\bar{ð}_0 I) - (1+I)^2 ð_0^2 I\cdot\bar{ð}_0^2 I - M^2(1+I)^2 ð_0\bar{ð}_0(R + \bar{R}). \tag{3.15}$$

Formally, this equation can be decomposed into spherical harmonics such that the $l = 0$ part gives the time dependence of the "mass" M, the $l = 1$ part gives the equation of motion in terms of $\dot{P}_0/P_0$, and the $l > 2$ parts give the time development of the internal degrees of freedom I. However, due to its extreme nonlinearity, it is more enlightening to consider the linearized version of (3.15).

Under the assumption that $\dot{P}_0/P_0$, I, and R are first-order quantities, the linearization of (3.15) yields

$$\dot{M} - 3M\dot{P}_0/P_0 - 3M\dot{I} = ð_0\bar{ð}_0ð_0\bar{ð}_0 I + 2ð_0\bar{ð}_0 I - M^2 ð_0\bar{ð}_0(R + \bar{R}). \tag{3.16}$$

Note that since ψ_0^0 is expandable in spin-2 spherical harmonics starting with $l = 2$, R must be expandable in $l \geq 2$ spherical harmonics. Because of the linearity of (3.16), we can (without loss of generality) let R have a definite l value, i.e., $ð_0\bar{ð}_0 R = -l(l+1)R$. Then the decomposition of (3.16) yields

$$l = 0, \quad \dot{M} = 0, \tag{3.17a}$$

$$l = 1, \quad M\dot{P}_0/P_0 = 0, \tag{3.17b}$$

$$l \geq 2, \quad \dot{I} + 3M^{-1}l(l+1)[l(l+1) - 2]I = \tfrac{1}{3}M\, l(l+1)(R + \bar{R}). \tag{3.17c}$$

Thus, from (3.17a) and (3.17b), we see that the singularity moves with a constant mass and zero acceleration, while from (3.17c) we get the solution

$$I = e^{-u/u_0} \times \left(I_0(\zeta,\bar\zeta) - \tfrac{1}{3}M\, l(l+1) \int (R+\bar R)\, e^{-u/u_0} du \right),$$

where (3.18)

$$(u_0)^{-1} = 3M^{-1} l(l+1)\,[l(l+1)-2]. \qquad (3.19)$$

Equation (3.18) shows how the internal degrees of freedom are driven by the incoming gravitational field ψ_0^0 or R.

In the test-particle limit ($M \to 0$), we, of course, obtain from (3.17a), (3.17b), and (3.18) the usual results $\dot P_0/P_0 = 0$ and $I = 0$, i.e., the test particle moves along a geodesic in the regular background space. However, if we constrain I to be zero before going to the test-particle limit, we obtain an interesting result: The world line of the particle is not only a geodesic but also part of a rigid geodesic congruence. To show this, we set $I = 0$ in (3.15) and decompose the resulting equation into spherical harmonics. Then we get

$$l = 0, \quad \dot M = 0 \quad \text{or } M = \text{const}, \qquad (3.20a)$$

$$l = 1, \quad M\dot P_0/P_0 = 0 \quad \text{or } \dot P_0/P_0 = 0, \qquad (3.20b)$$

$$l \geq 2, \quad M^2(R+\bar R) = 0 \quad \text{or } R+\bar R = 0. \qquad (3.20c)$$

In the limit $M \to 0$, (3.20b) implies that the world line $r = 0$ is a geodesic while (3.20c) implies that R is pure imaginary, i.e.,

$$R = i\chi, \qquad (3.21)$$

where χ is real. It follows from this that

$$\psi_0^0 = i\eth_0^2\chi, \qquad (3.22)$$

which shows that ψ_0^0 is pure magnetic. As we shall now prove, the vanishing of the electric part of ψ_0^0 implies that neighboring geodesics have zero relative acceleration with respect to the world line $r = 0$.

Given a timelike geodesic congruence, the relative acceleration between any two neighboring geodesics of the congruence, L_1 and L_2 say, is expressed by the equation of geodesic deviation[8]

$$\frac{D^2\eta^\mu}{Du^2} = R^{\mu\nu\rho\sigma} t_\nu t_\rho \eta_\sigma, \qquad (3.23)$$

where t^μ is the tangent vector to the congruence of timelike geodesics parametrized by the proper time $u(t^\mu t_\mu = 1)$, η^μ is a vector orthogonal to t^μ which connects points of L_1 and L_2, D denotes absolute differentiation along t^μ, and $R^{\mu\nu\rho\sigma}$ is the Rieman tensor. The tangent vector t^μ may be written in terms of the null tetrad vectors $(l^\mu, n^\mu, m^\mu, \bar m^\mu)$ as

$$t^\mu = 2^{-1/2}(l^\mu + n^\mu), \qquad (3.24)$$

and in empty space $R^{\mu\nu\rho\sigma}$ may be replaced by the Weyl tensor $C^{\mu\nu\rho\sigma}$. Hence, the equation for geodesic deviation can be rewritten in empty space as

$$\frac{D^2\eta^\mu}{Du^2} = C^{\mu\sigma}\eta_\sigma, \qquad (3.25)$$

where $C^{\mu\sigma}$ is given by

$$C^{\mu\sigma} = 2C^{\mu\nu\rho\sigma} t_\nu t_\rho = C^{\mu\nu\rho\sigma}(l_\nu + n_\nu)(l_\rho + n_\rho) \qquad (3.26)$$

and has the properties

$$C^{\mu\sigma} = C^{(\mu\sigma)}, \quad C^\mu_\mu = 0, \quad C_{\mu\nu}t^\nu = 0. \qquad (3.27)$$

It can be seen from these properties that $C_{\mu\nu}$ has only five independent real components. We choose these components to be the two complex scalars, Ω_1 and Ω_2 and the real scalar Ω_3, defined by

$$\Omega_1 = -C_{\mu\nu}m^\mu m^\nu, \quad \Omega_2 = -C_{\mu\nu}l^\mu m^\nu, \quad \Omega_3 = -C_{\mu\nu}\bar m^\mu m^\nu. \qquad (3.28)$$

From the definitions of the tetrad components of the Weyl tensor, we can also express (3.28) as

$$\Omega_1 = -(\psi_0 + \bar\psi_4), \quad \Omega_2 = \psi_1 - \bar\psi_3, \quad \Omega_3 = \psi_2 + \bar\psi_2. \qquad (3.29)$$

Now, let $I = 0$ and $M \to 0$ so that the world line $r = 0$ becomes a timelike geodesic, which we can identify with L_1, and ψ_0^0 becomes pure magnetic, $\psi_0^0 = i\eth_0^2\chi$. From (3.7h) we find that in the limit $M \to 0$

$$\eth_0\bar\eth_0\chi = -6\chi, \qquad (3.30)$$

which shows that χ is an $l = 2$ spherical harmonic. Then, using this in (3.3a)–(3.3e), we get the following values for ψ_0 to ψ_4 on the world line $r = 0$:

$$\psi_0 = \psi_0^0 = i\eth_0^2\chi, \qquad (3.31a)$$

$$\psi_1 = -\tfrac{1}{4}\bar\eth_0\psi_0^0 = i\eth_0\chi, \qquad (3.31b)$$

$$\psi_2 = \tfrac{1}{12}\bar\eth_0^2\psi_0^0 = 2i\chi, \qquad (3.31c)$$

$$\psi_3 = -\tfrac{1}{24}\bar\eth_0^3\psi_0^0 = -i\bar\eth_0\chi, \qquad (3.31d)$$

$$\psi_4 = \tfrac{1}{24}\bar\eth_0^4\psi_0^0 = i\bar\eth_0^2\chi. \qquad (3.31e)$$

[Note that the $O(1)$ term in ψ_4 was explicitly evaluated by adding another term to ψ_0, i.e., $\psi_0 = \psi_0^0 + \psi_0^1 r + \psi_0^2 r^2 + O(r^3)$.]

Substituting (3.31a)–(3.31e) into (3.29), we obtain

$$\Omega_1 = \Omega_2 = \Omega_3 = 0, \qquad (3.32)$$

which means that $C_{\mu\nu} = 0$, or

$$\frac{D^2\eta^\mu}{Du^2} = 0.$$

Therefore, the vanishing of the electric part of ψ_0^0 (under the constraint $I = 0$ and in the test-particle limit $M \to 0$) implies that neighboring geodesics have zero geodesic deviation from the geodesic $r = 0$.

Finally, we consider how the incoming field ψ_0^0 and the radiation field ψ_4^0 are affected by the motion and structure of the singularity. The former is modified by the presence of the singularity through Eq. (3.7h), which can be rewritten as

$$\eth^2\bar{\eth}\eth R + 6K\eth^2 R = 3M\psi_0^1, \quad (3.33)$$

where use was made of the relation $(\bar{\eth}\eth - \eth\bar{\eth})\eta = 2sK\eta$. Thus the incoming field drives the internal degrees of freedom of the singularity and is in turn affected by the presence of the singularity. In the case of the radiation field, we can express (3.7j) as

$$\psi_4^0 = \eth^2[\tfrac{1}{4}(\bar{\eth}Z^0 + \eth\bar{Z}^0) - \dot{P}/P] + \tfrac{1}{3}\psi_2^0 \times (\eth\bar{\eth}\bar{\psi}_0^0 - 6K\bar{\psi}_0^0) = \eth^2[\tfrac{1}{3}M\eth\bar{\eth}(R + \bar{R}) - \dot{P}_0/P_0 - \dot{I}/(1+I)] + M(2K\bar{\psi}_0^0 - M\bar{\psi}_0^1). \quad (3.34)$$

In the linear approximation, this becomes

$$\psi_4^0 = \bar{\eth}_0^2[\tfrac{1}{3}M\,\eth_0\bar{\eth}_0 R - \dot{I}], \quad (3.35)$$

where the first term represents the contribution of the incoming field R and the second term represents radiation from a 2^l-pole source.[9]

4. MOTION IN THE EINSTEIN-MAXWELL THEORY

We now consider the motion and structure of singularities in the presence of both incoming gravitational and electromagnetic fields. Again, the Einstein-Maxwell equations are first integrated under the assumption $\rho = -r^{-1} + O(r)$ and $\sigma = O(r)$, and the solutions are then analyzed with the use of the regularity condition $P = P_0(1 + I)$. The calculations become much more tedious and the details, which can be found elsewhere,[6] will not be given here.

In the presence of a Maxwell field $F_{\mu\nu}$, the two "radial" spin-coefficient equations (3.1) get modified as follows:

$$\frac{\partial\rho}{\partial r} = \rho^2 + \sigma\bar{\sigma} + k\varphi_0\bar{\varphi}_0, \quad \frac{\partial\sigma}{\partial r} = 2\rho\sigma + \psi_0, \quad (4.1)$$

where φ_0, which represents the incoming electromagnetic field, is given by $\varphi_0 = F_{\mu\nu}l^\mu m^\nu$, and the coupling constant k is twice the Newtonian gravitational constant G. If we again integrate (4.1) under the condition $\rho = -r^{-1} + O(r)$ and $\sigma = O(r)$, we find that $\psi_0 = O(1)$ and $\varphi_0 = O(1)$.[6] Therefore, condition (2.3) excludes not only intrinsic mass quadrupole and higher multipole moments but also intrinsic electromagnetic dipole and higher moments (i.e., r^{-3} and higher singularities in φ_0). In integrating the radial equations, we take ψ_1^0, the coefficient of r^{-4} in the Weyl tensor, to be zero although it is very likely that, under condition (2.3), ψ_1^0 vanishes identically, as in the empty-space case.

With the information that the incoming fields ψ_0 and φ_0 have to be regular functions of r around $r = 0$, we may assume that they have the following explicit forms:

$$\psi_0 = \psi_0^0 + \psi_0^1 r + \psi_0^2 r^2 + O(r^3),$$
$$\varphi_0 = \varphi_0^0 + \varphi_0^1 r + \varphi_0^2 r^2 + O(r^3). \quad (4.2)$$

We can again integrate the "radial" spin-coefficient equations asymptotically around $r = 0$, obtaining at each step a "constant" independent of r. The results of the "radial" integration are extremely long, so we shall give here only the relationships among the "constants" and the differential equations for ψ_2^0 and φ_1^0, which are respectively the coefficients of r^{-3} in the Weyl tensor and of r^{-2} in the Maxwell tensor.

A. Relationships among the "constants":

$$\omega^0 = \psi_1^0 = \varphi_0^1 = 0, \quad \tau^0 = \bar{\alpha}^0 + \beta^0 = 0, \quad (4.3a)$$

$$\xi^{02} = i\xi^{03} = -P(u, \zeta, \bar{\zeta}), \quad P = \bar{P}, \quad (4.3b)$$

$$K \equiv \eth\bar{\eth}\log P, \quad (4.3c)$$

$$\alpha^0 = -\bar{\beta}^0 = -\frac{\partial P}{\partial\bar{\zeta}} - \frac{k}{2}\bar{\varphi}_0^0\varphi_1^0, \quad (4.3d)$$

$$\lambda^0 = k\bar{\varphi}_0^0\bar{\eth}\varphi_1^0 - k^2(\bar{\varphi}_0^0\varphi_1^0)^2, \quad (4.3e)$$

$$Z^0 \equiv P^{-1}(X^{02} + iX^{03}), \quad (4.3f)$$

$$\eth Z^0 = 2k\varphi_0^0\bar{\varphi}_2^0 - \tfrac{4}{3}\psi_2^0\psi_0^0 - k\psi_0^1|\varphi_1^0|^2, \quad (4.3g)$$

$$U^0 = -K + \tfrac{32}{3}k^2|\varphi_0^0|^2|\varphi_1^0|^2 - 2k\varphi_1^0\eth\bar{\varphi}_0^0 - 2k\bar{\varphi}_1^0\bar{\eth}\varphi_0^0, \quad (4.3h)$$

$$\mu^0 = -K + 8k^2|\varphi_0^0|^2|\varphi_1^0|^2 - 2k\varphi_1^0\eth\bar{\varphi}_0^0 - k\bar{\varphi}_1^0\bar{\eth}\varphi_0^0, \quad (4.3i)$$

$$\gamma^0 = -\tfrac{1}{2}\dot{P}/P + \tfrac{1}{4}\bar{\eth}Z^0 + \tfrac{1}{3}k\,\psi_2^0|\varphi_0^0|^2 + \tfrac{1}{2}\,\mathrm{Im}(Z^0\bar{\eth}\log P), \quad (4.3j)$$

$$\psi_2^0 = \bar{\psi}_2^0, \quad (4.3k)$$

$$\eth\psi_2^0 = 2k\varphi_1^0\bar{\varphi}_2^0 - 2k\psi_2^0\varphi_0^0\bar{\varphi}_1^0, \quad (4.3l)$$

$$\eth\varphi_1^0 = -3k\varphi_0^0|\varphi_1^0|^2, \quad (4.3m)$$

$$\eth\varphi_0^0 = -k\bar{\varphi}_1^0(\varphi_0^0)^2 - \tfrac{1}{3}\psi_0^0\varphi_1^0, \quad (4.3n)$$

$$\bar{\eth}\eth\psi_0^0 = -3\psi_2^0\psi_0^1 - \tfrac{12}{5}k\psi_0^2|\varphi_1^0|^2 + 6k\bar{\varphi}_0^0\varphi_1^0\eth\psi_0^0 + 2k\varphi_0^0\bar{\varphi}_1^0\bar{\eth}\psi_0^0 + 10k\varphi_0^2\eth\bar{\varphi}_1^0 - 6k\bar{\varphi}_1^0\eth\varphi_0^2 - 10k\psi_0^0\bar{\varphi}_1^0\bar{\eth}\varphi_0^0 + \tfrac{114}{15}k^2\psi_0^0|\varphi_0^0|^2|\varphi_1^0|^2, \tag{4.3o}$$

$$\begin{aligned}\psi_3^0 = {}&\bar{\eth}K - 3k\bar{\varphi}_0^0\varphi_1^0K + \tfrac{3}{2}k\bar{\varphi}_1^0\bar{\eth}^2\varphi_0^0 + \tfrac{5}{2}k\bar{\eth}\varphi_1^0\cdot\eth\bar{\varphi}_0^0 \\ &+ 3k^2\bar{\psi}_0^0\varphi_0^0\bar{\varphi}_1^0|\varphi_1^0|^2 - k^2\bar{\varphi}_0^2\varphi_1^0|\varphi_1^0|^2 \\ &- \tfrac{1}{2}k\,\varphi_1^0\eth(\bar{\psi}_0^0\bar{\varphi}_1^0) - 15k^2\bar{\varphi}_0^0|\varphi_1^0|^2\bar{\eth}\varphi_0^0 \\ &- \tfrac{41}{3}k^2\bar{\varphi}_1^0|\varphi_0^0|^2\bar{\eth}\varphi_1^0 - 3k^2\bar{\varphi}_0^0(\varphi_1^0)^2\eth\bar{\varphi}_0^0 \\ &+ \tfrac{89}{2}k^3\bar{\varphi}_0^0\varphi_1^0|\varphi_0^0|^2|\varphi_1^0|^2.\end{aligned} \tag{4.3p}$$

B. Differential Equations:

$$\begin{aligned}&\dot{\varphi}_1^0 - 2(\dot{P}/P)\,\varphi_1^0 + \tfrac{1}{2}[\eth(\varphi_1^0\bar{Z}^0) + \bar{\eth}(\varphi_1^0Z^0)] \\ &\quad = -\eth\varphi_2^0 - \bar{\eth}(\psi_2^0\varphi_0^0).\end{aligned} \tag{4.4}$$

$$\begin{aligned}&\dot{\psi}_2^0 - 3(\dot{P}/P)\psi_2^0 + k|\psi_2^0\varphi_0^0|^2 + \tfrac{3}{4}\psi_2^0(\eth\bar{Z}^0 + \bar{\eth}Z^0) \\ &+ \tfrac{1}{2}(Z^0\bar{\eth}\psi_2^0 + \bar{Z}^0\eth\psi_2^0) = -\eth\bar{\eth}K + 3k[\varphi_1^0\eth(\bar{\varphi}_0^0K) \\ &+ \bar{\varphi}_1^0\bar{\eth}(\varphi_0^0K)] + k\varphi_2^0\bar{\varphi}_2^0 + \tfrac{1}{4}k|\varphi_1^0|^2(\eth^2\bar{\psi}_0^0 \\ &+ \bar{\eth}^2\psi_0^0) + \tfrac{3}{4}k(\varphi_1^0\eth\bar{\varphi}_1^0\cdot\eth\bar{\psi}_0^0 + \bar{\varphi}_1^0\bar{\eth}\varphi_1^0\cdot\bar{\eth}\psi_0^0) \\ &+ \tfrac{1}{2}k(\psi_0^0\bar{\varphi}_1^0\bar{\eth}^2\varphi_1^0 + \bar{\psi}_0^0\varphi_1^0\eth^2\bar{\varphi}_1^0) - \tfrac{3}{2}k(\eth\bar{\varphi}_1^0\cdot\bar{\eth}^2\varphi_0^0 \\ &+ \bar{\eth}\varphi_1^0\cdot\eth^2\bar{\varphi}_0^0) - 36k^2|\varphi_0^0|^2|\varphi_1^0|^2K \\ &+ \tfrac{5}{2}k^2[(\varphi_1^0)^2\eth(\bar{\varphi}_0^2\bar{\varphi}_1^0) + (\bar{\varphi}_1^0)^2\bar{\eth}(\varphi_0^2\varphi_1^0)] \\ &+ 3k^2[(\varphi_1^0\eth\bar{\varphi}_0^0)^2 + (\bar{\varphi}_1^0\bar{\eth}\varphi_0^0)^2] - \tfrac{9}{2} \\ &\times k^2|\varphi_1^0|^2(\psi_0^0\bar{\varphi}_0^0\bar{\eth}\varphi_1^0 + \bar{\psi}_0^0\varphi_0^0\eth\bar{\varphi}_1^0) \\ &+ 9k^2|\varphi_0^0\eth\bar{\varphi}_1^0|^2 + \tfrac{27}{2}k^2(\varphi_0^0\bar{\varphi}_1^0\eth\bar{\varphi}_0^0\cdot\bar{\eth}\varphi_1^0 \\ &+ \bar{\varphi}_0^0\varphi_1^0\bar{\eth}\varphi_0^0\cdot\eth\bar{\varphi}_1^0) + 18k^2|\varphi_1^0\eth\bar{\varphi}_0^0|^2 \\ &+ 3k^2[\bar{\varphi}_0^0(\varphi_1^0)^2\eth^2\bar{\varphi}_0^0 + \varphi_0^0(\bar{\varphi}_1^0)^2\bar{\eth}^2\varphi_0^0] \\ &- \tfrac{9}{4}k^2|\varphi_1^0|^2(\varphi_0^0\bar{\varphi}_1^0\eth\bar{\psi}_0^0 + \bar{\varphi}_0^0\varphi_1^0\bar{\eth}\psi_0^0) \\ &- 15k^3|\varphi_1^0|^4(\varphi_0^0\bar{\varphi}_0^2 + \bar{\varphi}_0^0\varphi_0^2) - \tfrac{225}{2} \\ &\times k^3|\varphi_0^0|^2|\varphi_1^0|^2(\varphi_1^0\eth\bar{\varphi}_0^0 + \bar{\varphi}_1^0\bar{\eth}\varphi_0^0) \\ &- \tfrac{15}{2}k^3|\varphi_1^0|^2[\psi_0^0(\bar{\varphi}_0^0\varphi_1^0)^2 + \bar{\psi}_0^0(\varphi_0^0\bar{\varphi}_1^0)^2] \\ &- \tfrac{81}{2}k^3|\varphi_1^0|^2[\varphi_0^0(\bar{\varphi}_1^0)^2\bar{\eth}\varphi_1^0 + \bar{\varphi}_0^0(\varphi_1^0)^2\eth\bar{\varphi}_1^0] \\ &+ 423k^4|\varphi_0^0|^4|\varphi_1^0|^4.\end{aligned} \tag{4.5}$$

These results are obviously much more complicated and nonlinear than those of the empty-space calculations. Though in principle we could extract equations of motion from (4.5) and (4.4), it is more instructive to use a linear approximation procedure for the present. Thus, we impose the regularity condition $P = P_0(1 + I)$ and assume that P_0/P_0 and I are first-order quantities. In addition, we carry out the analysis only up to first order in the coupling constant k.

Now, since φ_0^0, φ_2^0, and ψ_0^0 have spin weights +1, −1, and +2, respectively, we can write them as

$$\varphi_0^0 = \eth A, \qquad \varphi_2^0 = \bar{\eth}B, \qquad \psi_0^0 = \eth^2 G, \tag{4.6}$$

where A, B, and G are all spin-weight zero variables. Next, from (4.3m) we find that

$$\eth_0\varphi_1^0 = O(k),$$

which implies that

$$\varphi_1^0 = E(u) + O(k). \tag{4.7}$$

Then, substituting $\psi_0^0 = \eth^2 G$ into (4.30) and using the commutation relation for $\eth$ and $\bar{\eth}$, we obtain

$$\bar{\eth}\eth^3 G = \eth^2\eth\bar{\eth}G + 6K\eth^2 G = O(k), \tag{4.8}$$

where we have also used the fact that there is a k in ψ_2^0 (c.f. Schwarzschild solution: $\psi_2^0 = -\sqrt{2}\,km$). In the linear approximation, Eq. (4.8) becomes

$$\eth_0^2(\eth_0\bar{\eth}_0 G + 6G) = O(k),$$

which implies that $G = R + O(k)$, where R is an $l = 2$ spherical harmonic, i.e.,

$$\eth_0\bar{\eth}_0 R = -6R. \tag{4.9}$$

Therefore, ψ_0^0 is given by

$$\psi_0^0 = \eth_0^2 R + O(k). \tag{4.10}$$

If we substitute this together with (4.7) into (4.3n), we get

$$\eth_0^2 A = -\tfrac{1}{3}E\,\eth_0^2 R + O(k), \tag{4.11}$$

whose homogeneous part has the solution $A = F$, F being an $l = 1$ spherical harmonic. Hence, the complete linearized solution of (4.11) is

$$A = F - \tfrac{1}{3}ER + O(k), \tag{4.12}$$

i.e.,

$$\varphi_0^0 = \eth_0 F - \tfrac{1}{3}E\eth_0 R + O(k). \tag{4.13}$$

From (4.3g) we find next that

$$\eth Z^0 = O(k).$$

Since the homogeneous part of this equation can be transformed away by means of the coordinate freedom $\zeta' = g(u, \zeta)$, we therefore have

$$Z^0 = O(k). \tag{4.14}$$

Now, linearizing (4.4), we obtain

$$\eth_0\bar{\eth}_0 B = -\dot{E} + 2E\dot{P}_0/P_0 + 2E\dot{I} + O(k). \quad (4.15)$$

If I is assumed to have a definite l value, i.e., $\eth_0\bar{\eth}_0 I = -l(l+1)I$, then (4.4) can be decomposed such that

$$\dot{E} = O(k) \quad (4.16a)$$

and

$$B = -E\dot{P}_0/P_0 - [2E/l(l+1)]\dot{I} + O(k). \quad (4.16b)$$

Equation (4.16a) implies that

$$E = e + O(k), \quad (4.17)$$

where the constant e, assumed to be real, is just the charge of the singularity (cf. Reissner–Nordström solution: $\varphi_1^0 = e$). With this result, φ_1^0, φ_0^0, and φ_2^0 become

$$\varphi_1^0 = e + O(k), \quad (4.18a)$$

$$\varphi_0^0 = \eth_0 F - \tfrac{1}{3}e\,\eth_0 R + O(k), \quad (4.18b)$$

$$\varphi_2^0 = -e\bar{\eth}_0(\dot{P}_0/P_0) - [2e/l(l+1)]\bar{\eth}_0\dot{I} + O(k), \quad (4.18c)$$

Substituting all these into (4.31), we then obtain

$$\eth_0\psi_2^0 = -2ke^2\eth_0(\dot{P}_0/P_0 + [2/l(l+1)]\dot{I}) + O(k^2),$$

which has the general solution

$$\psi_2^0 = -kW(u) - 2ke^2\dot{P}_0/P_0 - [4ke^2/l(l+1)\dot{I} + O(k^2), \quad (4.19)$$

where $-kW(u)$ is the solution of the homogeneous part.

Finally, we consider the linearization of (4.5). Substituting into this equation the expressions for $\varphi_1^0, \varphi_0^0, \varphi_2^0, \psi_0^0$, and ψ_2^0 obtained previously, we get to first order in k

$$k\dot{W} + 2ke^2(\ddot{P}_0/P_0 + \ddot{\xi}^2/2) + [4ke^2/l(l+1)\ddot{I} - 3kW\dot{P}_0/P_0 - 3kW\dot{I} = \eth_0\bar{\eth}_0\eth_0\bar{\eth}_0 I + 2\eth_0\bar{\eth}_0 I - 3ke\eth_0\bar{\eth}_0(F+\bar{F}) + ke^2\eth_0\bar{\eth}_0(R+\bar{R}) - \tfrac{1}{4}ke^2(\eth_0^2\bar{\eth}_0^2\bar{R} + \bar{\eth}_0^2\eth_0^2 R) + O(k^2), \quad (4.20)$$

where $\ddot{\xi}^2 \equiv \ddot{\xi}^\alpha\ddot{\xi}_\alpha$ comes from the identity[6]

$$\eth_0(\dot{P}_0/P_0)\cdot\bar{\eth}_0(\dot{P}_0/P_0) = -[(\dot{P}_0/P_0)^2 + \ddot{\xi}^2/2].$$

Since F and R are $l=1$ and $l=2$ spherical harmonics, respectively, and since $\eth_0\bar{\eth}_0 I = -l(l+1)I$, Eq. (4.20) can be simplified further to yield

$$k\dot{W} + 2ke^2(\ddot{P}_0/P_0 + \ddot{\xi}^2/2) + 4ke^2\ddot{I}/l(l+1) - 3kW(\dot{P}_0/P_0) - 3kW\dot{I} = l(l+1)[l(l+1)-2]I + 6ke(F+\bar{F}) - 12ke^2(R+\bar{R}) + O(k^2). \quad (4.21)$$

If we now decompose this into its different l values, then we obtain

$$l=0,\ \dot{W} = O(k), \quad (4.22)$$

$$l=1,\ W(\dot{P}_0/P_0) = -2e(F+\bar{F}) + \tfrac{2}{3}e^2(\ddot{P}_0/P_0 + \ddot{\xi}^2/2) + O(k) \quad (4.23)$$

$$l=2,\ \tfrac{2}{3}ke^2\ddot{I} - 3kW\dot{I} - 24I = -12ke^2(R+\bar{R}) + O(k^2). \quad (4.24)$$

From (4.22) it follows that

$$W = \sqrt{2}m + O(k), \quad (4.25)$$

where m is a constant which can be identified with the mass of the singularity. Eq. (4.24) shows that in this order of approximation only the $l=2$ part of I is excited by the incoming fields. Substituting (4.25) into (4.23) and taking the limit $k\to 0$, we get

$$\sqrt{2}\,m(\dot{P}_0/P_0) = -2e(F+\bar{F}) + \tfrac{2}{3}e^2(\ddot{P}_0/P_0 + \ddot{\xi}^2/2). \quad (4.26)$$

We will now prove that (4.26) is equivalent to the Lorentz–Dirac equation of motion.

If the Lorentz–Dirac equation is expressed in terms of a parameter which is $\sqrt{2}/2$ times the proper time on an arbitrary timelike world line in Minkowski space, it becomes

$$\sqrt{2}\,m\,\ddot{\xi}^\mu = 2e\dot{\xi}_\nu F^{\nu\mu} + \tfrac{2}{3}e^2(\dddot{\xi}^\mu + \tfrac{1}{2}\ddot{\xi}^2\dot{\xi}^\mu), \quad (4.27)$$

where $\dot{\xi}^\mu\dot{\xi}_\mu = 2$. Multiplying this by l_μ and using the relations, $l_\mu\ddot{\xi}^\mu = 1$ and $l_\mu\dddot{\xi}^\mu = \dot{P}_0/P_0$, we get

$$\sqrt{2}\,m(\dot{P}_0/P_0) = 2eF^{\nu\mu}\dot{\xi}_\nu l_\mu + \tfrac{2}{3}e^2(\ddot{P}_0/P_0 + \ddot{\xi}^2/2). \quad (4.28)$$

Now, since $\dot{\xi}_\nu$ can be expressed in terms of the tetrad vectors l_ν and n_ν as $\dot{\xi}_\nu = l_\nu + n_\nu$, and since $F^{\nu\mu}$ is antisymmetric, then

$$F^{\nu\mu}\dot{\xi}_\nu l_\mu = F^{\nu\mu}l_\mu n_\nu = -F^{\mu\nu}l_\mu n_\nu. \quad (4.29)$$

But from the definition of φ_1, i.e., $\varphi_1 = \tfrac{1}{2}F^{\mu\nu}(l_\mu n_\nu + \bar{m}_\mu m_\nu)$, we see that

$$F^{\mu\nu}l_\mu n_\nu = \varphi_1 + \bar{\varphi}_1.$$

Hence, the first term on the right of (4.28) can be written as

$$2eF^{\nu\mu}\dot{\xi}_\nu l_\mu = -2e(\varphi_1 + \bar{\varphi}_1). \quad (4.30)$$

Now, in the flat-space limit ($K\to 1, I\to 0, \psi_a\to 0$, $a = 0$–4) and in the test-charge limit ($\varphi_1^0 \to 0$) of the Einstein–Maxwell solutions, the world line $r=0$ becomes a regular world line in flat space and the value of φ_1 on this line can be shown to be[6]

$$\varphi_1 = -\tfrac{1}{2}\,\bar{\eth}_0 \varphi_0^0, \qquad (4.31)$$

where φ_0^0 satisfies the equation [see (4.3n)]

$$\eth_0 \varphi_0^0 = 0. \qquad (4.32)$$

Setting $\varphi_0^0 = \eth_0 A$, we see that then (4.32) implies that A is an $l = 1$ spherical harmonic, i.e., $A = F$. Therefore, (4.30) becomes

$$2eF^{\mu\nu}\dot{\xi}_\nu l_\mu = e\eth_0\bar{\eth}_0(F + \bar{F}) = -2e(F + \bar{F}). \qquad (4.33)$$

Substituting this back into (4.28), we get precisely (4.26). Thus, we have shown that (4.26) is equivalent to the Lorentz–Dirac equation, with the Lorentz force appearing in terms of a unique background field F and the Abraham radiation reaction force arising without the use of mass renormalization or ad hoc assumptions.

5. SUMMARY AND CONCLUSIONS

We have considered here the extension of a new approach[10] to equations of motion in general relativity that was presented in an earlier paper. This approach was based on an analysis of motion in terms of the structure and behavior of a family of null cones emanating from a special class of singularities, called elementary singularities. Imposing the condition $\rho = -r^{-1} + O(r)$ and $\sigma = O(r)$ on a family of null hypersurfaces u = const in a general curved space, we were able to define a fundamental 2-surface (F2S) whose metric is specified by a function $P = P(u, \zeta, \bar{\zeta})$. By assuming that this F2S is a deformed sphere, i.e., $P = P_0(1 + I)$, we were then able to give an alternative mode of describing motion, in which $\dot{P}_0/P_0$ is identified with the acceleration and I is interpreted as internal degrees of freedom. If the Weyl tensor is singular at $r = 0$, Einstein's field equations yield differential equations governing the behavior of the F2S, from which one could extract equations of motion for the singularity in terms of $\dot{P}_0/P_0$ as well as equations for the time development of its internal structure I.

In this paper we discussed the case where the singularity interacts with both incoming gravitational and electromagnetic fields. We showed (to lowest order) how equations of motion are obtained and how the internal degrees of freedom are driven by the incoming fields (which in turn are modified by the presence of the singularity). In the case of a charged singularity interacting with a Maxwell field, we were able to derive the Lorentz–Dirac equation as a first-order approximation. This is the major result of our work.

In conclusion, we would like to point out some of the difficulties in our approach that must be clarified before it can be considered as an acceptable theory of motion. The primary difficulty is that it appears almost certain that in the neighborhood of the singularity at $r = 0$, there exists a horizon that prohibits external fields from penetrating to $r = 0$. It thus leaves the meaning of the "external" fields ψ_0 and φ_0 obscure. Associated with this problem is that of the time development of each term in the expansion of ψ_0 and φ_0. We do not know the results of studying the higher order r behavior of the solution, e.g., do they lead to compatible equations? Our inclination is to believe that these are not insurmountable difficulties but they nevertheless must be faced.

The work presented here totally neglects the possibility of introducing singularities with internal angular momentum. It now appears that by generalizing the conditions

$$\rho = -1/r + O(r), \qquad \sigma = O(r),$$

to

$$\rho = -\frac{1}{r + i\Sigma} + O(r), \qquad \sigma = O(r),$$

it is possible to study singularities possessing a spin structure, the resulting equations of motion resembling the Frenkel–Mathisson–Papaetrou equations. The details of this work will be discussed in a future paper.

---

* Based in part on a thesis submitted by Roger Posadas to the University of Pittsburgh (1970) in partial fulfillment of the requirements for the Ph.D. degree.

† Research sponsored by the Aerospace Research Lab., OAR, U.S. Air Force, Contract No. F33615-70-C-1081.

‡ Research supported by a Rockefeller Foundation Scholarship. Present address: Department of Physics, University of the Philippines, Diliman, Quezon City D-505, Philippines.

1 E. T. Newman and R. Posadas, Phys. Rev. 187, 1784 (1969).

2 See, for example, F. Rohrlich, *Classical Charged Particles* (Addison-Wesley, Reading, Mass., 1965).

3 E. T. Newman and R. Penrose, J. Math. Phys. 3, 566 (1962).

4 The order symbol is defined as follows: $f(r,u,x^A) = O[g(r)]$ implies that $|f(r,u,x^A)| < g(r)\,F(u,x^A)$ for some function F independent of r and for all small r.

5 E. T. Newman and T. Unti, J. Math. Phys. 3, 891 (1962).

6 Roger Posadas, Ph.D. thesis, University of Pittsburgh, 1970.

7 E. T. Newman and R. Penrose, J. Math. Phys. 7, 863 (1966); J. Goldburg *et al.*, J. Math. Phys. 8, 2155 (1967).

8 F. A. E. Pirani, in *Lectures on General Relativity: 1964 Brandeis Summer Institute in Theoretical Physics* (Prentice-Hall, Englewood Cliffs, N.J., 1965), Vol. I.

9 A. Janis and E. Newman, J. Math. Phys. 6, 902 (1965).

10 For an alternate description of this new approach, see E. Newman, Proceedings of the "Seminar on the Bearings of Topology upon General Relativity", University of Berne, to be published in the new journal, General Relativity and Gravitation.

Relativistic Scattering of Electromagnetic Waves by Moving Obstacles*

Victor Twersky
Mathematics Department, University of Illinois, Chicago, Illinois 60680

(Received 8 December 1970)

The excitation for an obstacle moving with constant velocity in free space (Σ) is transformed to the scatterer's rest system (Σ'), and the corresponding far-field scattering $\mathbf{U}' \sim \mathbf{U}'_a(\mathbf{g})$ is transformed to Σ to obtain $\mathbf{U} \sim \mathbf{U}_a(\mathbf{G})$. A simple expression is derived for the scattering amplitude $\mathbf{G}$ in terms of the conventional $\mathbf{g}$, and known functional forms $\mathbf{U}[\mathbf{G}]$ give the scattered field in Σ as a complex integral and its inverse-distance expansion. In dyadic form, $\tilde{\mathbf{G}} = \tilde{\mathbf{p}}^r \cdot \tilde{\mathbf{g}} \cdot \tilde{\mathbf{p}}$, where $\tilde{\mathbf{p}}$ corresponds to transforming the excitation from Σ to Σ', and $\tilde{\mathbf{p}}^r$ (a planar reciprocal) to transforming the scattering from Σ' to Σ. Then we transform the Green's function surface and volume integral representations, and the multipole series for $\mathbf{U}'$, and apply the results to spherically symmetric scatterers, arbitrary small scatterers, large tenuous scatterers, and to cylinders and slabs.

INTRODUCTION

The scattering of a plane electromagnetic wave by an obstacle moving with costant velocity $\mathbf{v}$ in free space is determined by Einstein's procedure.[1] The wave $\mathbf{\Phi}(\mathbf{r},t)$ in the observer's system Σ is transformed to the scatterer's system Σ' as the incident wave $\mathbf{\Phi}'(\mathbf{r}'t')$, and the corresponding scattered wave $\mathbf{U}'(\mathbf{r}',t')$ is then transformed to Σ as the required function $\mathbf{U}$. We use known results of relativity[1-3] and scattering[4,5] theory, and transform explicit 3-vector forms in an invariant cylindrical basis $(\hat{\mathbf{v}}, \hat{\rho}, \hat{\varphi})$; initial forms are in spherical bases $(\hat{\mathbf{r}}, \hat{\theta}, \hat{\varphi}; \hat{\mathbf{r}}', \hat{\theta}, \hat{\varphi})$, and results are exhibited in retarded $(\hat{\mathbf{R}}, \hat{\Theta}, \hat{\varphi})$, present $(\hat{\mathbf{r}}_s, \hat{\theta}_s, \hat{\varphi})$, and mixed $(\hat{\mathbf{r}}_s, \hat{\Theta}, \hat{\varphi})$ bases in which $\hat{\varphi}$ is invariant. Earlier work of Yeh and Casey,[6] Censor,[7] Lee and Mittra,[8] and Restrick[9] and Tai[10] is cited in context.

Given $\mathbf{\Phi}$ with direction of propagation $\hat{\mathbf{r}}_i = \hat{\mathbf{k}}$ and polarization $\hat{\mathbf{p}} = \hat{\theta}_i p_1 + \hat{\varphi}_i p_2 = \hat{\alpha} p_1 + \hat{\delta} p_2$, we isolate a simple form $\hat{\mathbf{p}}' = \hat{\alpha}' p_1 + \hat{\delta} p_2$ in $\mathbf{\Phi}'(\hat{\mathbf{k}}' : p' \hat{\mathbf{p}}')$ and show it exhibits the invariance aspects of the transformation. Given the scattering amplitude $\mathbf{g}(\hat{\mathbf{r}}')$ for the conventional problem in Σ', we transform only the far-field $\mathbf{U}' \sim \mathbf{U}'_a(\mathbf{g})$ to obtain $\mathbf{U} \sim \mathbf{U}_a(\mathbf{G})$ with $\mathbf{G}(\hat{\mathbf{R}}; \hat{\mathbf{r}}') \propto \hat{\Theta} g_{\theta'} + \hat{\varphi} g_\varphi$; the known[4] functional forms $\mathbf{U}[\mathbf{G}]$ give the scattered field in Σ as a complex integral, and its inverse-distance expansion. (Far fields have been transformed before,[8-10] and a complex integral for $\mathbf{U}$ was obtained originally by Censor[7] by transforming the analogous integral for $\mathbf{U}'$.) The result $\hat{\mathbf{p}} \cdot \mathbf{G}(\hat{\mathbf{k}}; \hat{\mathbf{k}}') = \hat{\mathbf{p}}' \cdot \mathbf{g}(\hat{\mathbf{k}}')$ interrelates the interference effects in the two systems. In dyadic form, $\tilde{\mathbf{G}} = \tilde{\mathbf{p}}^r \cdot \tilde{\mathbf{g}} \cdot \tilde{\mathbf{p}}$, where $\tilde{\mathbf{p}} = (\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta}) p'(\hat{\mathbf{k}} \cdot \hat{\mathbf{v}})$ corresponds to transforming the excitation from Σ to Σ', $\tilde{\mathbf{p}}^r = (\hat{\Theta}\hat{\theta}' + \hat{\varphi}\hat{\varphi})/p'(\hat{\mathbf{R}} \cdot \hat{\mathbf{v}})$ (a planar reciprocal) to transforming the scattering from Σ' to Σ.

Then we transform surface and volume integral representations and multipole series, and apply the results to spheres, arbitrary small scatterers, large tenuous scatterers, cylinders and slabs.

1. THE SCATTERED FIELD

Preliminary Considerations

We assume that system Σ' has the constant velocity $\mathbf{v} = v\hat{\mathbf{z}}$ in Σ and that the origins coincide at $t = t' = 0$. An event $\mathbf{r}(z,x,y), t$ in Σ is specified in Σ' by $\mathbf{r}'(z',x',y'), t'$ where[1]

$$z' = \gamma(z - \beta ct), \quad x' = x, \quad y' = y, \quad t = \gamma(t - \beta z/c), \quad \beta = v/c, \quad \gamma = (1-\beta^2)^{-1/2} \tag{1}$$

with the velocity of light given by $c = (\epsilon_0 \mu_0)^{-1/2}$ in terms of the free-space electromagnetic parameters. Using the dyadic $\tilde{\mathbf{V}} = \hat{\mathbf{v}}\hat{\mathbf{v}}$ and the identity $\tilde{\mathbf{I}}$, we write

$$\mathbf{r}' = \tilde{\mathbf{L}} \cdot (\mathbf{r} - \mathbf{v}t), t' = \gamma(t - \mathbf{v}\cdot\mathbf{r}/c^2); \quad \tilde{\mathbf{L}} = \gamma\tilde{\mathbf{V}} + (\tilde{\mathbf{I}} - \tilde{\mathbf{V}}) = \gamma\tilde{\mathbf{V}} + \tilde{\mathbf{T}} \tag{2}$$

The fields transform as[1-3]

$$\mathbf{E}' = \tilde{\mathbf{\Gamma}} \cdot \mathbf{E} + \gamma \mathbf{v} \times \mathbf{H}\mu_0, \quad \mathbf{H}' = \tilde{\mathbf{\Gamma}} \cdot \mathbf{H} - \gamma \mathbf{v} \times \mathbf{E}\epsilon_0, \quad \tilde{\mathbf{\Gamma}} = \tilde{\mathbf{V}} + \gamma\tilde{\mathbf{T}} = \gamma\tilde{\mathbf{L}}^{-1}. \tag{3}$$

For the inverse of (2) or (3), we switch primes from left to right and replace $\mathbf{v}$ by $-\mathbf{v}$. For t-periodic $(e^{-i\omega t})$ fields, from $\nabla \times \mathbf{H} = \epsilon_0 \partial_t \mathbf{E}$ and $\nabla \times \mathbf{E} = -\mu_0 \partial_t \mathbf{H}$, we have

$$\mathbf{\Psi} = \frac{\nabla \times \nabla \times \mathbf{\Psi}}{k^2} = -\frac{\nabla \times \mathbf{\Psi}_M}{ik} = \begin{Bmatrix} \mathbf{E} \\ \mathbf{H} \end{Bmatrix}, \quad \mathbf{\Psi}_M = \frac{\nabla \times \mathbf{\Psi}}{ik} = \begin{Bmatrix} \mathbf{H}\mu_0 c \\ -\mathbf{E}\epsilon_0 c \end{Bmatrix}, \quad \nabla \cdot \mathbf{\Psi} = 0, \tag{4}$$

with $k = \omega/c$. Thus, $\mathbf{\Psi}'$ and its mate $\mathbf{\Psi}'_M$ are specified by $\mathbf{\Psi}$ as

$$\mathbf{\Psi}' = \tilde{\mathbf{\Gamma}} \cdot \mathbf{\Psi} + \gamma\beta\hat{\mathbf{v}} \times (\nabla \times \mathbf{\Psi}/ik), \quad \mathbf{\Psi}'_M = \tilde{\mathbf{\Gamma}} \cdot (\nabla \times \mathbf{\Psi}/ik) - \gamma\beta\hat{\mathbf{v}} \times \mathbf{\Psi}; \quad \nabla' \cdot \mathbf{\Psi}' = 0. \tag{5}$$

Similarly, to transform t'-periodic $(e^{-i\omega' t'})$ fields from Σ' to Σ we switch the primes and replace $\hat{\mathbf{v}}$ by $-\hat{\mathbf{v}}$ and k by k'.

We use (5), or its inverse, with explicit 3-vector forms in the invariant Cartesian basis $(\hat{\mathbf{z}} = \hat{\mathbf{v}}, \hat{\mathbf{x}}, \hat{\mathbf{y}})$ implicit in (1), or in the invariant cylindrical basis $(\hat{\mathbf{v}}, \hat{\rho} = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi, \hat{\varphi} = \hat{\mathbf{v}} \times \hat{\rho})$, or in spherical bases $(\hat{\mathbf{r}} = \hat{\mathbf{v}}\cos\theta + \hat{\rho}\sin\theta, \hat{\theta} = \hat{\varphi} \times \hat{\mathbf{r}}, \hat{\varphi}; \hat{\mathbf{r}}', \hat{\theta}', \hat{\varphi})$ in which only $\hat{\varphi}$ is invariant. Corresponding to $\mathbf{r} = \mathbf{z} + \boldsymbol{\rho} = \hat{\mathbf{z}}r\cos\theta + \hat{\rho}r\sin\theta$, we have $\mathbf{r}' = \mathbf{z}' + \boldsymbol{\rho}$, with $z' = r'\cos\theta' = \gamma(\hat{\mathbf{v}}\cdot\mathbf{r} - vt)$ and $\rho = r'\sin\theta' = r\sin\theta = (x^2 + y^2)^{1/2}$. The decompositions are general, since any direction $\hat{\mathbf{r}}$ can be written in terms of the invariant direction $\hat{\mathbf{v}}$ as $\hat{\mathbf{r}} = \hat{\mathbf{r}}\cdot\hat{\mathbf{v}}\hat{\mathbf{v}} + (\hat{\mathbf{v}} \times \hat{\mathbf{r}}) \times \hat{\mathbf{r}}$; then, we define in turn θ, then $\hat{\varphi}$, and then $\hat{\rho}$ and $\hat{\theta}$, by means of $\hat{\mathbf{v}}\cdot\hat{\mathbf{r}} = \cos\theta$, $\hat{\mathbf{v}} \times \hat{\mathbf{r}} = \hat{\varphi}\sin\theta$, $\hat{\varphi} \times \hat{\mathbf{v}} = \hat{\rho}$, and $\hat{\varphi} \times \hat{\mathbf{r}} = \hat{\theta}$.

Plane Waves

In Σ, we write a plane wave with direction of propagation $\hat{\mathbf{k}}$ and polarization $\hat{\mathbf{p}}$ as

$$\Phi = e^{i\nu(\hat{\mathbf{k}})}\hat{\mathbf{p}}(\hat{\mathbf{k}}), \quad \nu(\hat{\mathbf{k}}) = k\hat{\mathbf{k}}\cdot\mathbf{r} - \omega t, \quad \hat{\mathbf{k}}\cdot\hat{\mathbf{p}}(\hat{\mathbf{k}}) = 0, \tag{6}$$

where $\hat{\mathbf{k}}\cdot\hat{\mathbf{p}} = 0$ ensures $\nabla\cdot\Phi = 0$. In Σ', by (5) and (2),

$$\Phi' = e^{i\nu'(\hat{\mathbf{k}}')}\mathbf{p}', \quad \nu'(\hat{\mathbf{k}}') = k'\hat{\mathbf{k}}'\cdot\mathbf{r}' - \omega' t',$$
$$\mathbf{p}' = \tilde{\Gamma}\cdot\hat{\mathbf{p}} + \gamma\beta\hat{\mathbf{v}}\times(\hat{\mathbf{k}}\times\hat{\mathbf{p}}) = p'\hat{\mathbf{p}}', \tag{7}$$

where the phase $\nu'(\hat{\mathbf{k}}') = \nu(\hat{\mathbf{k}})$ is invariant[1,2] with

$$k'/k = \omega'/\omega = \gamma(1-\beta\cos\alpha) = 1/\gamma(1+\beta\cos\alpha) = p';$$
$$\cos\alpha' = (\cos\alpha - \beta)/(1-\beta\cos\alpha),$$
$$\sin\alpha' = \sin\alpha/[\gamma(1-\beta\cos\alpha)], \tag{8}$$

in terms of $\cos\alpha = \hat{\mathbf{k}}\cdot\hat{\mathbf{v}}$ and $\cos\alpha' = \hat{\mathbf{k}}'\cdot\hat{\mathbf{v}}$. All details of (7) but $\hat{\mathbf{p}}'$ have been discussed fully.[1-3] Since the isolation of a simple form $\hat{\mathbf{p}}'(\hat{\mathbf{p}})$ exhibiting the invariance aspects of the transformation is essential to our development (and provides the prototype for later work), we consider some elementary matters. See Censor[7] for work with $\mathbf{p}' = [(1-\gamma)\hat{\mathbf{v}} + \gamma\beta\hat{\mathbf{k}}]\hat{\mathbf{v}}\cdot\hat{\mathbf{p}} + \gamma(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}})\hat{\mathbf{p}}$, and Restrick[9] for work in rotated Cartesian systems.

We write $\hat{\mathbf{k}} = \hat{\mathbf{v}}\cdot\hat{\mathbf{k}}\hat{\mathbf{v}} + (\hat{\mathbf{v}}\times\hat{\mathbf{k}})\times\hat{\mathbf{v}}$, and introduce α, then $\hat{\delta}$, and then $\hat{\mu}$ and $\hat{\alpha}$ by means of $\hat{\mathbf{v}}\cdot\hat{\mathbf{k}} = \cos\alpha$, $\hat{\mathbf{v}}\times\hat{\mathbf{k}} = \hat{\delta}\sin\alpha$, and $\hat{\delta}\times\hat{\mathbf{v}} = \hat{\mu}$ and $\hat{\delta}\times\hat{\mathbf{k}} = \hat{\alpha}$. Thus, for a given $\hat{\mathbf{k}}$ there is an associated invariant cylindrical set $\hat{\mathbf{v}}, \hat{\mu}, \hat{\delta}$ (in $\hat{\mathbf{v}}, \hat{\rho}, \hat{\varphi}$), and a spherical set $\hat{\mathbf{k}}, \hat{\alpha}, \hat{\delta}$ (in $\hat{\mathbf{r}}, \hat{\theta}, \hat{\varphi}$) with $\hat{\delta}$ invariant. Since $\hat{\mathbf{p}}\cdot\hat{\mathbf{k}} = 0$, we may write $\hat{\mathbf{p}} = (\tilde{\mathbf{I}} - \hat{\mathbf{k}}\hat{\mathbf{k}})\cdot\hat{\mathbf{p}}$ or, equivalently,

$$\hat{\mathbf{p}} = (\hat{\alpha}\hat{\alpha} + \hat{\delta}\hat{\delta})\cdot\hat{\mathbf{p}} = \hat{\alpha}(\hat{\alpha}\cdot\hat{\mathbf{p}}) + \hat{\delta}(\hat{\delta}\cdot\hat{\mathbf{p}}) = \hat{\alpha}p_1 + \hat{\delta}p_2$$
$$= \hat{\alpha}\sin Q + \hat{\delta}\cos Q, \tag{9}$$

where Q is the polarization angle.

In the cylindrical basis, we have $\hat{\mathbf{k}} = \hat{\mathbf{v}}\cos\alpha + \hat{\mu}\sin\alpha$, $\hat{\alpha} = -\hat{\mathbf{v}}\sin\alpha + \hat{\mu}\cos\alpha$, and $\tilde{\Gamma} = \hat{\mathbf{v}}\hat{\mathbf{v}} + \gamma(\hat{\mu}\hat{\mu} + \hat{\delta}\hat{\delta})$; from (7), $\mathbf{p}' = [-\hat{\mathbf{v}}\sin\alpha + \hat{\mu}\gamma(\cos\alpha - \beta)]p_1 + \hat{\delta}\gamma(1-\beta\cos\alpha)p_2$, and by (8), $\mathbf{p}' = (-\hat{\mathbf{v}}\sin\alpha' + \hat{\mu}\cos\alpha')p_1 + \hat{\delta}p_2$. Thus, with $\hat{\alpha}' = -\hat{\mathbf{v}}\sin\alpha' + \hat{\mu}\cos\alpha'$,

$$\hat{\mathbf{p}}' = \hat{\alpha}'p_1 + \hat{\delta}p_2 = \hat{\alpha}'(\hat{\alpha}\cdot\hat{\mathbf{p}}) + \hat{\delta}(\hat{\delta}\cdot\hat{\mathbf{p}})$$
$$= (\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta})\cdot\hat{\mathbf{p}} = \hat{\alpha}'\sin Q + \hat{\delta}\cos Q; \tag{10}$$

since $\hat{\mathbf{k}}' = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{k}} - \beta\hat{\mathbf{v}})/p' = \hat{\mathbf{v}}\cos\alpha' + \hat{\mu}\sin\alpha'$, we have $\hat{\mathbf{p}}'\cdot\hat{\mathbf{k}}' = 0$ as required for $\nabla'\cdot\Phi' = 0$. The final forms of $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$ differ from those of Restrick[9] in that his corresponding pairs of base vectors plus $\hat{\mathbf{k}}$ or $\hat{\mathbf{k}}'$, respectively, form rotated Cartesian bases with one base vector in common.

In terms of $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$, the corresponding mates are

$$\Phi_M = \hat{\mathbf{k}}\times\Phi = \hat{\mathbf{p}}_M e^{i\nu},$$
$$\hat{\mathbf{p}}_M = \hat{\mathbf{k}}\times\hat{\mathbf{p}} = (-\hat{\alpha}\hat{\delta} + \hat{\delta}\hat{\alpha})\cdot\hat{\mathbf{p}} = -\hat{\alpha}\cos Q + \hat{\delta}\sin Q,$$
$$\Phi'_M = \hat{\mathbf{k}}'\times\Phi' = p'\hat{\mathbf{p}}'_M e^{i\nu},$$
$$\hat{\mathbf{p}}'_M = \hat{\mathbf{k}}'\times\hat{\mathbf{p}}' = (-\hat{\alpha}'\hat{\delta} + \hat{\delta}\hat{\alpha})\cdot\hat{\mathbf{p}}' = -\hat{\alpha}'\cos Q + \hat{\delta}\sin Q, \tag{11}$$

and we also have $\hat{\mathbf{p}}_M = (\hat{\alpha}\hat{\alpha} + \hat{\delta}\hat{\delta})\cdot(\hat{\mathbf{k}}\times\hat{\mathbf{p}})$ and $\hat{\mathbf{p}}'_M = (\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta})\cdot(\hat{\mathbf{k}}\times\hat{\mathbf{p}})$, as well as the analogs of (11) for $\hat{\mathbf{p}}(\hat{\mathbf{p}}_M)$ and $\hat{\mathbf{p}}'(\hat{\mathbf{p}}'_M)$. (For some purposes, the sets $\hat{\mathbf{k}}, \hat{\mathbf{p}}, \hat{\mathbf{p}}_M$ and $\hat{\mathbf{k}}', \hat{\mathbf{p}}', \hat{\mathbf{p}}'_M$ provide natural rotated Cartesian bases, but we do not use them in the present development.)

The polarization angle Q is preserved in the sense

$$\hat{\delta}\cdot\hat{\mathbf{p}} = \hat{\delta}\cdot\hat{\mathbf{p}}' = \cos Q, \quad \hat{\alpha}\cdot\hat{\mathbf{p}} = \hat{\alpha}'\cdot\hat{\mathbf{p}}' = \sin Q. \tag{12}$$

Thus, if for fixed $\hat{\mathbf{k}}$ we consider two different polarizations, $\hat{\mathbf{p}}_1 = \hat{\alpha}\sin Q_1 + \hat{\delta}\cos Q_1 = \hat{\mathbf{p}}[Q_1]$ and $\hat{\mathbf{p}}_2 = \hat{\mathbf{p}}[Q_2]$, then

$$\hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2 = \hat{\mathbf{p}}'_1\cdot\hat{\mathbf{p}}'_2 = \cos(Q_1 - Q_2) \tag{13}$$

is invariant, i.e., the angle between two different polarizations along a ray is invariant under transformation. This follows from (12), which is simply a consequence of the invariance of the $\hat{\mathbf{v}}$ components of the field (3) or (5). Thus, from $\hat{\mathbf{v}}\cdot\Phi_M = \hat{\mathbf{v}}\cdot\Phi'_M$, i.e., $\hat{\mathbf{v}}\cdot\hat{\mathbf{p}}_M = p'\hat{\mathbf{v}}\cdot\hat{\mathbf{p}}_M$, we have $\hat{\mathbf{v}}\cdot(\hat{\mathbf{k}}\times\hat{\mathbf{p}}) = p'\hat{\mathbf{v}}\cdot(\hat{\mathbf{k}}'\times\hat{\mathbf{p}}')$; since $\hat{\mathbf{v}}\times\hat{\mathbf{k}} = \hat{\delta}\sin\alpha$ and $\hat{\mathbf{v}}\times\hat{\mathbf{k}}' = \hat{\delta}\sin\alpha'$, we obtain $\hat{\delta}\cdot\hat{\mathbf{p}}\sin\alpha = \hat{\delta}\cdot\hat{\mathbf{p}}'p'\sin\alpha'$ which by (8) reduces to $\hat{\delta}\cdot\hat{\mathbf{p}} = \hat{\delta}\cdot\hat{\mathbf{p}}'$ of (12). Similarly, $\hat{\mathbf{v}}\cdot\Phi = \hat{\mathbf{v}}\cdot\Phi'$ gives $\hat{\delta}\cdot\hat{\mathbf{p}}_M = \hat{\delta}\cdot\hat{\mathbf{p}}'_M$ or, equivalently, $\hat{\delta}\cdot(\hat{\mathbf{k}}\times\hat{\mathbf{p}}) = \hat{\delta}\cdot(\hat{\mathbf{k}}'\times\hat{\mathbf{p}}')$ which reduces to $\hat{\alpha}\cdot\hat{\mathbf{p}} = \hat{\alpha}'\cdot\hat{\mathbf{p}}'$ of (12) on using $\hat{\delta}\times\hat{\mathbf{k}} = \hat{\alpha}$ and $\hat{\delta}\times\hat{\mathbf{k}}' = \hat{\alpha}'$. Thus, the invariants $\hat{\mathbf{v}}\cdot\Phi_M$ and $\hat{\mathbf{v}}\cdot\Phi$ correspond, respectively, to the invariants $\hat{\delta}\cdot\hat{\mathbf{p}}$ and $\hat{\delta}\cdot\hat{\mathbf{p}}_M$, and both are exhibited in (12) and in the basic form $\hat{\mathbf{p}}'(\hat{\mathbf{p}})$ of (10). The relation $\Phi'\cdot\Phi_M = \Phi\cdot\Phi'_M$ required by (5) is shown in $\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}}_M = \hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'_M = \cos Q\sin Q[1 - \cos(\alpha' - \alpha)]$.

Similarly, if we transform from Σ' the wave

$$\Phi'_s(\hat{\mathbf{R}}') = p'e^{i\nu'(\hat{\mathbf{R}}')}\hat{\mathbf{G}}(\hat{\mathbf{R}}'), \quad \nu'(\hat{\mathbf{R}}') = k'\hat{\mathbf{R}}'\cdot\mathbf{r}' - \omega' t',$$
$$\hat{\mathbf{G}}' = (\hat{\Theta}'\hat{\Theta}' + \hat{\varphi}\hat{\varphi})\cdot\hat{\mathbf{G}}' = \hat{\Theta}'\sin\mathfrak{Q} + \hat{\varphi}\cos\mathfrak{Q}; \tag{14}$$

where $\hat{\mathbf{R}}', \hat{\Theta}', \hat{\varphi}$ form a special spherical set (in $\hat{\mathbf{r}}', \hat{\theta}, \hat{\varphi}$), we obtain in Σ in terms of the corresponding set $\hat{\mathbf{R}}, \hat{\Theta}, \hat{\varphi}$ (in $\hat{\mathbf{r}}, \hat{\theta}, \hat{\varphi}$)

$$\Phi_s(\hat{\mathbf{R}};\hat{\mathbf{R}}') = p'p_s e^{i\nu_s}\hat{\mathbf{G}} = Pe^{iP\nu(\hat{\mathbf{R}})}\hat{\mathbf{G}}(\hat{\mathbf{R}});$$
$$\hat{\mathbf{G}}(\hat{\mathbf{R}}) = (\hat{\Theta}\hat{\Theta}' + \hat{\varphi}\hat{\varphi})\cdot\hat{\mathbf{G}}' = \hat{\Theta}\sin\mathfrak{Q} + \hat{\varphi}\cos\mathfrak{Q};$$
$$\nu_s = k_s\hat{\mathbf{R}}\cdot\mathbf{r} - \omega_s t = \nu'(\hat{\mathbf{R}}') = P\nu(\hat{\mathbf{R}}),$$
$$\nu(\hat{\mathbf{R}}) = k\hat{\mathbf{R}}\cdot\mathbf{r} - \omega t, \quad P = p'p_s = k_s/k = \omega_s/\omega;$$
$$p_s = k_s/k' = \omega_s/\omega' = \gamma(1+\beta\cos\Theta')$$
$$= [\gamma(1-\beta\cos\Theta)]^{-1};$$
$$\cos\Theta = (\cos\Theta' + \beta)/(1+\beta\cos\Theta'),$$
$$\sin\Theta = \sin\Theta'/[\gamma(1+\beta\cos\Theta')]. \tag{15}$$

Essentially as before for (7), the form for $\hat{\mathbf{G}}$ follows from $p_s\hat{\mathbf{G}} = \tilde{\Gamma}\cdot\hat{\mathbf{G}}' - \gamma\beta\hat{\mathbf{v}}\times(\hat{\mathbf{R}}'\times\hat{\mathbf{G}}')$ with $\tilde{\Gamma} = \hat{\mathbf{v}}\hat{\mathbf{v}} + \gamma(\hat{\rho}\hat{\rho} + \hat{\varphi}\hat{\varphi})$, etc. We have $\hat{\mathbf{R}} = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{R}}' +$

$\beta\hat{\mathbf{v}})/p_s = \hat{\mathbf{v}}\cos\Theta + \hat{\boldsymbol{\rho}}\sin\Theta$, and $\hat{\mathbf{\Theta}} = \tilde{\Gamma}\cdot(\hat{\Theta}' + \beta\hat{\rho})/p_s = \hat{\varphi}\times\hat{\mathbf{R}}$; the forms $\Theta(\Theta')$ are the same as $\alpha(\alpha')$ of (8), and the function p_s is reciprocal to p'. The corresponding mates are

$$\begin{aligned}\mathbf{\Phi}'_{sM} &= \hat{\mathbf{R}}'\times\mathbf{\Phi}'_s = \hat{\mathbf{G}}'_M e^{i\nu'},\\ \hat{\mathbf{G}}'_M &= \hat{\mathbf{R}}'\times\hat{\mathbf{G}}' = (-\hat{\mathbf{\Theta}}'\hat{\varphi} + \hat{\varphi}\hat{\mathbf{\Theta}}')\cdot\hat{\mathbf{G}}',\\ \mathbf{\Phi}_{sM} &= \hat{\mathbf{R}}\times\mathbf{\Phi}_s = \hat{\mathbf{G}}_M P e^{iP\nu},\\ \hat{\mathbf{G}}_M &= \hat{\mathbf{R}}\times\hat{\mathbf{G}} = (\hat{\mathbf{\Theta}}\hat{\mathbf{\Theta}}' + \hat{\varphi}\hat{\varphi})\cdot(\hat{\mathbf{R}}\times\hat{\mathbf{G}}')\\ &= (-\hat{\mathbf{\Theta}}\hat{\varphi} + \hat{\varphi}\hat{\mathbf{\Theta}}')\cdot\mathbf{G}'.\end{aligned}\tag{16}$$

If $\hat{\mathbf{R}}' = \hat{\mathbf{k}}'$, then $\hat{\mathbf{R}} = \hat{\mathbf{k}}$ (and $\omega_s = \omega$, etc.), and (14) and (15) reduce to (7) and (6) with different polarizations; by (13),

$$\hat{\mathbf{p}}'(\hat{\mathbf{k}}')\cdot\hat{\mathbf{G}}'(\hat{\mathbf{k}}') = \hat{\mathbf{p}}(\hat{\mathbf{k}})\cdot\hat{\mathbf{G}}(\hat{\mathbf{k}}) = \cos(Q - \mathcal{Q}).\tag{17}$$

More generally, for fixed $\hat{\mathbf{R}}'$, in terms of $\hat{\mathbf{G}}_1 = \mathbf{G}[\mathcal{Q}_1]$, etc,

$$\hat{\mathbf{G}}'_1(\hat{\mathbf{R}}')\cdot\hat{\mathbf{G}}'_2(\hat{\mathbf{R}}') = \hat{\mathbf{G}}_1(\hat{\mathbf{R}})\cdot\hat{\mathbf{G}}_2(\hat{\mathbf{R}}) = \cos(\mathcal{Q}_1 - \mathcal{Q}_2)\tag{18}$$

is invariant. Essentially as before for $\hat{\mathbf{p}}$, (18) is a consequence of $\hat{\varphi}\cdot\hat{\mathbf{G}} = \hat{\varphi}\cdot\hat{\mathbf{G}}'$ and $\hat{\varphi}\cdot\hat{\mathbf{G}}_M = \hat{\varphi}\cdot\mathbf{G}'_M$, which follow from the invariance of $\hat{\mathbf{v}}\cdot\mathbf{\Phi}'_{sM}$ and $\hat{\mathbf{v}}\cdot\mathbf{\Phi}'_s$ respectively.

In terms of the dyadics $\tilde{\phi}$ and $\tilde{\mathbf{\Phi}}$, we rewrite the fields as

$$\mathbf{\Phi}'_s = e^{-i\omega't'}p'\tilde{\phi}(\hat{\mathbf{R}}')\cdot\hat{\mathbf{G}}',\quad \tilde{\phi}(\hat{\mathbf{R}}') = (\hat{\mathbf{\Theta}}'\hat{\mathbf{\Theta}}' + \hat{\varphi}\hat{\varphi})e^{ik'\hat{\mathbf{R}}'\cdot\mathbf{r}'},\tag{19}$$

$$\mathbf{\Phi}_s = \tilde{\mathbf{\Phi}}\cdot\hat{\mathbf{G}},\quad \Phi(\hat{\mathbf{R}},\hat{\mathbf{R}}') = (\hat{\mathbf{\Theta}}\hat{\mathbf{\Theta}}' + \hat{\varphi}\hat{\varphi})Pe^{iP\nu(\hat{\mathbf{R}})},\quad \nu(\hat{\mathbf{R}}) = k(\hat{\mathbf{R}}\cdot\mathbf{r} - ct)\tag{20}$$

Statement of the Problem

We consider $\mathbf{\Phi} = \hat{\mathbf{p}}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}$ of (6) exciting a scatterer moving with $\mathbf{v} = v\hat{\mathbf{z}}$ in Σ. The scatterer is specified in its rest system Σ' by its volume ($\mathcal{V}'$), surface ($\mathcal{A}'$), electromagnetic parameters (ϵ', μ'), etc.; the center ($r' = 0$) of its smallest circumscribing sphere ($r' = a'$) is the origin. The excitation in Σ' is $\mathbf{\Phi}'$ of (7), which we rewrite as

$$\mathbf{\Phi}' = e^{-i\omega't'}p'\boldsymbol{\phi},\quad \boldsymbol{\phi} = \hat{\mathbf{p}}'e^{i\mathbf{k}'\cdot\mathbf{r}'}\tag{21}$$

with $\mathbf{k}' = \tilde{\mathbf{L}}\cdot(\mathbf{k} - k\beta\hat{\mathbf{v}}) = kp'\hat{\mathbf{k}}'$ and $\hat{\mathbf{p}}' = (\hat{\boldsymbol{\alpha}}'\hat{\alpha} + \hat{\delta}\hat{\delta})\cdot\hat{\mathbf{p}}$ as in (8)–(10). The corresponding scattered wave is

$$\mathbf{U}' = e^{-i\omega't'}p'\mathbf{u}\tag{22}$$

such that $\boldsymbol{\phi} + \mathbf{u} = \boldsymbol{\psi}$ is the solution of the conventional scattering problem.[4] For $r' \sim \infty$, with $h(x) = h_0^{(1)}(x) = e^{ix}/ix$, we have

$$\begin{aligned}\mathbf{u} \sim \mathbf{u}_a &= h(k'r')\mathbf{g}(\hat{\mathbf{r}}'),\\ \mathbf{g}(\hat{\mathbf{r}}') &= (\hat{\theta}'\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\mathbf{g}(\hat{\mathbf{r}}') = \hat{\theta}'g_{\theta'} + \hat{\varphi}g_\varphi,\end{aligned}\tag{23}$$

where $\mathbf{g}(\hat{\mathbf{r}}') = \mathbf{g}(\hat{\mathbf{r}}', \hat{\mathbf{k}}' : \hat{\mathbf{p}}')$ is the corresponding scattering amplitude. The normalization is such that

$$-\operatorname{Re}\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') = (k'^2/4\pi)\sigma'_T = \mathfrak{M}\,|\mathbf{g}(\hat{\mathbf{r}}')|^2 + (k'^2/4\pi)\sigma'_A,$$
$$\sigma'_T = \sigma'_S = \sigma'_A,\quad \mathfrak{M} = (1/4\pi)\int d\Omega(\hat{\mathbf{r}}'),\tag{24}$$

where $\mathfrak{M}$ indicates the mean over all directions of observation, and σ'_T, σ'_S, and σ'_A are the total, scattering, and absorption cross sections. (The usual normalization corresponds to $\mathbf{g}/ik' = f$.) We regard $\mathbf{g}$ as known, so that $\mathbf{u}$ is known at least for $r' > a'$.

We may write $\mathbf{u}$ functionally in terms of $\mathbf{g}$ as the complex integral of plane waves with complex direction $\hat{\mathbf{R}}'_c(\hat{\Theta}'_c, \hat{\varphi}_c)$ and amplitude $\mathbf{g}(\hat{\mathbf{R}}'_c)$ given in (27),[4] or as the series (convergent and asymptotic) in powers of $1/k'r'$ and of derivatives of $\mathbf{g}(\hat{\mathbf{r}}')$ with respect to θ' and φ as in (29)[4] and (54).[4] We indicate these functional forms symbolically by

$$\begin{aligned}\mathbf{u}[\mathbf{g}] &= \int e^{ik'\mathbf{r}'\cdot\hat{\mathbf{R}}'_c}\mathbf{g}(\hat{\mathbf{R}}'_c) = \int\tilde{\boldsymbol{\phi}}(\hat{\mathbf{R}}'_c)\cdot\mathbf{g}(\hat{\mathbf{R}}'_c)\\ &= h(k'r')\tilde{\mathfrak{D}}\cdot\mathbf{g}(\hat{\mathbf{r}}'),\end{aligned}\tag{25}$$

where $\int = (1/2\pi)\int d\Omega(\hat{\mathbf{R}}'_c)$ with paths as for $h_0^{(1)}$, and $\tilde{\mathfrak{D}} = \tilde{\mathbf{I}} + (i/2k'r')\tilde{\mathbf{D}} + \cdots$, with $\tilde{\mathbf{D}}$ as a Beltrami operator; see Ref. 4 for details. For the mate $\mathbf{u}_M$, we replace $\mathbf{g}$ by $\hat{\mathbf{R}}'_c\times\mathbf{g}$ (or by $\hat{\mathbf{r}}'\times\mathbf{g}$ for the last form).

Thus, since $\mathbf{g}$ determines $\mathbf{u}$, and since $\mathbf{U}' \sim e^{-i\omega't'}p'\mathbf{u}_a = e^{-i\omega't'}hp'\mathbf{g} = \mathbf{U}'_a$ for $r' \sim \infty$, we need only transform

$$\begin{aligned}\mathbf{U}'_a &= e^{i(k'r'-\omega't')}\mathbf{G}'/ik'r',\\ \mathbf{G}'(\hat{\mathbf{r}}') &= p'\mathbf{g} = p'(\hat{\theta}'g_{\theta'} + \hat{\varphi}g_\varphi) = g(\hat{\mathbf{r}}')p'\hat{\mathbf{G}}'(\hat{\mathbf{r}}').\end{aligned}\tag{26}$$

Then, in Σ we isolate the corresponding amplitude $\mathbf{G}$ and use it in the functional forms (25) to construct $\mathbf{U}$.

Solution

From (5), the transform of $\mathbf{U}'_a$ for $r' \sim \infty$ is

$$\begin{aligned}\mathbf{U}_a &= e^{-i\omega't'}h(k'r')\mathbf{G} = e^{i\nu_s}\mathbf{G}/ik'r',\\ \nu_s &= P(k\hat{\mathbf{R}}\cdot\mathbf{r} - \omega t) = k'r' - \omega't',\\ \mathbf{G}(\hat{\mathbf{R}};\hat{\mathbf{r}}') &= g(\hat{\mathbf{r}}')P\hat{\mathbf{G}}(\hat{\mathbf{R}}) = P(\hat{\Theta}g_{\theta'} + \hat{\varphi}g_\varphi)\\ &= P(\hat{\mathbf{\Theta}}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\mathbf{g}(\hat{\mathbf{r}}'),\end{aligned}\tag{27}$$

where $\hat{\mathbf{R}} = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{r}}' + \beta\hat{\mathbf{v}})/p_s$ and $P = p'p_s(\theta')$ as in (15) in terms of $\mathbf{\Theta}' = \theta'$ (corresponding essentially to the transform of (14) for $\hat{\mathbf{R}}' = \hat{\mathbf{r}}'$). The mates to $\mathbf{U}'_a$ and $\mathbf{U}_a$ are $\mathbf{U}'_{aM} = \hat{\mathbf{r}}'\times\mathbf{U}'_a$ and $\mathbf{U}_{aM} = \hat{\mathbf{R}}\times\mathbf{U}_a$.

The scattered wave in Σ is thus

$$\begin{aligned}\mathbf{U} &= e^{-i\omega't'}\int e^{ik'\mathbf{r}'\cdot\hat{\mathbf{R}}_c}\mathbf{G}(\hat{\mathbf{R}}_c;\hat{\mathbf{R}}'_c) = \int\tilde{\mathbf{\Phi}}(\hat{\mathbf{R}}_c;\hat{\mathbf{R}}'_c)\cdot\mathbf{g}(\hat{\mathbf{R}}'_c)\\ &= e^{-i\omega't'}h(k'r')\tilde{\mathfrak{D}}\cdot\mathbf{G}(\hat{\mathbf{R}};\hat{\mathbf{r}}'),\end{aligned}\tag{28}$$

where $\mathbf{G}(\hat{\mathbf{R}}_c;\hat{\mathbf{R}}'_c) = (\hat{\mathbf{\Theta}}_c\hat{\mathbf{\Theta}}'_c + \hat{\varphi}_c\hat{\varphi}_c)\cdot\mathbf{g}(\hat{\mathbf{R}}'_c)p'p_s(\Theta'_c)$, with Θ_c and Θ'_c related by the forms in (15). For the mate $\mathbf{U}_M$ we replace $\mathbf{G}$ by $\hat{\mathbf{R}}_c \times \mathbf{G}$ (or by $\hat{\mathbf{R}} \times \mathbf{G}$ for the last form) and $\mathbf{g}$ by $\hat{\mathbf{R}}'_c \times \mathbf{g}$. Although $\mathbf{G}$ differs essentially from $\mathbf{g}$ in that $\mathbf{G}\cdot\hat{\mathbf{r}}' \neq 0$, we showed by (58)[4] and (60)[4] that the operations in (28) are also equivalent for the present generalization.

The procedure of transforming $\mathbf{U}'_a$ to obtain $\mathbf{U}_a$ was used by Lee and Mittra[8] for the cylinder, and by Restrick[9] for the sphere; the present form differs from Restrick's in the isolation of $\mathbf{G} = P(\hat{\mathbf{\Theta}}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\mathbf{g}$. The corresponding results for $\mathbf{U}'$ and $\mathbf{U}$ that follow from the functional equation (27)[4] may be written in terms of the wave forms of (14) and (15) as

$$\mathbf{U}' = \int e^{i\nu'}\mathbf{G}' = \int \mathbf{\Phi}'_s(\hat{\mathbf{R}}'_c) g(\hat{\mathbf{R}}'_c),$$
$$\mathbf{U} = \int e^{i\nu_s}\mathbf{G} = \int \mathbf{\Phi}_s(\hat{\mathbf{R}};\hat{\mathbf{R}}'_c) g(\hat{\mathbf{R}}'_c) \tag{29}$$

The second follows from the first on transforming the plane wave in the complex integral, the procedure used by Censor[7] with different representations for $\mathbf{\Phi}_s$ and $\mathbf{G}$.

The present form $\mathbf{G} = p_s(\hat{\mathbf{\Theta}}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\mathbf{G}'$ makes the structure of the transformation of the scattering from Σ' to Σ explicit. As discussed after (18) and (13), the form corresponds to the invariance of $\hat{\varphi}\cdot\hat{\mathbf{G}}'$ and $\hat{\varphi}\cdot\hat{\mathbf{G}}'_M$, which follow from the invariance of $\hat{\mathbf{v}}\cdot\mathbf{U}'_M$ and $\hat{\mathbf{v}}\cdot\mathbf{U}'$, respectively (or equivalently of $\hat{\mathbf{v}}\cdot\mathbf{\Phi}'_{sM}$ and $\hat{\mathbf{v}}\cdot\mathbf{\Phi}'_s$). A particular consequence of the form of $\mathbf{G}$ is that (17) applies, and since $P = 1$ for $\hat{\mathbf{R}} = \hat{\mathbf{k}}$, we obtain $\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') = \hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}};\hat{\mathbf{k}}')$. Thus, we may rewrite (24) as

$$\mathrm{Re}\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') = \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}};\hat{\mathbf{k}}') = -k'^2\sigma'_T/4\pi,$$
$$\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') = \hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}};\hat{\mathbf{k}}'), \tag{30}$$

which enables us to interrelate the interference effects in Σ' and Σ. Similarly for the generalization of (24) as in (23),[4] we may use (17) and (18) to replace the scalar products of unit vectors in Σ' by the corresponding ones in Σ.

Dyadic Amplitudes

We now complete the development by introducing a form of $\mathbf{G}$ that also makes the transformation of the excitation explicit.

We rewrite the transformation (6) to (7) from Σ Σ' as

$$\mathbf{\Phi}' = \tilde{\mathbf{p}}'\cdot\mathbf{\Phi}, \quad \tilde{\mathbf{p}}' = \tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}}) = \gamma(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}})(\hat{\boldsymbol{\alpha}}'\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}}), \tag{31}$$

where the operator $\tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}})$ accounts for the change in magnitude and direction of the Σ polarization $\hat{\mathbf{p}} = (\hat{\boldsymbol{\alpha}}\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})\cdot\hat{\mathbf{p}}$, i.e., $\mathbf{p}' = p'\hat{\mathbf{p}}' = \tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}})\cdot\hat{\mathbf{p}}$. Similarly, for the transformation (14) to (15) from Σ' to Σ,

$$\mathbf{\Phi}_s = \tilde{\mathbf{p}}_s\cdot\mathbf{\Phi}'_s,$$
$$\tilde{\mathbf{p}}_s = \tilde{\mathbf{p}}^r(\hat{\mathbf{R}},\hat{\mathbf{R}}') = (\hat{\mathbf{\Theta}}\hat{\mathbf{\Theta}}' + \hat{\varphi}\hat{\varphi})/\gamma(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{R}}), \tag{32}$$

where $\tilde{\mathbf{p}}^r$ accounts for the change in the Σ' polarization. Thus the inverse of (31) is $\mathbf{\Phi} = \tilde{\mathbf{p}}^r(\hat{\mathbf{k}},\hat{\mathbf{k}}')\cdot\mathbf{\Phi}'$, where $\tilde{\mathbf{p}}^r(\hat{\mathbf{k}},\hat{\mathbf{k}}')$ is the reciprocal of $\tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}})$ in the plane perpendicular to $\hat{\mathbf{k}}$, i.e., $\tilde{\mathbf{p}}^r(\hat{\mathbf{k}},\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}}) = \tilde{\mathbf{I}} - \hat{\mathbf{k}}\hat{\mathbf{k}}$. The transformation of $\mathbf{G}'$ of (26) to $\mathbf{G}$ of (27), in the form (32), is

$$\mathbf{G} = \tilde{\mathbf{p}}_s\cdot\mathbf{G}' = \tilde{\mathbf{p}}^r(\hat{\mathbf{R}},\hat{\mathbf{r}}')\cdot\mathbf{G}'. \tag{33}$$

The conventional scattering amplitude $\mathbf{g}(\hat{\mathbf{r}}') = \mathbf{g}(\hat{\mathbf{r}}',\hat{\mathbf{k}}':\hat{\mathbf{p}}')$ can be expressed in terms of the dyadic amplitude[11,12,4] as

$$\mathbf{g}(\hat{\mathbf{r}}',\hat{\mathbf{k}}':\hat{\mathbf{p}}') = \tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}')\cdot\hat{\mathbf{p}}',$$
$$\tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}') = \mathbf{g}(\hat{\mathbf{r}}',\hat{\mathbf{k}}':\hat{\boldsymbol{\alpha}}')\hat{\boldsymbol{\alpha}}' + \mathbf{g}(\hat{\mathbf{r}}',\hat{\mathbf{k}}':\hat{\boldsymbol{\delta}})\hat{\boldsymbol{\delta}}, \tag{34}$$

where $\tilde{\mathbf{g}}$ is independent of $\hat{\mathbf{p}}'$, i.e.,

$$\tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}') = (\hat{\boldsymbol{\theta}}'\hat{\boldsymbol{\theta}}' + \hat{\varphi}\hat{\varphi})\cdot\tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}')\cdot(\hat{\boldsymbol{\alpha}}'\hat{\boldsymbol{\alpha}}' + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})$$
$$= \hat{\boldsymbol{\theta}}'\hat{\boldsymbol{\alpha}}' g_{\theta'\alpha'} + \hat{\boldsymbol{\theta}}'\hat{\boldsymbol{\delta}} g_{\theta'\delta} + \hat{\varphi}\hat{\boldsymbol{\alpha}}' g_{\varphi\alpha'} + \hat{\varphi}\hat{\boldsymbol{\delta}} g_{\varphi\delta}. \tag{35}$$

In terms of $\tilde{\mathbf{g}}$ and $\tilde{\mathbf{p}}$, we rewrite $\mathbf{G}'$ of (26) as

$$\mathbf{G}' = \tilde{\mathbf{g}}\cdot\hat{\mathbf{p}}'p' = \tilde{\mathbf{g}}\cdot\tilde{\mathbf{p}}'\cdot\hat{\mathbf{p}} = \tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}})\cdot\hat{\mathbf{p}} \tag{36}$$

Thus we may rewrite $\mathbf{G}$ of (27) and (33) as

$$\mathbf{G} = \tilde{\mathbf{p}}_s\cdot\mathbf{G}' = \tilde{\mathbf{p}}_s\cdot\tilde{\mathbf{g}}\cdot\tilde{\mathbf{p}}'\cdot\hat{\mathbf{p}} = \tilde{\mathbf{G}}\cdot\hat{\mathbf{p}}, \tag{37}$$

where the dyadic amplitude

$$\hat{\mathbf{G}}(\hat{\mathbf{R}},\hat{\mathbf{k}}) = \tilde{\mathbf{p}}_s\cdot\tilde{\mathbf{g}}\cdot\tilde{\mathbf{p}}' = \tilde{\mathbf{p}}^r(\hat{\mathbf{R}},\hat{\mathbf{r}}')\cdot\tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}(\hat{\mathbf{k}}',\hat{\mathbf{k}}) \tag{38}$$

is independent of $\hat{\mathbf{p}}$. The operator $\tilde{\mathbf{p}}$ corresponds to transforming the excitation from Σ to Σ', and the reciprocal $\tilde{\mathbf{p}}^r$ to transforming the scattering from Σ' to Σ; since $\tilde{\mathbf{g}}(\hat{\mathbf{r}}',\hat{\mathbf{k}}')$ is transverse to $\hat{\mathbf{r}}'$ on the left and to $\hat{\mathbf{k}}'$ on the right, $\tilde{\mathbf{p}}^r$ performs essentially as the inverse of $\tilde{\mathbf{p}}$ for the operands at hand. In view of the discussions after (13) and (18), the forms

$$\tilde{\mathbf{G}} = p_s(\hat{\mathbf{\Theta}}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\tilde{\mathbf{g}}\cdot(\hat{\boldsymbol{\alpha}}'\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})p$$
$$= p_s(\hat{\mathbf{\Theta}}\hat{\boldsymbol{\alpha}} g_{\theta'\alpha'} + \hat{\mathbf{\Theta}}\hat{\boldsymbol{\delta}} g_{\theta'\delta} + \hat{\varphi}\hat{\boldsymbol{\alpha}} g_{\varphi\alpha'} + \hat{\varphi}\hat{\boldsymbol{\delta}} g_{\varphi\delta})p' \tag{39}$$

exhibit the consequences of the invariance of $\hat{\mathbf{v}}\cdot\mathbf{\Phi}$, $\hat{\mathbf{v}}\cdot\mathbf{\Phi}_M$, $\hat{\mathbf{v}}\cdot\mathbf{U}'$, and $\hat{\mathbf{v}}\cdot\mathbf{U}'_M$.

In terms of dyadics, (30) equals $\mathrm{Re}\hat{\mathbf{p}}'\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}',\hat{\mathbf{k}}')\cdot\hat{\mathbf{p}}' = \mathrm{Re}\,\hat{\mathbf{p}}\cdot\tilde{\mathbf{G}}(\hat{\mathbf{k}},\hat{\mathbf{k}})\cdot\hat{\mathbf{p}}$. To consider reciprocity, we must show more of the dependence of $\mathbf{G}$ on the parameters than required here, or elsewhere in the text. We therefore reserve discussion for the Appendix.

Interpretation

The phase of the incident wave $\mathbf{\Phi}'$ at $\mathbf{r}' = \mathbf{r}'_0 = 0$ and $t' = t'_0$ is $\nu'(\hat{\mathbf{k}}') = \nu'_0 = -\omega' t'_0$ and this is also the phase ν' of $\mathbf{U}'_a$ at $\mathbf{r}'$ and $t' = t'_0 + r'/c$. The displacement $\mathbf{R}' = \mathbf{r}' - \mathbf{r}'_0$ and the interval $t' - t'_0 = R'/C$ are observed in Σ as

$$\mathbf{R} = \mathbf{r} - \mathbf{r}_0 = \tilde{\mathbf{L}}\cdot(\mathbf{r}' + \beta r'\hat{\mathbf{v}}) = R\hat{\mathbf{R}}, \quad R = r'p_s,$$
$$t - t_0 = R/c, \tag{40}$$

where p_s and $\hat{\mathbf{R}}$ are the same as for (27). The transform of the incidence event $\mathbf{r}'_0, t'_0$ is the retarded event $\mathbf{r}_0, t_0$ with $\mathbf{r}_0 = \hat{\mathbf{v}}\gamma(vt' - \beta r') = \hat{\mathbf{v}}(vt - \beta R) = \mathbf{v}t_0$ and $t_0 = \gamma t'_0 = t - R/c$; the displacement $\mathbf{R}$ is the retarded vector from $\mathbf{r}_0$ to the observation position $\mathbf{r}$ at the present time t, and $t - t_0$ is the time for light to travel from $\mathbf{r}_0$ to $\mathbf{r}$. The form $R^2 = |\mathbf{r} - \mathbf{v}t_0|^2 = c^2(t - t_0)^2$ corresponds to a spherical wave emitted from the retarded position $\mathbf{v}t_0$ at the retarded time t_0. The scattered phase $\nu_s(\mathbf{r}, t) = \nu'(\mathbf{r}', t')$ is the same in both systems and equals the phase $\nu'_0 = -\omega'_0 t'_0$ of the incident wave Φ' at $\mathbf{r}'_0, t'$ and of Φ at the retarded event $\mathbf{r}_0, t_0$, i.e., $\nu_0 = \mathbf{k}\cdot\mathbf{r}_0 - \omega t_0 = -\omega(1 - \beta\cos\alpha)t_0 = -\omega' t_0/\gamma$; thus

$$\nu_s = P(k\hat{\mathbf{R}}\cdot\mathbf{r} - \omega t) = k'r' - \omega't' = -\omega't'_0$$
$$= -\omega(1 - \beta\cos\alpha)t_0 = (1 - \beta\cos\alpha)(kR - \omega t), \tag{41}$$

where $-\omega(1 - \beta\cos\alpha)t = \mathbf{k}\cdot\mathbf{v}t - \omega t = -\omega't/\gamma$ is the phase of Φ at the present position $\mathbf{v}t$.

By (2), we may rewrite $\mathbf{U}_a(\mathbf{r}', t')$ and $\mathbf{U}(\mathbf{r}', t')$ in terms of $\mathbf{r}, t$, and by (40), in terms of $\mathbf{R}, t$ [with $\hat{\mathbf{R}}, \hat{\mathbf{\Theta}}, \hat{\varphi}$ as before for (27) and (28)]. We may also work with present (simultaneous) coordinates originating from $\mathbf{v}t$ (the position of $r' = 0$ at t):

$$\mathbf{r}_s = \mathbf{r} - \mathbf{v}t = \mathbf{R} - R\beta\hat{\mathbf{v}}, \quad \hat{\mathbf{r}}_s, \hat{\theta}_s, \hat{\varphi}. \tag{42}$$

Since, from (2),

$$\mathbf{r}' = \tilde{\mathbf{L}}\cdot\mathbf{r}_s = \tilde{\mathbf{L}}\cdot(\mathbf{R} - R\beta\hat{\mathbf{v}}), \tag{43}$$

it follows that

$$r' = r_s/q = R/p_s,$$
$$q = 1/\gamma(1 - \beta^2\sin^2\theta_s)^{1/2} = (1 - \beta^2\cos^2\theta')^{1/2},$$
$$\cos\theta' = \gamma q\cos\theta_s = \gamma p_s(\cos\Theta - \beta),$$
$$\sin\theta' = q\sin\theta_s = p_s\sin\Theta. \tag{44}$$

We also use mixed forms

$$\cos(\theta_s - \Theta) = (1 - \beta^2\sin^2\theta_s)^{1/2} = 1/\gamma q = \cos\zeta$$
$$\sin(\theta_s - \Theta) = \beta\sin\theta_s = \sin\zeta \tag{45}$$

such that $\hat{\mathbf{r}}_s = \hat{\mathbf{R}}\cos\zeta + \hat{\mathbf{\Theta}}\sin\zeta$, etc. From (44) and (45),

$$r_s/R = q/p_s = \sin\theta_s/\sin\Theta = (1 - 2\beta\cos\Theta + \beta^2)^{1/2}$$
$$= \cos\zeta - \beta\cos\theta_s \tag{46}$$

as well as $R/r_s = \gamma^2(\cos\zeta + \beta\cos\theta_s) = (1 + \beta\cos\theta')^{1/2}/(1 - \beta\cos\theta')^{1/2}$, etc.

From (44) we see that $r' \sim \infty$ corresponds to $R \sim r_s \sim \infty$, and that (27) may be rewritten as

$$\mathbf{U}_a = (e^{i\nu'}/ik'R)p_s\mathbf{G} = (e^{i\nu_s}/ikR)p_s^2(\hat{\mathbf{\Theta}}g_{\theta'} + \hat{\varphi}g_\varphi),$$
$$\nu' = k'r' - \omega't' = \nu_s. \tag{47}$$

We may also rewrite $\mathbf{G}$ of (27) as

$$\mathbf{G} = -p_s\hat{\mathbf{R}}\times\tilde{\mathbf{L}}\cdot(\hat{\mathbf{r}}'\times\mathbf{G}') = -qp_s\hat{\mathbf{R}}\times(\hat{\mathbf{r}}_s\times\tilde{\mathbf{\Gamma}}\cdot\mathbf{G}')$$
$$= -p_s^2\mathbf{R}\times(\mathbf{r}_s\times\tilde{\mathbf{\Gamma}}\cdot\mathbf{G}')/R^2. \tag{48}$$

In particular, from (48) and the first form of (47) we obtain

$$\mathbf{U}_a = (e^{i\nu'}/ik'R)[-p_s^2q\hat{\mathbf{R}}\times(\hat{\mathbf{r}}_s\times\tilde{\mathbf{\Gamma}}\cdot\mathbf{G}')]$$
$$= -\frac{e^{i\nu'}\mathbf{R}\times(\mathbf{r}_s\times\tilde{\mathbf{\Gamma}}\cdot\mathbf{G}')}{ik'\gamma^3R^3(1 - \beta\cos\Theta)^3}. \tag{49}$$

Comparison of $\mathbf{U}_a$ with the $\mathbf{E}$-radiation field[2] of a moving dipole of charge e and acceleration $\dot{\mathbf{v}}$ shows that for this case $e^{i\nu'}\mathbf{G}'/ik'$ corresponds to $-(e/4\pi c^2\epsilon_0)\dot{\mathbf{v}}'$ with $\dot{\mathbf{v}}' = \gamma^3\tilde{\mathbf{\Gamma}}^{-1}\cdot\dot{\mathbf{v}} = \gamma^2\tilde{\mathbf{L}}\cdot\dot{\mathbf{v}}$ as the acceleration in Σ'.

From (41) in retarded or present coordinates, $\mathbf{U}_a$ is a periodic function of t with period $T_s = 2\pi\gamma/\omega'$, an interval that by (1) transforms to Σ' as the period $T' = 2\pi/\omega'$ of the t'-periodic function $\mathbf{U}'$, i.e.,

$$T' = 2\pi/\omega', \quad T_s = 2\pi\gamma/\omega' = 2\pi/\omega(1 - \beta\cos\alpha), \tag{50}$$

with T_s as the dilation of T'. From the final form of (28), i.e., (47) with G replaced by $\tilde{\mathbf{\mathfrak{D}}}\cdot\mathbf{G}$, we see that this result for $\mathbf{U}_a$ also holds for $\mathbf{U}$. Thus when in Σ' we consider quadratic functions (energy and momentum) of $\mathbf{U}'$ that have been averaged over one cycle T' in t', the analogs in Σ in retarded and present coordinates may be interpreted as t averages over T_s. We illustrate this in the following, but reserve discussion of the quadratic functions and of conservation of energy and momentum for a sequel.

Thus, we interpret $\mathbf{S}_s = \frac{1}{2}\mathrm{Re}\,\mathbf{E}_s\times\mathbf{H}_s^*$ in $\mathbf{R}, t$ as the scattered Poynting vector averaged over T_s. With $\mathbf{U} = \mathbf{E}_s$, and $S_0 = \epsilon_0 c/2$, we have

$$\mathbf{S}_s = S_0\mathrm{Re}\,\mathbf{U}\times\mathbf{U}_M^*$$
$$\sim S_0|\mathbf{G}|^2\hat{\mathbf{R}}/(k'r')^2 = (\mathcal{S}p_s^4|\mathbf{g}|^2/R^2)\hat{\mathbf{R}} = S_{sa}\hat{\mathbf{R}},$$
$$\mathcal{S} = S_0/k^2 = S_0p'^2/k'^2. \tag{51}$$

In general, the interval T_s is small enough for the implicit t variation of (51) in $\mathbf{r}, t$ to be neglected for practical purposes. Plots of S_{sa} for a small perfectly conducting sphere are given by Restrick[9]; he interprets $\mathbf{S}_{sa}$ as the limit of the t average over an infinite interval. Since $d\Omega(\hat{\mathbf{R}}) = d\Omega(\hat{\mathbf{r}}')(\partial_{\theta'}\cos\Theta)/\partial_\theta\cos\theta' = d\Omega(\hat{\mathbf{r}}')/p_s^2$, the scattered flux $\Delta\mathcal{P}_s$ through $\Delta\mathbf{A}(\hat{\mathbf{R}})$ with $\hat{\mathbf{R}}dA(\hat{\mathbf{R}}) = \hat{\mathbf{R}}R^2d\Omega(\hat{\mathbf{R}}) = \hat{\mathbf{R}}r'^2d\Omega(\hat{\mathbf{r}}')$ equals

$$\Delta\mathcal{P}_s = \mathcal{S}\int_\Delta p_s^2|\mathbf{g}(\hat{\mathbf{r}}')|^2d\Omega(\hat{\mathbf{r}}'), \quad p_s = \gamma(1 + \beta\cos\theta'),$$
$$\Delta = \Delta\Omega(\hat{\mathbf{R}}). \tag{52}$$

From (51) or (52), $d\mathcal{P}_s/d\Omega(\hat{\mathbf{R}}) = \mathcal{S}p_s^4|\mathbf{g}|^2$.

The corresponding energy density is

$$W_s = \tfrac{1}{4}\epsilon_0(|\mathbf{U}|^2 + |\mathbf{U}_M|^2) = \tfrac{1}{2}\epsilon_0|\mathbf{U}|^2 \sim S_{sa}/c = W_{sa}, \tag{53}$$

and from (51) and (53) we construct

$$\mathbf{S}_s - \mathbf{v}W_s \sim \mathbf{S}_{sa} - \mathbf{v}W_{sa} = S_{sa}(\hat{\mathbf{R}} - \beta\hat{\mathbf{v}}) = S_{sa}(q/p_s)\hat{\mathbf{r}}_s = \frac{\mathcal{S}p_s^4|\mathbf{g}|^2}{R^2}(\hat{\mathbf{R}} - \beta\hat{\mathbf{v}}) = \frac{\mathcal{S}p_s q^3|\mathbf{g}|^2}{r_s^2}\hat{\mathbf{r}}_s. \quad (54)$$

Since $d\Omega(\hat{\mathbf{r}}_s) = d\Omega(\hat{\mathbf{r}}')(\partial_\theta, \cos\theta_s)/\partial_\theta, \cos\theta' = d\Omega(\hat{\mathbf{r}}')/\gamma q^3$, the flux of (54) (say $\Delta\mathcal{P}_R$) through $\Delta\mathbf{A}_s$ with $\hat{\mathbf{r}}_s dA_s = \hat{\mathbf{r}}_s r_s^2 d\Omega(\hat{\mathbf{r}}_s) = \hat{\mathbf{r}}_s p'^2 d\Omega(\hat{\mathbf{r}}')/\gamma q$ is

$$\Delta\mathcal{P}_R = \mathcal{S}\int_{\Delta_s}(1 + \beta\cos\theta')|\mathbf{g}(\hat{\mathbf{r}}')|^2 d\Omega(\hat{\mathbf{r}}), \quad \Delta_s = \Delta\Omega(\hat{\mathbf{r}}_s); \quad (55)$$

for the corresponding flux through $\Delta\mathbf{A}(\hat{\mathbf{R}})$, we replace Δ_s by Δ. We regard (55) as the fundamental reradiated flux measure in Σ. It yields $d\mathcal{P}_R/d\Omega(\hat{\mathbf{R}}) = \mathcal{S}p_s^3|\mathbf{g}|^2/\gamma$ and $d\mathcal{P}_R/d\Omega(\hat{\mathbf{r}}_s) = \mathcal{S}p_s q^3|\mathbf{g}|^2$.

Several special values of $\mathbf{U}_a$ are of particular interest; we list key vectors and P. Corresponding to the forward-scattering direction in Σ',

$$\begin{aligned} \hat{\mathbf{r}}' &= \hat{\mathbf{k}}' = \hat{\mathbf{v}}\cos\alpha' + \hat{\mu}\sin\alpha', \\ \hat{\mathbf{R}} &= \hat{\mathbf{k}} = \hat{\mathbf{v}}\cos\alpha + \hat{\mu}\sin\alpha, \\ \hat{\mathbf{r}}_s &= \hat{\mathbf{r}}_f = \hat{\mathbf{v}}\cos\theta_f + \hat{\mu}\sin\theta_f = (\hat{\mathbf{k}} - \beta\hat{\mathbf{v}})/\mathcal{C}, \\ \cos\theta_f &= (\cos\alpha - \beta)/\mathcal{C}, \sin\theta_f = \sin\alpha/\mathcal{C}, \\ \mathcal{C} &= (1 - 2\beta\cos\alpha + \beta^2)^{1/2} P = 1. \end{aligned} \quad (56a)$$

For back scattering in Σ',

$$\begin{aligned} \hat{\mathbf{r}}' &= -\hat{\mathbf{k}}', \quad \hat{\mathbf{R}} = \hat{\mathbf{k}}_b = -\hat{\mathbf{z}}\cos\alpha_b - \hat{\mu}\sin\alpha_b, \\ \hat{\mathbf{r}}_s &= \hat{\mathbf{r}}_b = -\hat{\mathbf{r}}_f, \\ \cos\alpha_b &= (\cos\alpha - \beta_2)/(1 - \beta_2\cos\alpha), \\ \sin\alpha_b &= \sin\alpha/[\gamma_2(1 - \beta_2\cos\alpha)], \\ \beta_2 &= 2\beta/(1 + \beta^2), \\ \gamma_2 &= (1 - \beta_2^2)^{-1/2} = (1 + \beta^2)/(1 - \beta^2) \\ P &= P_b = \gamma^2\mathcal{C}^2 = (1 - 2\beta\cos\alpha + \beta^2)/(1 - \beta^2) \\ &= \gamma_2(1 - \beta_2\cos\alpha). \end{aligned} \quad (56b)$$

For back scattering in retarded coordinates

$$\begin{aligned} \hat{\mathbf{R}} &= -\hat{\mathbf{k}}, \quad \hat{\mathbf{r}}' = \hat{\mathbf{k}}_b' = -\hat{\mathbf{z}}\cos\alpha_b' - \hat{\mu}\sin\alpha_b', \\ \hat{\mathbf{r}}_s &= -(\hat{\mathbf{k}} + \beta\hat{\mathbf{v}})/(1 + 2\beta\cos\alpha + \beta^2)^{1/2} \\ \cos\alpha_b' &= (\cos\alpha + \beta)/(1 + \beta\cos\alpha) \\ &= (\cos\alpha' + \beta_2)/(1 + \beta_2\cos\alpha'), \\ \sin\alpha_b' &= \sin\alpha'/[\gamma_2(1 + \beta_2\cos\alpha')], \\ P &= (1 - \beta\cos\alpha)/(1 + \beta\cos\alpha) \\ &= [\gamma_2(1 + \beta_2\cos\alpha')]^{-1}, \end{aligned} \quad (56c)$$

where β_2 corresponds to the relativistic sum of two identical velocities. For geometrical reflection from $z' = 0$,

$$\begin{aligned} \hat{\mathbf{r}}' &= \hat{\mathbf{k}}_r' = -\hat{\mathbf{z}}\cos\alpha' + \hat{\mu}\sin\alpha', \\ \hat{\mathbf{R}} &= \hat{\mathbf{k}}_r = -\hat{\mathbf{z}}\cos\alpha_b + \hat{\mu}\sin\alpha_b, \\ \hat{\mathbf{r}}_s &= \hat{\mathbf{r}}_r = -\hat{\mathbf{z}}\cos\theta_f + \mu\sin\theta_f, \quad P_r = P_b. \end{aligned} \quad (56d)$$

For observation in the direction of motion,

$$\begin{aligned} \hat{\mathbf{r}}_s &= \hat{\mathbf{R}} = \hat{\mathbf{r}}' = \hat{\mathbf{v}}, \quad \theta_s = \Theta = \theta' = 0, \\ P &= P(0) = (1 - \beta\cos\alpha)/(1 + \beta). \end{aligned} \quad (56e)$$

For observation back from the motion,

$$\begin{aligned} \hat{\mathbf{r}}_s &= \hat{\mathbf{R}} = \hat{\mathbf{r}}' = -\hat{\mathbf{v}}', \quad \theta_s = \Theta = \theta' = \pi, \\ P &= P(\pi) = (1 - \beta\cos\alpha)/(1 - \beta). \end{aligned} \quad (56f)$$

For observation perpendicular to the motion, $\theta_s = \theta' = \pi/2$,

$$\begin{aligned} \hat{\mathbf{r}}_s &= \hat{\mathbf{r}}' = \hat{\rho}, \quad \hat{\mathbf{R}} = \hat{\mathbf{v}}\beta + \hat{\rho}(1 - \beta^2)^{1/2}, \\ P &= P(\pi/2) = (1 - \beta\cos\alpha)/(1 - \beta^2). \end{aligned} \quad (56g)$$

For $\Theta = \pi/2$,

$$\begin{aligned} \hat{\mathbf{R}} &= \hat{\rho}, \quad \hat{\mathbf{r}}' = -\hat{\mathbf{v}}\beta + \hat{\rho}(1 - \beta^2)^{1/2}, \\ \hat{\mathbf{r}}_s &= (-\hat{\mathbf{v}}\beta + \hat{\rho})/(1 + \beta^2)^{1/2}, \quad P = 1 - \beta\cos\alpha. \end{aligned} \quad (56h)$$

Finally, for forward and back scattering in present coordinates,

$$\hat{\mathbf{r}}_s = \pm\hat{\mathbf{k}}, \quad \hat{\mathbf{r}}' = \pm\hat{\mathbf{r}}_f' = \pm\frac{\hat{\mathbf{v}}\cos\alpha + \hat{\rho}(\sin\alpha)/\gamma}{(1 - \beta^2\sin^2\alpha)^{1/2}},$$

$$P = \frac{(1 - \beta\cos\alpha)}{1 - \beta^2}\left[1 \pm \frac{\beta\cos\alpha}{(1 - \beta^2\sin^2\alpha)^{1/2}}\right]. \quad (56i)$$

The Doppler effects are determined primarily by P in the form $P\nu(\hat{\mathbf{R}}) = \nu_s$ of the phase given in (27); see Lee and Mittra[8] for discussion, and also for graphs of $P(0)$ and $P(\pi)$. In terms of θ_s,

$$\begin{aligned} P &= p'(\alpha)p_s(\theta') = p'(\alpha)\gamma\left[1 + \frac{\beta\cos\theta_s}{\cos(\theta_s - \Theta)}\right] \\ &= \frac{1 - \beta\cos\alpha}{1 - \beta^2}\left[1 + \frac{\beta\cos\theta_s}{(1 - \beta^2\sin^2\theta_s)^{1/2}}\right]; \end{aligned} \quad (57)$$

the approximation $P \approx \gamma^2(1 - \beta\cos\alpha)(1 + \beta\cos\theta_s)$, correct at least to order β^2, is rigorous for $\theta_s = 0, \pi/2$, and π.

2. ALTERNATIVE REPRESENTATIONS

Surface and Volume Integrals

As discussed before,[4] we may write $\mathbf{u}$ of (22) in the form (12)[4]

$$\begin{aligned} \mathbf{u}(\mathbf{r}') &= \{\tilde{\mathbf{h}}(k'|\mathbf{r}' - \mathbf{r}''|), \mathbf{u}(\mathbf{r}'')\} = \{\tilde{\mathbf{h}}, \psi\} \\ &= (-k'^2/4\pi)\int[(\tilde{\mathbf{h}} \times \hat{\mathbf{n}}')\cdot\mathbf{u}_M + \tilde{\mathbf{h}}_M\cdot(\mathbf{u} \times \hat{\mathbf{n}}')]dA', \end{aligned} \quad (58)$$

$$\begin{aligned} \tilde{\mathbf{h}} &= \nabla' \times \nabla' \times \tilde{\mathbf{I}}\,h_0/k'^2 = (\mathbf{I} + \nabla'\nabla'/k'^2)h_0, \\ \tilde{\mathbf{h}}_M &= \nabla' \times \tilde{\mathbf{h}}/ik' = \nabla' \times \tilde{\mathbf{I}}h_0/ik', \\ h_0 &= h_0^{(1)}(k'|\mathbf{r}' - \mathbf{r}''|), \end{aligned} \quad (59)$$

where $A'(\mathbf{r}'')$ is any surface enclosing the scatterer's surface $\mathcal{a}'$ and excluding $\mathbf{r}'$, and $\hat{\mathbf{n}}'$ is the outward normal. [Equation (58) differs from (12)[4] in that it contains $\mathbf{u}_M$ instead of $\nabla'' \times \mathbf{u}(\mathbf{r}'')/ik'$ and $\tilde{\mathbf{h}}_M$

instead of $-\nabla''\times\tilde{\mathbf{h}}/ik'$.] If $A'=\mathcal{A}'$, the usual boundary or transition conditions lead to alternative surface ($\mathcal{A}'$) or volume ($\mathcal{V}'$) integral representations, and provide integral equations for $\boldsymbol{\psi}=\boldsymbol{\phi}+\mathbf{u}$. In particular, essentially as in (14),[4] we may represent $\mathbf{u}$ for constant parameters by

$$\mathbf{u}(\mathbf{r}')=\left(\frac{-k'^3}{4\pi i}\right)\int[(\eta'^2B-1)\tilde{\mathbf{h}}\cdot\boldsymbol{\psi}-(1-B)\tilde{\mathbf{h}}_M\cdot\boldsymbol{\psi}_M]d\mathcal{V}',$$
$$\eta'=\frac{K'}{k'}=\left(\frac{\mu'\epsilon'}{\mu_0\epsilon_0}\right)^{1/2},\quad B=\begin{Bmatrix}B_e\\B_m\end{Bmatrix}=\begin{Bmatrix}\mu_0/\mu'\\\epsilon_0/\epsilon'\end{Bmatrix},\qquad(60)$$

where the ordering for B corresponds to that in (4). For dispersive scattering material, the rest system parameters ϵ', μ' and index of refraction η' depend on ω' and therefore on v and α.

For $r'\sim\infty$, we have $h_0(k|\mathbf{r}'-\mathbf{r}''|)\sim h(k'r')\times e^{-ik'\hat{\mathbf{r}}'\cdot\mathbf{r}''}$, and (59) reduces to

$$\tilde{\mathbf{h}}\sim\tilde{\mathbf{h}}_a=(\hat{\theta}'\hat{\theta}'+\hat{\varphi}\hat{\varphi})e^{-ik'\hat{\mathbf{r}}'\cdot\mathbf{r}''}h=\tilde{\boldsymbol{\phi}}(-\hat{\mathbf{r}}';\mathbf{r}'')h(k'r'),$$
$$\tilde{\mathbf{h}}_M\sim\hat{\mathbf{r}}'\times\tilde{\mathbf{h}}_a=\hat{\mathbf{r}}'\times\tilde{\boldsymbol{\phi}}h=\tilde{\boldsymbol{\phi}}_M h,\qquad(61)$$

where $\tilde{\boldsymbol{\phi}}$ is the form in (19). By using (61) in (58) or (60), it follows from $\mathbf{u}\sim h\mathbf{g}$ that

$$\mathbf{g}(\hat{\mathbf{r}}')=\{\tilde{\boldsymbol{\phi}}(-\hat{\mathbf{r}}';\hat{\mathbf{r}}''),\boldsymbol{\psi}(\mathbf{r}'')\},\qquad(62)$$

where $\{\ \}$ represents integration over any surface inclosing the scatterer, or over $\mathcal{V}$. From (26),[4]

$$\tilde{\mathbf{h}}(k'|\mathbf{r}'-\mathbf{r}''|)=\int(\hat{\boldsymbol{\Theta}}_c'\hat{\boldsymbol{\Theta}}_c'+\hat{\varphi}_c\hat{\varphi}_c)e^{ik'(\mathbf{r}'-\mathbf{r}'')\cdot\hat{\mathbf{R}}_c'}=\int\tilde{\boldsymbol{\phi}}(\hat{\mathbf{R}}_c';\mathbf{r}')\cdot\tilde{\boldsymbol{\phi}}(-\hat{\mathbf{R}}_c';\mathbf{r}''),\quad\tilde{\mathbf{h}}_M=\int\tilde{\boldsymbol{\phi}}\cdot\tilde{\boldsymbol{\phi}}_M.\qquad(63)$$

Substituting (63) into (58) gives the integral representation (25) with $\mathbf{g}$ as in (62).

We may rewrite $\mathbf{U}'$ of (22) as

$$\mathbf{U}'=\{\tilde{\mathcal{H}}',\boldsymbol{\psi}\},\quad\tilde{\mathcal{H}}'=\tilde{\mathbf{h}}(k'|\mathbf{r}'-\mathbf{r}''|)p'e^{-i\omega't'},$$
$$\tilde{\mathcal{H}}_M'=\tilde{\mathbf{h}}_M p'e^{-i\omega't'},\qquad(64)$$

and, by (61),

$$\mathbf{U}'\sim\mathbf{U}_a'=he^{-i\omega't'}\mathbf{G}',\quad\mathbf{G}'=p'\{\tilde{\boldsymbol{\phi}},\boldsymbol{\psi}\}=p'\mathbf{g}.\qquad(65)$$

By (5), the transform of $\mathbf{U}'$ in Σ is

$$\mathbf{U}=\{\tilde{\mathcal{H}},\boldsymbol{\psi}\},\quad\tilde{\mathcal{H}}=\cdot\tilde{\Gamma}(\tilde{\mathbf{h}}-\gamma\beta\hat{\mathbf{v}}\times\tilde{\mathbf{h}}_M)p'e^{-i\omega't'},$$
$$\tilde{\mathcal{H}}_M=(\tilde{\Gamma}\cdot\tilde{\mathbf{h}}_M+\gamma\beta\hat{\mathbf{v}}\times\tilde{\mathbf{h}})p'e^{-i\omega't'}\qquad(66)$$

For $r'\sim\infty$, from (61) and the forms in (19) and (20),

$$\tilde{\mathcal{H}}\sim\tilde{\mathcal{H}}_a=P(\hat{\boldsymbol{\Theta}}\hat{\theta}+\hat{\varphi}\hat{\varphi})\cdot\tilde{h}_a e^{-i\omega't'}=\tilde{\boldsymbol{\Phi}}(\hat{\mathbf{R}},\hat{\mathbf{r}}';\mathbf{r}')\cdot\tilde{\boldsymbol{\phi}}(-\hat{\mathbf{r}}';\mathbf{r}'')/ik'r',$$
$$\tilde{\mathcal{H}}_M\sim\hat{\mathbf{R}}\times\tilde{\mathcal{H}}_a=\frac{\tilde{\boldsymbol{\Phi}}_M\cdot\tilde{\boldsymbol{\phi}}}{ik'r'}=\frac{\tilde{\boldsymbol{\Phi}}\cdot\tilde{\boldsymbol{\phi}}_M}{ik'r'}.\qquad(67)$$

Substituting (67) into (66), we obtain

$$\mathbf{U}\sim\mathbf{U}_a=he^{-i\omega't'}\mathbf{G},$$
$$\mathbf{G}=P(\hat{\boldsymbol{\Theta}}\hat{\theta}'+\hat{\varphi}\hat{\varphi})\cdot\{\tilde{\boldsymbol{\phi}},\boldsymbol{\psi}\}=P(\hat{\boldsymbol{\Theta}}\hat{\theta}'+\hat{\varphi}\hat{\varphi})\cdot\mathbf{g}\qquad(68)$$

as given originally in (27). Using (63) in $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}_M$, we have

$$\tilde{\mathcal{H}}=\int\tilde{\boldsymbol{\Phi}}(\hat{\mathbf{R}}_c,\hat{\mathbf{R}}_c';\mathbf{r}')\cdot\tilde{\boldsymbol{\phi}}(-\hat{\mathbf{R}}_c';\mathbf{r}'')=\int P(\hat{\boldsymbol{\Theta}}_c\hat{\boldsymbol{\Theta}}_c'+\hat{\varphi}_c\hat{\varphi}_c)e^{ik'(\mathbf{r}'-\mathbf{r}'')\cdot\hat{\mathbf{R}}_c'-i\omega't'},$$
$$\tilde{\mathcal{H}}_M=\int\tilde{\boldsymbol{\Phi}}\cdot\tilde{\boldsymbol{\phi}}_M,\qquad(69)$$

which when substituted into (66) gives the integral representation of (28) in terms of (62). Alternatively, we could start from (28) in terms of $\mathbf{G}$ as given in (68), then identify $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}_M$ of (69) in the result, and then relate $\tilde{\mathcal{H}}$ to $\tilde{\mathbf{h}}$, etc.

In terms of spherical waves,

$$\tilde{\mathbf{h}}=(\hat{\theta}'\hat{\theta}'+\hat{\varphi}\hat{\varphi})\mathcal{H}_1+\hat{\mathbf{r}}'\hat{\mathbf{r}}'H_1,$$
$$\tilde{\mathbf{h}}_M=(-\hat{\theta}'\hat{\varphi}+\hat{\varphi}\hat{\theta}')ih_1,$$
$$h_1=h_1(x)=h_1^{(1)}(k|\mathbf{r}'-\mathbf{r}''|),\quad H_1=2h_1/x,$$
$$\mathcal{H}_1=\partial_x(xh_1)/x,\qquad(70)$$

where $h_1=h(-i+1/x)$ and $\mathcal{H}_1=ih_1-h/x^2$. If $r'\sim\infty$, we have $\mathcal{H}_1\sim ih_1\sim h(k'|\mathbf{r}'-\mathbf{r}''|)\sim h(k'r')e^{-ik'\hat{\mathbf{r}}'\cdot\mathbf{r}''}$ and $H_1\sim O(r'^{-2})$, then (70) simplifies to (61). The corresponding $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}_M$ of (66) may be represented in various ways in different coordinate systems. It is useful to keep the right-hand vectors in $\hat{\mathbf{r}}',\hat{\theta}',\hat{\varphi}$ and to express the left-hand vectors in terms of $\hat{\mathbf{r}}_s,\hat{\boldsymbol{\Theta}}$, and $\hat{\varphi}$.

Thus

$$\tilde{\mathcal{H}}/p'e^{-i\omega't'}=(\hat{\boldsymbol{\Theta}}\hat{\theta}'+\hat{\varphi}\hat{\varphi})\mathcal{N}_1^1+\hat{\mathbf{r}}_s(\hat{\theta}'\mathcal{N}_1^2+\hat{\mathbf{r}}'\mathcal{N}_1^3),$$
$$\mathcal{N}_1^1=\gamma(\mathcal{H}_1+ih_1\beta\cos\theta'),$$
$$\mathcal{N}_1^2=[(ih_1-\mathcal{H}_1)\gamma\beta\sin\Theta]/\cos\zeta,$$
$$\mathcal{N}_1^3=H_1/\cos\zeta,$$
$$\tilde{\mathcal{H}}_M/p'e^{-i\omega't'}=(-\hat{\boldsymbol{\Theta}}\hat{\varphi}+\hat{\varphi}\hat{\theta}')\mathcal{M}_1^1+\hat{\mathbf{r}}_s\hat{\varphi}\mathcal{M}_1^2+\hat{\varphi}\hat{\mathbf{r}}'\mathcal{M}_1^3,$$
$$\mathcal{M}_1^1=\gamma(ih_1+\mathcal{H}_1\beta\cos\theta'),$$
$$\mathcal{M}_1^2=\mathcal{N}_1^2,$$
$$\mathcal{M}_1^3=H_1\gamma\beta\sin\theta'=H_1\gamma\beta p_s\sin\Theta,\qquad(71)$$

where the basis reciprocal to $\hat{\mathbf{r}}_s,\hat{\boldsymbol{\Theta}},\hat{\varphi}$ is $\hat{\mathbf{R}}/\cos\zeta$, $\hat{\boldsymbol{\theta}}_s/\cos\zeta,\hat{\varphi}$. Since $\hat{\mathbf{r}}_s=\hat{\mathbf{R}}\cos\zeta+\hat{\boldsymbol{\Theta}}\sin\zeta$, we could regroup into forms $\hat{\mathbf{R}}\,\mathbf{A}_1+\hat{\boldsymbol{\Theta}}\mathbf{A}_2+\hat{\varphi}\,\mathbf{A}_3$, but the present forms are simpler and more similar to (70). If $r'\sim\infty$, we have $\mathcal{N}_1^1\sim\mathcal{M}_1^1\sim p_sh$ and the remaining terms are $O(r'^{-2})$; then (71) simplifies to (67). We always have $\mathcal{N}_1^2=\mathcal{M}_1^2\propto h/x^2=O(x^{-3})$.

Special Function Series

Similarly the procedures discussed before[4] for generating the series representation of **u** can be generalized to **u**. The Hansen functions satisfy[11,4]

$$\begin{Bmatrix}\mathbf{M}\\\mathbf{N}\end{Bmatrix} = \frac{\nabla'}{k'}\times\begin{Bmatrix}\mathbf{N}\\\mathbf{M}\end{Bmatrix} = i^{-n}\int e^{-ik'\mathbf{r}'\cdot\hat{\mathbf{R}}'_c}\begin{Bmatrix}\mathbf{C}(\hat{\mathbf{R}}'_c)\\ i\mathbf{B}(\hat{\mathbf{R}}'_c)\end{Bmatrix}$$

$$\sim hi^{-n}\begin{Bmatrix}\mathbf{C}(\hat{\mathbf{r}}')\\ i\mathbf{B}(\hat{\mathbf{r}}')\end{Bmatrix}, \qquad (72)$$

$$\mathbf{B} = \hat{\mathbf{r}}'\times\mathbf{C}, \quad \mathbf{C} = -\hat{\mathbf{r}}'\times\mathbf{B}, \quad \mathbf{M} = i\mathbf{N}_M, \ \mathbf{N} = i\mathbf{M}_M,$$

where $\mathbf{M} = \mathbf{M}_{nm}(k',\mathbf{r}')$, $\mathbf{C} = \mathbf{C}_n^m(\hat{\mathbf{r}}')$, etc., with subscripts usually suppressed. In terms of

$$h_n = h_n^{(1)}(x), \quad H_n = n(n+1)h_n/x, \quad \mathcal{H}_n = \partial_x(xh_n)/x, \quad x = k'r', \qquad (73)$$

and the spherical harmonics $Y_n^m(\theta',\varphi)$ normalized as before[4],

$$\mathbf{M}_{nm} = h_n\mathbf{C}_n^m = h_n(\hat{\boldsymbol{\theta}}'\partial - \hat{\boldsymbol{\varphi}}\partial_{\theta'})Y_n^m, \quad \partial = (\sin\theta')^{-1}\partial_\varphi,$$

$$\mathbf{N}_{nm} = \mathcal{H}_n\mathbf{B}_n^m + H_n\mathbf{P}_n^m = \mathcal{H}_n(\hat{\boldsymbol{\theta}}'\partial_{\theta'} + \hat{\boldsymbol{\varphi}}\partial)Y_n^m + H_n\hat{\mathbf{r}}'Y_n^m. \qquad (74)$$

If $r'\sim\infty$, then $h_n\sim i^{-n}h$, $\mathcal{H}_n\sim i^{-n+1}h$ and $H_n\sim O(x^{-2})$. The analogs with $h_n^{(1)}$ replaced by j_n are written $\mathbf{M}^1$, $\mathbf{N}^1$. The Green's function (59) may be written [11,4]

$$\tilde{\mathbf{h}} = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}[\mathbf{M}_{nm}(\mathbf{r}')\mathbf{M}^1_{n,-m}(\mathbf{r}'') + \mathbf{N}\mathbf{N}^1](-1)^m d_n,$$

$$d_n = (2n+1)/n(n+1), \qquad (75)$$

and $\tilde{\mathbf{h}}_M$ has $\mathbf{M}(\mathbf{r}')$ and $\mathbf{N}(\mathbf{r}')$ replaced by $-i\mathbf{N}$ and $-i\mathbf{M}$ (corresponding to $\mathbf{M}_M$ and $\mathbf{N}_M$). By substituting into **u** of (58) we obtain (36)[4]

$$\mathbf{u} = \sum(\mathbf{M}c - i\mathbf{N}b)i^n = \mathbf{u}(c,b), \quad \mathbf{u}_M = \mathbf{u}(b,-c) = \mathbf{w} \qquad (76)$$

where $c = c_{nm} = i^{-n}(-1)^m d_n\{\mathbf{M}^1_{n,-m},\boldsymbol{\Psi}\}$, and $b = b_{nm}$ has $\mathbf{M}^1$ replaced by $\mathbf{N}^1$. Similarly, as in (37)[4],

$$\mathbf{g} = \sum(\mathbf{C}c + \mathbf{B}b)$$
$$= \sum[\hat{\boldsymbol{\theta}}'(c\partial + b\partial_{\theta'}) + \hat{\boldsymbol{\varphi}}(-c\partial_{\theta'} + b\partial)]Y_n^m \qquad (77)$$
$$= \hat{\boldsymbol{\theta}}'g_{\theta'} + \hat{\boldsymbol{\varphi}}g_\varphi.$$

The corresponding form of $\tilde{\mathcal{H}}$ is

$$\tilde{\mathcal{H}} = \sum[\mathfrak{M}\mathbf{M}^1 + \mathfrak{N}\mathbf{N}^1](-1)^m d_n,$$

$$\mathfrak{M} = (\tilde{\Gamma}\cdot\mathbf{M} + i\gamma\beta\hat{\mathbf{v}}\times\mathbf{N})p'e^{-i\omega't'} = \mathfrak{M}(\mathbf{M},\mathbf{N}),$$

$$\mathfrak{N} = \mathfrak{M}(\mathbf{N},\mathbf{M}) \qquad (78)$$

and $\tilde{\mathcal{H}}_M$ has $\mathfrak{M}$ and $\mathfrak{N}$ replaced by $-i\mathfrak{N}$ and $-i\mathfrak{M}$. Substituting into (66), we obtain

$$\mathbf{U} = \sum(\mathfrak{M}c - i\mathfrak{N}b)i^n = \mathbf{U}(c,b), \quad \mathbf{U}_M = \mathbf{U}(b,-c), \qquad (79)$$

which also follows directly from (5) on transforming $\mathbf{U}' = p'e^{-i\omega't'}\mathbf{u}$ with **u** as in (76). The corresponding scattering amplitude is

$$\mathbf{G} = \sum(\mathfrak{C}c + \mathfrak{B}b) = P(\hat{\boldsymbol{\Theta}}g_{\theta'} + \hat{\boldsymbol{\varphi}}g_\varphi),$$

$$\mathfrak{C}_n^m = (\tilde{\Gamma}\cdot\mathbf{C}_n^m - \gamma\beta\hat{\mathbf{v}}\times\mathbf{B}_n^m)p' = P(\hat{\boldsymbol{\Theta}}\partial - \hat{\boldsymbol{\varphi}}\partial_{\theta'})Y_n^m,$$

$$\mathfrak{B}_n^m = (\tilde{\Gamma}\cdot\mathbf{B} + \gamma\beta\hat{\mathbf{v}}\times\mathbf{C})p' = P(\hat{\boldsymbol{\Theta}}\partial_{\theta'} + \hat{\boldsymbol{\varphi}}\partial)Y_n^m$$
$$= \hat{\mathbf{R}}\times\mathfrak{C}_n^m. \qquad (80)$$

Since $h_n(x)$ has the form e^{ix} times a polynomial in $1/x$, we may factor **u** in the form $e^{i\nu_s}[\ ]$, where the phase factor $e^{i\nu_s}$ was discussed for $\mathbf{U}_a$.

The functional forms $\mathbf{M}(\mathbf{C})$ and $\mathbf{N}(\mathbf{B})$ of (72) are also satisfied by $\mathfrak{M}(\mathfrak{C})$ and $\mathfrak{N}(\mathfrak{B})$; thus, if we substitute the present series $\mathbf{G}(\mathfrak{C},\mathfrak{B})$ into the complex integral in (28), we again obtain (79). Censor[7] decomposed $\tilde{\Gamma}\cdot\mathbf{g} - \gamma\beta\hat{\mathbf{v}}\times(\hat{\mathbf{R}}'_c\times\mathbf{g})$ as a series of vector spherical harmonics involving $\mathbf{P}_n^m$ as well as $\mathbf{C}_n^m$ and $\mathbf{B}_n^m$, and obtained a series for **U** involving $\mathbf{L}_{nm}(\mathbf{r}')$ as well as $\mathbf{M}_{nm}$ and $\mathbf{N}_{nm}$.

Essentially as before for $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}_M$, we resolve the analogs $\mathfrak{N}$ and $\mathfrak{M}/i$ into components along $\hat{\mathbf{r}}_s$, $\hat{\boldsymbol{\Theta}}$, and $\hat{\boldsymbol{\varphi}}$:

$$\mathfrak{N}_{nm}/p'e^{-i\omega't'}$$
$$= [\mathfrak{N}_n^1(\hat{\boldsymbol{\Theta}}\partial_{\theta'} + \hat{\boldsymbol{\varphi}}\partial) + \hat{\mathbf{r}}_s(\mathfrak{N}_n^2\partial_{\theta'} + \mathfrak{N}_n^3)]Y_n^m,$$

$$\mathfrak{M}_{nm}/ip'e^{-i\omega't'}$$
$$= [\mathfrak{M}_n^1(-\hat{\boldsymbol{\Theta}}\partial + \hat{\boldsymbol{\varphi}}\partial_{\theta'}) + \mathbf{r}_s\mathfrak{M}_n^2\partial + \hat{\boldsymbol{\varphi}}\mathfrak{M}_n^3]Y_n^m, \qquad (81)$$

where $\mathfrak{N}_n^1$, $\mathfrak{N}_n^2 = \mathfrak{M}_n^2$, etc. are the forms given in (71) for $\mathfrak{N}_1^1$, $\mathfrak{N}_1^2$, etc., with $h_1(h|\mathbf{r}'-\mathbf{r}''|)$, H_1, and $\mathcal{H}_1$, replaced by $h_n(k'r')$, H_n, and $\mathcal{H}_n$.

Alternative representations may also be constructed by using (106)[4] and (108)[4],

$$\tilde{\mathbf{h}} = \hat{\mathbf{z}}\mathbf{N}_{10} + \hat{\mathbf{x}}\,\mathrm{Re}\,\mathbf{N}_{11} + \hat{\mathbf{y}}\,\mathrm{Im}\,\mathbf{N}_{11} = \tilde{\mathbf{h}}(\mathbf{N}),$$
$$\tilde{\mathbf{h}}_M/i = \tilde{\mathbf{h}}(\mathbf{M}), \qquad (82)$$

and the analogs

$$\tilde{\mathcal{H}}(\mathbf{N},\mathbf{M})/p'e^{-i\omega't'} = \hat{\mathbf{z}}\mathbf{N}_{10} + \hat{\mathbf{x}}\gamma(\mathrm{Re}\,\mathbf{N}_{11} + i\beta\,\mathrm{Im}\,\mathbf{M}_{11})$$
$$+ \hat{\mathbf{y}}\gamma(\mathrm{Im}\,\mathbf{N}_{11} - i\beta\,\mathrm{Re}\,\mathbf{M}_{11}), \quad \tilde{\mathcal{H}}_M = \tilde{\mathcal{H}}(\mathbf{M},\mathbf{N}). \qquad (83)$$

General Decompositions

Alternative representations and decompositions may be more useful for special computations. Thus from (5) in the form

$$\mathbf{U}/p'e^{-i\omega't'} = \mathfrak{U} = \tilde{\Gamma}\cdot\mathbf{u} - \gamma\beta\hat{\mathbf{v}}\times\mathbf{w},$$
$$\mathbf{w} = \mathbf{u}_M = \nabla'\times\mathbf{u}/ik', \qquad (84)$$

we have in the invariant cylindrical basis

$$\mathfrak{U} = \hat{z}u_z + \hat{\rho}\gamma(u_\rho - \beta w_\varphi) + \hat{\varphi}\gamma(u_\varphi - \beta w_\rho)$$
$$= \hat{z}\mathfrak{U}_z + \hat{\rho}\mathfrak{U}_\rho + \hat{\varphi}\mathfrak{U}_\varphi. \quad (85)$$

We rewrite the scalars in terms of the spherical components as

$$\mathfrak{U}_z = u_{r'} \cos\theta' - u_{\theta'} \sin\theta',$$
$$\mathfrak{U}_\rho/\gamma = u_{r'} \sin\theta' + u_{\theta'} \cos\theta' + \beta w_\varphi,$$
$$\mathfrak{U}_\varphi = \gamma(u_\varphi - w_{\theta'}\beta \cos\theta') - w_{r'}\beta\gamma \sin\theta'$$
$$= \mathfrak{U}_{\varphi 1} - w_{r'}\beta\gamma \sin\theta' \quad (86)$$

and can express $(\hat{z}, \hat{\rho})$ in $(\hat{R}, \hat{\Theta})$, or $(\hat{r}_s, \hat{\theta}_s)$, or $(\hat{r}', \hat{\theta}')$, or in a mixed system.

In $\hat{R}, \hat{\Theta}, \hat{\varphi}$, we have

$$\mathfrak{U} = \hat{R}\mathfrak{U}_R + \hat{\Theta}\mathfrak{U}_\Theta + \hat{\varphi}\mathfrak{U}_\varphi,$$
$$\mathfrak{U}_R = u_{r'} - (u_{\theta'} - w_\varphi)\gamma\beta \sin\Theta,$$
$$\mathfrak{U}_\Theta = (u_{r'}\gamma\beta \sin\Theta + u_{\theta'})p_s - (u_{\theta'} - w_\varphi)\gamma\beta \cos\Theta, \quad (87)$$

with $\mathfrak{U}_{\varphi'}$ as in (86). The representation in $\hat{r}_s, \hat{\Theta}, \hat{\varphi}$ is simpler:

$$\mathfrak{U} = \hat{r}_s \mathfrak{U}_R/\cos\zeta + \hat{\Theta}\mathfrak{U}^\Theta + \hat{\varphi}\mathfrak{U}_\varphi,$$
$$\mathfrak{U}^\Theta = \gamma(u_{\theta'} + w_\varphi\beta \cos\theta'). \quad (88)$$

Here $\mathfrak{U}^\Theta$ is similar to $\mathfrak{U}_{\varphi 1}$, and all terms but these become negligible as $r' \sim \infty$. The behavior of the terms can be seen from (76) and (74):

$$\mathbf{u}(c, b) = \sum [\hat{\mathbf{r}}'f_1 + \hat{\theta}'f_2 + \hat{\varphi}f_3] Y_n^m i^n,$$
$$\mathbf{w} = \mathbf{u}(-b, c),$$
$$f_1 = -ibH, \quad f_2 = ch\partial - ib\mathcal{H}\partial_{\theta'},$$
$$f_3 = -ch\partial_{\theta'} - ib\mathcal{H}\partial,$$
$$\mathfrak{U} = i\sum[\hat{\mathbf{r}}_S F_1 + \hat{\Theta}F_2 + \hat{\varphi}F_3] Y_n^m i^n,$$
$$F_1 = \mathfrak{M}^2(c\partial - b\partial_{\theta'}) - \mathfrak{N}^3 b,$$
$$F_2 = -\mathfrak{M}^1 c\partial - \mathfrak{N}^1 b\partial_{\theta'},$$
$$F_3 = \mathfrak{M}^1 c\partial_{\theta'} - \mathfrak{N}^1 b\partial + \mathfrak{M}^3 c. \quad (89)$$

As $r' \sim \infty$, $\mathfrak{U}^\Theta(\partial, \partial_{\theta'})$ and $\mathfrak{U}_{\varphi 1} = \mathfrak{U}^\Theta(-\partial_{\theta'}, \partial)$ reduce to $h_0 p_s g_{\theta'}$ and $h_0 p_s g_\varphi$. On the other hand $u_{\theta'} - w_\varphi = \Sigma(h + i\mathcal{H})(c\partial - b\partial_{\theta'})Yi^n$, as well as $u_{r'}$ and $w_{r'}$, become negligible.

Spherical Scatterers

For spherically symmetric scatterers we have $c_{nm} = \hat{\mathbf{p}}' \cdot \mathbf{C}_n^{-m}(\hat{\mathbf{k}}')(-1)^m c_n$, and similarly for b_{nm}. For a homogeneous sphere,[11] with $\Phi = \mathbf{E}_0$ in terms of $x = k'a'$ and $X = K'a' = \eta' x$

$$a_n(B) = -\frac{j_n(X)\mathcal{J}_n(x) - j_n(x)\mathcal{J}_n(X)B\eta'}{j_n(X)\mathcal{H}_n(x) - h_n(x)\mathcal{J}_n(X)B\eta'} d_n,$$

$$c_n = a_n(\mu_0/\mu'), \quad b_n = a_n(\epsilon_0/\epsilon'), \quad (90)$$

where $\mathcal{J}_n$ is the form $\mathcal{H}_n$ of (73) with h_n replaced by j_n. Restrick[9] discusses a different decomposition of $\mathbf{U}_a$ in terms of the coefficients c_n and b_n for a sphere, and gives numerical results for a perfect conductor ($B_e \to \infty$ in c_n, and $B_m \to 0$ in b_n) for small $k'a'$. Censor[7] considers a different decomposition of $\mathbf{U}$ and specializes the result to dipoles.

For spherical symmetry, we write the dyadic scattering amplitude (35) for the conventional problem essentially as in (90),[4]

$$\tilde{\mathbf{g}}(\hat{\mathbf{r}}', \hat{\mathbf{k}}') = \sum_{n=1}^{\infty} (\tilde{\mathbf{C}}_n c_n + \tilde{\mathbf{B}}_n b_n),$$
$$\tilde{\mathbf{B}}_n = (r'\nabla_{r'})(k'\nabla_{k'})P_n(\hat{\mathbf{r}}'\cdot\hat{\mathbf{k}}'), \quad \tilde{\mathbf{C}}_n = -\hat{\mathbf{r}}' \times \tilde{\mathbf{B}}_n \times \hat{\mathbf{k}}' \quad (91)$$

such that $\mathbf{g} = \tilde{\mathbf{g}}\cdot\hat{\mathbf{p}}'$. Here $r'\nabla_{r'} = \hat{\theta}'\partial_{\theta'} + \hat{\varphi}\partial_\varphi/\sin\theta'$, etc., and P_n is the Legendre Polynomial. In terms of

$$\tilde{\mathbf{Q}}_n = \tilde{\mathbf{I}}\partial_x P_n(x) + \hat{\mathbf{k}}'\hat{\mathbf{r}}'\partial_x^2 P_n(x), \quad x = \hat{\mathbf{k}}'\cdot\hat{\mathbf{r}}' \quad (92)$$

We obtain

$$\tilde{\mathbf{B}}_n = (\hat{\theta}'\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\tilde{\mathbf{Q}}_n\cdot(\hat{\alpha}'\hat{\alpha}' + \hat{\delta}\hat{\delta}),$$
$$\tilde{\mathbf{C}}_n = -(-\hat{\theta}'\hat{\varphi} + \hat{\varphi}\hat{\theta}')\cdot\tilde{\mathbf{Q}}_n\cdot(-\hat{\alpha}'\hat{\delta} + \hat{\delta}\hat{\alpha}')$$
$$= -\hat{\mathbf{r}}' \times \tilde{\mathbf{Q}}_n \times \hat{\mathbf{k}}'. \quad (93)$$

Thus, for the corresponding relativistic problem, $\tilde{\mathbf{G}}$ of (38) equals

$$\tilde{\mathbf{G}} = \sum_{n=1}^{\infty} (\tilde{\mathfrak{C}}_n c_n + \tilde{\mathfrak{B}}_n b_n), \quad \tilde{\mathfrak{B}}_n = \tilde{\mathbf{p}}_s\cdot\tilde{\mathbf{Q}}_n\cdot\tilde{\mathbf{p}}',$$
$$\tilde{\mathfrak{C}}_n = -\hat{\mathbf{R}} \times \mathfrak{B}_n \times \hat{\mathbf{k}} = -\tilde{\mathbf{p}}_s\cdot(\hat{\mathbf{r}}' \times \tilde{\mathbf{Q}}_n \times \hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}',$$
$$\tilde{\mathfrak{B}}_n = \mathbf{p}_s(\hat{\Theta}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\tilde{\mathbf{Q}}_n\cdot(\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta})p',$$
$$\tilde{\mathfrak{C}}_n = -p_s(-\hat{\Theta}\hat{\varphi} + \hat{\varphi}\hat{\theta}')\cdot\tilde{\mathbf{Q}}_n\cdot(-\hat{\alpha}'\hat{\delta} + \hat{\delta}\hat{\alpha})p', \quad (94)$$

from which we obtain $\mathbf{G} = \tilde{\mathbf{G}}\cdot\hat{\mathbf{p}}$. If $\Phi = \mathbf{E}_0$, then b_n and c_n correspond to electric and magnetic multipoles, respectively. If only the dipoles are significant, we retain only $P_1 = x$, and $\tilde{\mathbf{Q}}_1$ reduces to the identity $\tilde{\mathbf{I}}$. For the perfect conductor, $b_1 \approx -2c_1 \approx i(k'a')^3$ (the case considered by Restrick[9]), and for homogeneous spherical dipoles, $b_1 \approx i(k'a')^3 \times (\epsilon' - \epsilon_0)/(\epsilon' + 2\epsilon_0) = b(\epsilon', \epsilon_0)$ and $c_1 \approx b(\mu', \mu_0)$; to include scattering losses, we replace these first approximations for b_1 or c_1 by $b - 2|b|^2/3$. If the quadrupoles are also significant, then, from $P_2 = \frac{1}{2}(3x^2 - 1)$, we get $\tilde{\mathbf{Q}}_2 = 3\hat{\mathbf{k}}'\cdot\hat{\mathbf{r}}'\mathbf{I} + 3\hat{\mathbf{k}}'\hat{\mathbf{r}}'$, etc.

The corresponding dyadic scattered wave $\tilde{\mathbf{u}}$ such that $\mathbf{u} = \tilde{\mathbf{u}}\cdot\hat{\mathbf{p}}'$ is

$$\tilde{\mathbf{u}} = \sum_{n=1}^{\infty} (\tilde{\mathbf{M}}_n c_n - i\tilde{\mathbf{N}} b_n) i^n,$$

$$\tilde{\mathbf{M}}_n = \sum_{m=-n}^{n} \mathbf{M}_{nm}(\mathbf{r}')\mathbf{C}_n^{-m}(\hat{\mathbf{k}}')(-1)^m = h_n\tilde{\mathbf{C}}_n$$
$$= h_n(-\hat{\theta}'\hat{\varphi} + \hat{\varphi}\hat{\theta}')\cdot\tilde{\mathbf{B}}_n \times \hat{\mathbf{k}}',$$

$$\tilde{\mathbf{N}}_n = \sum_{m=-n}^{n} \mathbf{N}_{nm}(\mathbf{r}')\mathbf{B}_n^{-m}(\hat{\mathbf{k}}')(-1)^m$$
$$= \mathcal{H}_n\tilde{\mathbf{B}}_n + H_n\hat{\mathbf{r}}'\hat{\mathbf{r}}'\cdot\tilde{\mathbf{P}}_n,$$
$$\tilde{\mathbf{P}}_n = \partial_x P_n(\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta}). \tag{95}$$

Similarly, the relativistic dyadic $\tilde{\mathbf{U}}$, such that $\mathbf{U} = \tilde{\mathbf{U}}\cdot\hat{\mathbf{p}}$, equals

$$\tilde{\mathbf{U}} = \sum_{n=1}^{\infty} (\tilde{\mathfrak{M}}_n c_n - i\tilde{\mathfrak{N}}_n b_n)i^n,$$
$$\tilde{\mathfrak{M}}_n = \sum_{n=-m}^{m} \mathfrak{M}_{nm}\mathbf{C}_n^{-m}(\hat{\mathbf{k}}')\cdot\tilde{p}'(-1)^m,$$
$$\tilde{\mathfrak{N}} = \sum \mathfrak{N}\mathbf{B}\cdot\tilde{p}'(-1)^m,$$
$$\tilde{\mathfrak{N}}_n/e^{-i\omega't'} = [\mathfrak{N}_n^1(\hat{\Theta}\hat{\theta}' + \hat{\varphi}\hat{\varphi}) + \mathfrak{N}_n^2\hat{\mathbf{r}}_s\hat{\theta}']\cdot\tilde{\mathbf{B}}_n\cdot\tilde{\mathbf{p}}' + \mathfrak{N}_n^3\hat{\mathbf{r}}_s\hat{\mathbf{r}}'\cdot\tilde{\mathbf{P}}_n\cdot\tilde{\mathbf{p}}',$$
$$\tilde{\mathfrak{M}}_n/ie^{-i\omega't'} = [\mathfrak{M}_n^1(-\hat{\Theta}\hat{\varphi} + \hat{\varphi}\hat{\theta}') + \mathfrak{M}_n^2\hat{\mathbf{r}}_s\hat{\varphi}]\cdot(\tilde{\mathbf{B}}_n\times\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}' + \mathfrak{M}_n^3\hat{\varphi}\hat{\mathbf{r}}'\cdot(\tilde{\mathbf{P}}_n\times\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}' \tag{96}$$

where $\tilde{\mathbf{B}} = (\hat{\theta}'\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\tilde{\mathbf{B}}$ for comparison with (95), and we may rewrite $\mathfrak{M}$ in terms of $\tilde{\mathbf{p}}'_M = \hat{\mathbf{k}}'\times\tilde{\mathbf{p}}' = \tilde{\mathbf{p}}'\times\hat{\mathbf{k}}$. We obtain a form of $\tilde{\mathfrak{M}}$ more similar to the final form of $\tilde{\mathbf{M}}$ in (95) by replacing the terms in $\mathfrak{M}^1$ and $\mathfrak{M}^2$ by $[\mathfrak{M}_n^1(\hat{\Theta}\hat{\theta}' + \hat{\varphi}\hat{\varphi}) - \mathfrak{M}_n^2\hat{\mathbf{r}}_s\hat{\theta}']\cdot\tilde{\mathbf{C}}_n\cdot\tilde{\mathbf{p}}'$, where the form in brackets is now close to the corresponding one of $\tilde{\mathfrak{N}}$. The dyadics $\tilde{\mathfrak{N}}_1$ and $\tilde{\mathfrak{M}}_1/i$ are identically the dipole dyadics $\tilde{\mathcal{H}}(k'r')\cdot\tilde{\mathbf{p}}'/p'$ and $\tilde{\mathcal{H}}_M\cdot\tilde{\mathbf{p}}'/p'$ of (71). The set $\tilde{\mathfrak{N}}_2$ and $\tilde{\mathfrak{M}}_2/i$ are symmetrical quadrupole dyadics, etc.

Arbitrary Dipoles

If $\Phi = \mathbf{E}_0$, in terms of (99),[4] the scattered wave for a general electric dipole with moment $\tilde{\mathbf{b}}$ is

$$\mathbf{E}_s = \tilde{\mathbf{U}}_e\cdot\hat{\mathbf{p}} \sim he^{-i\omega't'}\tilde{\mathbf{G}}_e\cdot\hat{\mathbf{p}},$$
$$\tilde{\mathbf{U}}_e = \tilde{\mathcal{H}}(k'r', \omega't')\cdot\tilde{\mathbf{b}}\cdot\tilde{\mathbf{p}}',$$
$$\tilde{\mathbf{G}}_e = \tilde{\mathbf{p}}_s\cdot\tilde{\mathbf{b}}\cdot\tilde{\mathbf{p}}' = p_s(\hat{\Theta}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\tilde{\mathbf{b}}\cdot(\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta})p'. \tag{97}$$

For a magnetic dipole with moment $\tilde{\mathbf{c}}$, we have

$$\mathbf{E}_s = \tilde{\mathbf{U}}_m\cdot\hat{\mathbf{p}} \sim he^{-i\omega't'}\tilde{\mathbf{G}}_m\cdot\hat{\mathbf{p}}, \quad \tilde{\mathbf{U}}_m = -\tilde{\mathcal{H}}_M\cdot\tilde{\mathbf{c}}\cdot\tilde{\mathbf{p}}'_m,$$
$$\tilde{\mathbf{G}}_m = -\tilde{\mathbf{p}}_{sM}\cdot\tilde{\mathbf{c}}\cdot\tilde{\mathbf{p}}'_M = -\hat{\mathbf{R}}\times[\tilde{\mathbf{p}}_s\cdot\tilde{\mathbf{c}}\cdot\tilde{\mathbf{p}}']\times\hat{\mathbf{k}}$$
$$= -\tilde{\mathbf{p}}_s\cdot[\hat{\mathbf{r}}'\times\tilde{\mathbf{c}}\times\hat{\mathbf{k}}']\cdot\tilde{\mathbf{p}}', \tag{98}$$

where $\tilde{\mathbf{p}}_{sM} = p_s(-\hat{\Theta}\hat{\varphi} + \hat{\varphi}\hat{\theta}')$ and $\tilde{\mathbf{p}}'_M = p'(-\hat{\alpha}'\hat{\delta} + \hat{\delta}\hat{\alpha})$. The sum $\tilde{\mathbf{U}}_e + \tilde{\mathbf{U}}_m = \tilde{\mathbf{U}}$ is the result for a general particle with dimensions small compound to $1/k'$. We have

$$\mathbf{E}_s = (\tilde{\mathbf{U}}_e + \tilde{\mathbf{U}}_m)\cdot\hat{\mathbf{p}} \sim h(k'r')e^{-i\omega't'}\tilde{\mathbf{G}}\cdot\hat{\mathbf{p}},$$
$$\tilde{\mathbf{G}} = \tilde{\mathbf{p}}_s\cdot(\tilde{\mathbf{b}} - \hat{\mathbf{r}}'\times\tilde{\mathbf{c}}\times\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}', \tag{99}$$

which follows directly on substituting $\tilde{\mathbf{g}}$ of (101)[4] into (38). If $\beta \sim 1$ and $\hat{\mathbf{k}} = \hat{\mathbf{v}}$ (i.e., for large velocities and excitation along the motion) then all particles become small compared to $1/k' = (\lambda/2\pi) \times (1+\beta)^{1/2}/(1-\beta)^{1/2}$, where $\lambda = 2\pi/k$ is the original wavelength. If $\tilde{\mathbf{b}} = b_1\tilde{\mathbf{I}}$ and $\tilde{\mathbf{c}} = c_1\tilde{\mathbf{I}}$, we get the corresponding special results for a small sphere.

Tenuous Scatterers

From (66) and (60), we have

$$\mathbf{E}_s = (ik'^3/4\pi)\int\{[(\epsilon' - \epsilon_0)/\epsilon_0]\,\tilde{\mathcal{H}}\cdot\psi - [(\mu' - \mu_0)/\mu']\,\tilde{\mathcal{H}}_M\cdot\psi_M\}\,d\mathcal{V}'. \tag{100}$$

If $\epsilon' \approx \epsilon_0$ and $\mu' \approx \mu_0$, we may use the Rayleigh–Born approximation $\psi \approx \phi$. For small $k'^3\mathcal{V}'$, we obtain the special case of (99) with

$$\tilde{\mathbf{b}} = \tilde{\mathbf{I}}ik'^3\mathcal{V}'(\epsilon' - \epsilon_0)/4\pi\epsilon_0 = \tilde{\mathbf{I}}b = \tilde{\mathbf{b}}_0(\epsilon', \epsilon_0),$$
$$\tilde{\mathbf{c}} = \tilde{\mathbf{b}}_0(\mu', \mu_0) = \tilde{\mathbf{I}}c. \tag{101}$$

If $k'^3\mathcal{V}'$ is not small, we use $\mathbf{G} = \tilde{\mathbf{G}}\cdot\hat{\mathbf{p}}$,

$$\tilde{\mathbf{G}} = \tilde{\mathbf{p}}_s\cdot(\tilde{\mathbf{b}}_0 - \hat{\mathbf{r}}'\times\tilde{\mathbf{c}}_0\times\hat{\mathbf{k}}')\cdot\tilde{\mathbf{p}}'\,\mathcal{g},$$
$$\mathcal{g} = \int e^{ik'(\hat{\mathbf{k}}'-\hat{\mathbf{r}}')\cdot\mathbf{r}''}\,d\mathcal{V}'(\mathbf{r}'')/\mathcal{V}', \tag{102}$$

where $\mathcal{g}$ is the conventional Rayleigh-Born integral. The usual explicit results for $\mathcal{g}(\hat{\mathbf{r}}', \hat{\mathbf{k}}')$ may be rewritten in $\hat{\mathbf{r}}, \hat{\mathbf{k}}$ in terms of $\hat{\mathbf{k}}' = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{k}} - \beta\hat{\mathbf{v}})/p'$ and $\hat{\mathbf{r}}' = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{R}} - \beta\hat{\mathbf{v}})p_s = \tilde{\mathbf{L}}\cdot\hat{\mathbf{r}}_s q$.

In the forward direction $\hat{\mathbf{r}}' = \hat{\mathbf{k}}'$, $\hat{\mathbf{R}} = \hat{\mathbf{k}}$, from the eikonal approximation,

$$\tilde{\mathbf{G}} = (\hat{\alpha}\hat{\alpha} + \hat{\delta}\hat{\delta})(b + c)\,\mathcal{g}_e,$$
$$\mathcal{g}_e = \int e^{i(K'-k')(\zeta'-\zeta_0')}\,d\mathcal{V}'(\mathbf{r}') \approx 1 + ik'(\eta' - 1)\ell', \tag{103}$$

where ℓ' is approximately half the scatterer's mean thickness[13] along $\hat{\mathbf{k}}'$. We used $\zeta' = \hat{\mathbf{k}}'\cdot\mathbf{r}'$ and $\psi = \phi(\zeta_0')\exp[iK'(\zeta' - \zeta_0')]$ with $\zeta_0'\hat{\mathbf{k}}'$ as the impact point on $\mathcal{A}'$ for the ray through $\mathbf{r}'$.

Cylindrical Scatterer

Results analogous to (21) ff. hold outside the smallest circumscribing circle (of radius a') for an arbitrary cylinder with generator along $\hat{\mathbf{y}}$, and $\hat{\mathbf{k}}'$ and $\hat{\mathbf{r}}'$ in the plane $y = 0$. For this case we use[5]

$$h(x) = e^{ix}(2/\pi x)^{1/2}e^{-i\pi/4}, \quad \mathfrak{M} = (1/2\pi)\int_0^{2\pi} d\theta',$$
$$\int = (1/\pi)\int d\Theta_c, \tag{104}$$

where h is now the asymptotic form of $H_0^{(1)}$, and the path of $\int$ is as for $H_0^{(1)}$; also $h\mathfrak{D}(k'r'; \partial_{\theta'}^2)$ of (11)[5] provides the complete asymptotic series, and (34)[14] the converging series. Thus, since $\hat{\mu} = \hat{\rho} = \hat{\mathbf{x}}$ and $\hat{\delta} = \hat{\varphi} = \hat{\mathbf{y}}$, the analog of (27) is

$$\mathbf{U} \sim \mathbf{U}_a = e^{-i\omega't'}h(k'r')\,\mathbf{G} = e^{i\nu_s}\mathbf{G}(2/\pi k'r')^{1/2}e^{-i\pi/4},$$
$$\mathbf{G} = P(\hat{\Theta}\hat{\theta}' + \hat{\mathbf{y}}\hat{\mathbf{y}})\cdot\mathbf{g} \tag{105}$$

with $\mathbf{k}\cdot\mathbf{r} = kr\cos(\theta - \alpha)$ and $\hat{\mathbf{p}} = \hat{\alpha}\sin Q + \hat{\mathbf{y}}\cos Q$ in the incident wave and $\nu_s = P\nu(\mathbf{R}) = P[kr\cos(\Theta - \theta) - \omega t]$ for the scattered phase. The rest follows through (30) with the factor $k'^2/4\pi$ in (24) and (30) replaced by $k'/4$. The essential difference is that now we cannot factor $e^{i\nu_s}$ in the form of **U** obtained from (34)[14] [which involves $e^{-i\omega' t'} H_0^{(1)}(k'r')$ and $e^{-i\omega' t'} H_1^{(1)}(k'r')$]; however, we can factor the complete asymptotic series (11)[5] so there is full correspondance for moderate to large $k'r'$.

The scattering amplitude **g** for $\Phi = \mathbf{E}_0$ may be written

$$\mathbf{g} = \hat{\theta}' g_{\theta'} + \hat{\mathbf{y}} g_y = \hat{\theta}' g_m \sin Q + \hat{\mathbf{y}} g_e \cos Q, \quad (106)$$

where g_m corresponds to the standard function for the scalar problem of **H** parallel to a generator, and g_e corresponds to **E** parallel.[13] In terms of the dyadic

$$\tilde{\mathbf{g}}(\hat{\theta}, \hat{\alpha}') = \hat{\theta}'\hat{\alpha}' g_m + \hat{\mathbf{y}}\hat{\mathbf{y}} g_e, \quad (107)$$

we have the same development (31) to (39) with $\hat{\delta} = \hat{\varphi} = \hat{\mathbf{y}}$, $g_{\theta' y} = g_{y\alpha'} = 0$.

The analog of (51) is

$$\mathbf{S}_s \sim (2S_0/\pi k'r')|\mathbf{G}|^2\hat{\mathbf{R}} = (\mathcal{S}_2 p_s^3 |g|^2/R)\hat{\mathbf{R}},$$
$$\mathcal{S}_2 = 2S_0 p'^2/\pi k' = 2S_0 p'/\pi k, \quad (108)$$

and since $d\Theta = d\theta'/p_s$ the flux through $\Delta\mathbf{A} = R\hat{\mathbf{R}}\Delta\Theta$ equals (52) in terms of $\mathbf{S}_2$ and $d\Omega_2 = d\theta'$. Thus, $d\mathcal{P}_s/d\Theta = \mathcal{S}_2 p_s^3 |\mathbf{g}|^2$.

Similarly the analog of (54) is

$$\mathbf{S}_s - \mathbf{v}W_s \sim \mathcal{S}_2 p_s^3 |\mathbf{g}|^2 (\hat{\mathbf{R}} - \beta\hat{\mathbf{v}})/R$$
$$= \mathcal{S}_2 p_s q^2 |\mathbf{g}|^2 \hat{\mathbf{r}}_s / r_s, \quad (109)$$

and since $d\theta_s = d\theta'/\gamma q^2$, the flux through $\Delta\mathbf{A}_s = \hat{\mathbf{r}}_s r_s \Delta\theta_s$ is the form (55) in terms of $\mathcal{S}_2$ and $d\Omega_2$. Thus, $d\mathcal{P}_R/d\Theta = \mathcal{S}_2 p_s^2 |\mathbf{g}|^2/\gamma$ and $d\mathcal{P}_R/d\theta_s = \mathcal{S}_2 p_s q^2 |\mathbf{g}|^2$.

The Green's function development is essentially as in (58)–(69) with

$$\{\ \} = -(k'/4)\int [\ ]\, dA' = -(k'^2/4i)\int [\ ]\, d\mathcal{V}'$$

as line and surface integrals, and with $h_0^{(1)}$ of (59) replaced by $H_0^{(1)}$; the analogs of (58)–(60) follow directly from (9)[4] to (14)[4]. From the Sommerfeld representation[11] for $H_0^{(1)}(k|\mathbf{r}' - \mathbf{r}''|)$ as a complex integral, we construct

$$\tilde{\mathbf{h}}_2 = (\tilde{\mathbf{I}} + \nabla'\nabla'/k'^2) H_0^{(1)}$$
$$= (1/\pi)\int (\hat{\Theta}_c'\hat{\Theta}_c' + \hat{\mathbf{y}}\hat{\mathbf{y}}) e^{ik'(\mathbf{r}'-\mathbf{r}'')\cdot\hat{\mathbf{R}}_c'} d\Theta_c', \quad (110)$$

and using this in $\mathbf{u} = \{\tilde{\mathbf{h}}_2, \psi\}$ gives the cylindrical analog of (25). This is one way of generalizing our earlier scalar result (9),[5] i.e.,

$$\mathbf{u}[g] = (1/\pi)\int e^{ik'r'\cos(\Theta_c' - \theta')} g(\Theta_c')\, d\Theta_c' \quad (111)$$

to the problem at hand; see Ref. 5 for discussion of paths.

The cylindrical dyadics corresponding to (70) are

$$\tilde{\mathbf{h}} = \hat{\theta}'\hat{\theta}'\mathcal{H}_1 + \hat{\mathbf{y}}\hat{\mathbf{y}} H_0 + \hat{\mathbf{r}}'\hat{\mathbf{r}}'\overline{H}_1,$$
$$\tilde{\mathbf{h}}_M = (-\hat{\theta}'\hat{\mathbf{y}} + \hat{\mathbf{y}}\hat{\theta}') iH_1,$$
$$H_0 = H_0(x) = H_0^{(1)}(k'|\mathbf{r}' - \mathbf{r}''|),$$
$$H_1 = H_1^{(1)} = -\partial_x H_0, \qquad \overline{H}_1 = H_1/x,$$
$$\mathcal{H}_1 = \partial_x H_1 = H_0 - H_1/x. \quad (112)$$

If $r' \sim \infty$, then $\mathcal{H}_1 \sim iH_1 \sim H_0 \sim h e^{-ik'\hat{\mathbf{r}}'\cdot\mathbf{r}''}$ with $h(k'r')$ as in (104), and $\overline{H}_1 \sim O(x^{-3/2})$.

Similarly, corresponding to (71),

$$\tilde{\boldsymbol{\mathcal{H}}}/p'e^{-i\omega' t'} = \hat{\Theta}\hat{\theta}'\gamma(\mathcal{H}_1 + iH_1\beta\cos\theta')$$
$$+ \hat{\mathbf{y}}\hat{\mathbf{y}}\gamma(H_0 + iH_1\beta\cos\theta')$$
$$+ \hat{\mathbf{r}}_s\hat{\theta}'(iH_1 - \mathcal{H}_1)\gamma\beta\sin\Theta/\cos\zeta$$
$$+ \hat{\mathbf{r}}_s\hat{\mathbf{r}}'\overline{H}_1/\cos\zeta,$$
$$\tilde{\boldsymbol{\mathcal{H}}}_M/p'e^{-i\omega' t'} = -\hat{\Theta}\hat{\mathbf{y}}\gamma(iH_1 + H_0\beta\cos\theta')$$
$$+ \hat{\mathbf{y}}\hat{\theta}'\gamma(iH_1 + \mathcal{H}_1\beta\cos\theta')$$
$$+ \hat{\mathbf{r}}_s\hat{\mathbf{y}}(iH_1 - H_0)\gamma\beta\sin\Theta/\cos\zeta$$
$$+ \hat{\mathbf{y}}\hat{\mathbf{r}}'\overline{H}_1\gamma\beta\sin\theta'. \quad (113)$$

Because (112) and (113) involve H_0 (a monopole term) as well as $\mathcal{H}_1$, the present functions are not quite as symmetrical as those of (70) and (71).

The cylindrical Hansen functions subject to (72), in terms of

$$H_n = H_n(x) = H_n^{(1)}(k'r'), \qquad \overline{H}_n = nH_n/x,$$
$$\mathcal{H}_n = \partial_x H_n, \quad (114)$$

may be written[15]

$$\mathbf{M}_n = \hat{\mathbf{y}} M_n = \hat{\mathbf{y}} H_n e^{in\theta'} = H_n \mathbf{C}_n,$$
$$\mathbf{C}_n = \hat{\mathbf{y}} e^{in\theta'} = -\hat{\mathbf{r}}' \times \mathbf{B}_n$$
$$\mathbf{N}_n = \mathcal{H}_n \mathbf{B}_n + \overline{H}_n \mathbf{P}_n = (-\hat{\theta}'\mathcal{H}_n + \hat{\mathbf{r}}' i\overline{H}_n) e^{in\theta'}$$
$$= \hat{\mathbf{z}} i\tfrac{1}{2}(M_{n-1} + M_{n+1}) - \hat{\mathbf{x}}\tfrac{1}{2}(M_{n-1} - M_{n+1}), \quad (115)$$

where $H_n^{(1)} \sim i\mathcal{H}_n \sim hi^{-n+1}$, and $\overline{H}_n \sim O(x^{-3/2})$ for $r' \sim \infty$. The analogs with $H_n^{(1)}$ replaced by J_n are written $\mathbf{M}_n^1, \mathbf{N}_n^1$.

The Green's function is

$$\tilde{\mathbf{h}}_2(k'|\mathbf{r}' - \mathbf{r}''|)$$
$$= \sum_{n=-\infty}^{\infty} [\mathbf{M}_n(\mathbf{r}')\mathbf{M}_{-n}^1(\mathbf{r}'') + \mathbf{N}_n\mathbf{N}_{-n}^1](-1)^n \quad (116)$$

and the development of (76) to (79) carries over in terms of the present functions. We have

$$\mathbf{u} = \sum_{n=-\infty}^{\infty} (\mathbf{M}_n c_n - i\mathbf{N}_n b_n) i^n$$
$$= \Sigma(\hat{\mathbf{r}}'\overline{H}b + \hat{\theta}' i\mathcal{H}b + \hat{\mathbf{y}}Hc) e^{in\theta'} i^n \quad (117)$$

and we obtain (106) in the form

$$\mathbf{g} = \sum_{n=-\infty}^{\infty} (\mathbf{C}_n c_n + \mathbf{B}_n b_n) = \Sigma (\hat{\mathbf{y}} c_n - \hat{\theta}' b_n) e^{in\theta'},$$
$$c_n = \bar{c}_n \cos Q, \quad b_n = -\bar{b}_n \sin Q, \quad (118)$$

where $\bar{c}_n$ and $\bar{b}_n$ are the coefficients for the standard scalar problems. For circularly symmetric scatterers, for either set, $a_{\pm n}(\alpha') = a_n e^{\mp i\alpha'}$. If the scatterer is homogeneous, then we use the form (90) with d_n replaced by unity; we work with J_n and H_n instead of j_n and h_n, and $\mathcal{J}_n$ and $\mathcal{H}_n$ correspond to ∂J_n and ∂H_n (differentiated with respect to argument). Similarly we obtain

$$\mathbf{G} = \sum (\mathbf{C}_n c_n + \mathbf{B}_n b_n) = P(\hat{\Theta} g_{\theta'} + \hat{\mathbf{y}} g_y),$$
$$\mathbf{C}_n = P\hat{\mathbf{y}} e^{in\theta'}, \quad \mathbf{B}_n = -P\hat{\Theta} e^{in\theta'} = \hat{\mathbf{R}} \times \mathbf{C}_n \tag{119}$$

In the present version of (79), i.e.,

$$\mathbf{U} = \sum_{n=-\infty}^{\infty} (\mathfrak{M}_n c_n - i\mathfrak{N}_n b_n) i^n = \mathbf{U}(c, b),$$
$$\mathbf{U}_M = \mathbf{U}(b, -c), \tag{120}$$

we decompose $\mathfrak{N}$ and $\mathfrak{M}$ essentially as for (81),

$$\mathfrak{M}_n/ip'e^{-i\omega' t'} = -\hat{\mathbf{y}}(\mathfrak{M}_n^1 - i\mathfrak{M}_n^3)e^{in\theta'},$$
$$\mathfrak{M}_n^1 = \gamma(iH_n + \mathcal{H}_n \beta \cos\theta'),$$
$$\mathfrak{M}_n^3 = \bar{H}_n \gamma\beta \sin\theta',$$
$$\mathfrak{N}_n/p'e^{-i\omega' t'} = [-\hat{\Theta}\mathfrak{N}_n^1 + \hat{\mathbf{r}}_s(-\mathfrak{N}_n^2 + i\mathfrak{N}_n^3)]e^{in\theta'},$$
$$\mathfrak{N}_n^1 = \gamma(\mathcal{H}_n + iH_n \beta \cos\theta'),$$
$$\mathfrak{N}_n^2 = [(iH_n - \mathcal{H}_n)\gamma\beta \sin\Theta]/\cos\zeta,$$
$$\mathfrak{N}_n^3 = \bar{H}_n/\cos\zeta. \tag{121}$$

Equivalently, in the Cartesian basis

$$\mathfrak{M}_n/p'e^{-i\omega' t} = \hat{\mathbf{y}}\gamma[M_n - i\beta(M_{n-1} - M_{n+1})/2],$$
$$\mathfrak{N}_n/p'e^{-i\omega' t'} = \hat{\mathbf{z}} i(M_{n-1} + M_{n+1})/2$$
$$- \hat{\mathbf{x}}\gamma[(M_{n-1} - M_{n+1})/2 + i\beta M_n]. \tag{122}$$

The scalar problem for $\hat{\mathbf{p}} = \hat{\mathbf{y}}$ corresponds to

$$U' = p'e^{-i\omega' t'} \sum i^n a_n M_n, \quad p' = \gamma(1 - \beta\cos\alpha), \tag{123}$$

and by (5), to

$$U = \gamma[1 - (i\beta/k')\partial_{z'}]U'$$
$$= \gamma p' e^{-i\omega' t'} \sum i^n a_n [M_n - i\beta(M_{n-1} - M_{n+1})/2] \tag{124}$$

in terms of $\partial_{z'} M_n = (M_{n-1} - M_{n+1})k'/2$. The series in (124) was obtained originally by Censor[7] by transforming the plane waves in the complex integral $p'e^{-i\omega' t'}u'$ of (111), and the corresponding asymptotic form $U \sim he^{-i\omega' t'}p'\gamma(1 + \beta\cos\theta')g$ was obtained directly by Lee and Mittra;[8] see Refs. 7 and 8 for detailed discussion.

Similarly for the mates to $\mathbf{U}' = U'\hat{\mathbf{y}}$ and $\mathbf{U} = U\hat{\mathbf{y}} = \sum i^n a_n \mathfrak{M}_n$ of (123) and (124), the transform of

$$\mathbf{U}'_M = p'e^{-i\omega' t'} \sum i^{n-1} a_n \mathbf{N}_n \tag{125}$$

as obtained directly from (5) is

$$\mathbf{U}_M = [\hat{\mathbf{z}}\partial_x - \hat{\mathbf{x}}\gamma(ik'\beta + \partial_{z'})]U'/ik'$$
$$= \sum i^{n-1} a_n \mathfrak{N}_n \tag{126}$$

in terms of $\mathfrak{N}_n$ of (122), or, more conventionally, of (121). From (124) and (126), we obtain the general case (120) by superposition.

Slab Scatterer

Similarly for a slab $-a' \leq z' \leq a'$, and $\hat{\mathbf{k}}$ in the plane $y = 0$, we use $h = \exp[i|\mathbf{k}'\cdot\mathbf{z}'| + i\mathbf{k}'\cdot\mathbf{x}]$ and take $\mathfrak{M}$ as the mean over the forward and reflected directions. We obtain $\mathbf{U} = \mathbf{U}_a$ in the form (105) in terms of (106), i.e.,

$$\mathbf{U} = \mathbf{G}e^{i\nu_s} = P[\hat{\Theta} g_m \sin Q + \hat{\mathbf{y}} g_e \cos Q]e^{i\nu_s}, \quad g = g(\Theta'), \tag{127}$$

where $g(\alpha') = \mathcal{T} - 1$ and $g(\pi - \alpha') = \mathcal{R}$ with $\mathcal{T}$ and $\mathcal{R}$ as the usual[13] transmission and reflection coefficients for the scalar problem of the slab. In the forward scattering direction $\Theta' = \alpha'$, corresponding to (56a), we have

$$\mathbf{U} = (\hat{\alpha} g_m \sin Q + \hat{\mathbf{y}} g_e \cos Q)e^{i\nu},$$
$$\Psi = \Phi + \mathbf{U} = (\hat{\alpha}\mathcal{T}_m \sin Q + \hat{\mathbf{y}}\mathcal{T}_e \cos Q)e^{i\nu} = \mathcal{T} e^{i\nu} \tag{128}$$

and the mate $\Psi_M = \hat{\mathbf{k}} \times \Psi$. In the reflected direction, $\Theta' = \pi - \alpha'$,

$$\mathbf{U} = P_r(\hat{\alpha}_r \mathcal{R}_m \sin Q + \hat{\mathbf{y}}\,\mathcal{R}_e \cos Q)e^{iP_r \nu(\hat{\mathbf{k}}_r)}$$
$$= P_r \mathcal{R} e^{iP_r\nu(\hat{\mathbf{k}}_r)}, \quad \mathbf{U}_M = \hat{\mathbf{k}}_r \times \mathbf{U}, \tag{129}$$

where $\nu(\hat{\mathbf{k}}_r) = kr\cos(\alpha_r - \theta) - \omega t$, with P_r and $\hat{\mathbf{k}}_r$ as before in (56d).

The analog of the scattered flux (51) is

$$\mathbf{S}_s = S_o|\mathbf{G}|^2\hat{\mathbf{R}} = \mathcal{S}_1 p_s^2 |\mathbf{g}|^2\hat{\mathbf{R}}, \quad \mathcal{S}_1 = S_o p'^2, \tag{130}$$

which reduces to $S_o|\mathbf{g}|^2\hat{\mathbf{k}}$ in the forward direction; the corresponding transmitted flux is $\mathbf{S} = S_o|\mathbf{g} + \hat{\mathbf{p}}|^2 \times \hat{\mathbf{k}} = S_o|\mathcal{T}|^2\hat{\mathbf{k}}$. In the reflected direction, $\mathbf{S}_s = S_o P_r^2 |\mathcal{R}|^2\hat{\mathbf{k}}_r$. Similarly, the analog of (54) is

$$\mathbf{S}_s - \mathbf{v}W_s = \mathcal{S}_1 p_s^2 |\mathbf{g}|^2(\hat{\mathbf{R}} - \beta\hat{\mathbf{v}}) = \mathcal{S}_1 p_s q |\mathbf{g}|^2\hat{\mathbf{r}}_s$$
$$= [\mathcal{S}_1(1 + \beta\cos\Theta')|\mathbf{g}|^2]\gamma q\hat{\mathbf{r}}_s \tag{131}$$

with $\hat{\mathbf{r}}_s = \hat{\mathbf{r}}_f$ as in (56a) for $\Theta' = \alpha'$ and $\hat{\mathbf{r}}_s = \hat{\mathbf{r}}_r$ as in (56d) for $\Theta' = \pi - \alpha'$. The beam width of the flux from unit area of slab surface is proportional to $\cos\Theta'$ along $\hat{\mathbf{R}}'$ and to $\cos\theta_s$ along $\hat{\mathbf{r}}_s$, and, from (44), $\cos\theta_s = (\cos\Theta')/\gamma q$; we isolated $\mathcal{S}_1(1 + \beta\cos\Theta')|\mathbf{g}|^2$ for comparison with (55). The reradiated flux density along $\hat{\mathbf{R}}$ is $\mathcal{S}_1 p_s |\mathbf{g}|^2/\gamma$, and that along $\hat{\mathbf{r}}_s$ is $\mathcal{S}_1 p_s q |\mathbf{g}|^2$.

For a homogeneous slab, in terms of

$$\xi = (1 - Z')/(1 + Z'),$$
$$Z' = (B\mathbf{K}'\cdot\hat{\mathbf{v}})/(\mathbf{k}'\cdot\hat{\mathbf{v}}) = B(\eta'^2 - \sin^2\alpha)^{1/2}/\cos\alpha', \tag{132}$$

with B and η' as in (60), we have[13]

$$\mathcal{T} = (1-\xi^2)e^{i(\mathbf{K}'-\mathbf{k}')\cdot\mathbf{d}'}D,$$
$$\mathcal{R} = \xi e^{-i\mathbf{k}'\cdot\mathbf{d}'}(1-e^{i2\mathbf{k}'\cdot\mathbf{d}'})D,$$
$$D = (1-\xi^2 e^{i2\mathbf{k}'\cdot\mathbf{d}'})^{-1} \tag{133}$$

where $\mathbf{d}' = 2a'\hat{\mathbf{v}}$.

The scalar problem ($Q = 0$) is discussed in detail for the perfect conductor ($\mathcal{R} = 1, \mathcal{T} = 0$) by Einstein[1] and Pauli[2] and for the homogeneous slab by Yeh and Casey[6] and Censor.[7]

APPENDIX

The usual reciprocity relation in dyadic form is[12,4]

$$\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1) = \tilde{\mathbf{g}}^T(-\hat{\mathbf{k}}_1, -\hat{\mathbf{k}}_2),$$
$$\tilde{\mathbf{g}}(-\hat{\mathbf{k}}_1, -\hat{\mathbf{k}}_2) = \tilde{\mathbf{g}}^T(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1) \tag{A1}$$

where $\tilde{\mathbf{g}}^T$ is the transpose (Gibb's conjugate) of $\tilde{\mathbf{g}}$. Similarly, the generalization of (24) for lossless scatterers is

$$\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1) + \tilde{\mathbf{g}}^\dagger(\hat{\mathbf{k}}_1, \hat{\mathbf{k}}_2) = \tilde{\mathbf{g}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1) + \tilde{\mathbf{g}}^*(-\hat{\mathbf{k}}_2, -\hat{\mathbf{k}}_1)$$
$$= -2\mathfrak{M}[\tilde{\mathbf{g}}^\dagger(\hat{\mathbf{k}}_3, \hat{\mathbf{k}}_2)\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}_3, \hat{\mathbf{k}}_1)], \tag{A2}$$

where $\tilde{\mathbf{g}}^\dagger = \tilde{\mathbf{g}}^{T*}$ is the Hermitian adjoint of $\tilde{\mathbf{g}}$, and we integrate over $d\Omega(\hat{\mathbf{k}}_3)$.

For the present problem, the rest system $\hat{\mathbf{g}}$ depends not only on $\hat{\mathbf{k}}_1'$ and $\hat{\mathbf{k}}_2'$ as shown in the above, but also on the direction of incidence in Σ (and the direction $\hat{\mathbf{v}}$) as it enters the wavenumber

$$k_i' = kp_i',$$
$$p_i' = \gamma(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}}_i) = p'(\hat{\mathbf{v}}, \hat{\mathbf{k}}_i) = p'(-\hat{\mathbf{v}}, -\hat{\mathbf{k}}_i). \tag{A3}$$

Thus instead of (A1), we have

$$\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_1'; p_1') = \tilde{\mathbf{g}}^T(-\hat{\mathbf{k}}_1', -\hat{\mathbf{k}}_2'; p_1'),$$
$$\tilde{\mathbf{g}}(-\hat{\mathbf{k}}_1', -\hat{\mathbf{k}}_2'; p_2') = \tilde{\mathbf{g}}^T(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_1'; p_2'), \tag{A4}$$

where $\hat{\mathbf{k}}_1'$ is the direction of incidence for the first relation, and $-\hat{\mathbf{k}}_2'$ for the second. To seek analogs involving $\tilde{\mathbf{G}}$ of (38), if we reverse $\hat{\mathbf{k}}_i$, then we must also reverse $\hat{\mathbf{v}}$ to insure that the relation between $-\hat{\mathbf{k}}_i$ and $\hat{\mathbf{k}}_i'$ is preserved, i.e., as determined by

$$\hat{\mathbf{k}}_i = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{k}}_i' + \beta\hat{\mathbf{v}})p_i', \quad \hat{\mathbf{k}}_i' = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{k}}_i - \beta\hat{\mathbf{v}})/p_i'. \tag{A5}$$

Since $\tilde{\mathbf{p}}(\hat{\mathbf{k}}_i', \hat{\mathbf{k}}_i) = \tilde{\mathbf{p}}_i$ of (31) is unaltered by reversing both $\hat{\mathbf{v}}$ and $\hat{\mathbf{k}}_i$ (and thereby reversing $\hat{\mathbf{k}}_i'$), i.e.,

$$\tilde{\mathbf{p}}_i = \tilde{\mathbf{p}}(\hat{\mathbf{k}}_i', \hat{\mathbf{k}}_i; \hat{\mathbf{v}}) = (\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta})p_i'$$
$$= [(\hat{\delta}\times\hat{\mathbf{k}}')(\hat{\delta}\times\hat{\mathbf{k}}) + \hat{\delta}\hat{\delta}]p_i' = \tilde{\mathbf{p}}(-\hat{\mathbf{k}}_i', -\hat{\mathbf{k}}_i; -\hat{\mathbf{v}}), \tag{A6}$$

we may write corresponding forms of $\tilde{\mathbf{G}}$ of (38) as

$$\tilde{\mathbf{G}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1; \hat{\mathbf{v}}) = \tilde{\mathbf{p}}_2^r\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_1'; p_1')\cdot\tilde{p}_1$$
$$= [\tilde{\mathbf{p}}_1^T\cdot\tilde{\mathbf{g}}(-\hat{\mathbf{k}}_1', -\hat{k}_2'; p_1')\cdot\tilde{p}_2^{rT}]^T, \tag{A7}$$

$$\tilde{\mathbf{G}}(-\hat{\mathbf{k}}_1, -\hat{\mathbf{k}}_2; -\hat{\mathbf{v}}) = \tilde{\mathbf{p}}_1^r\cdot\tilde{\mathbf{g}}(-\hat{\mathbf{k}}_1', -\hat{\mathbf{k}}_2'; p_2')\cdot\tilde{\mathbf{p}}_2$$
$$= [\tilde{\mathbf{p}}_2^T\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_1'; p_2')\cdot\tilde{p}_1^{rT}]^T. \tag{A8}$$

Thus, in general, there is no direct relation between $\tilde{\mathbf{G}}$ of (A7) and $\tilde{\mathbf{G}}^T$ of (A8); to stress this we write

$$\tilde{\mathbf{G}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1; \hat{\mathbf{v}}) = \tilde{\mathbf{G}}^T(-\hat{\mathbf{k}}_1, -\hat{\mathbf{k}}_2; -\hat{\mathbf{v}})\,|_{p_2' \rightleftharpoons p_1'}, \tag{A9}$$

where $p_2' \rightleftharpoons p_1'$ indicates an ad hoc interchange.

For an arbitrary scatterer, a simple relation exists for the forward scattered direction $\hat{\mathbf{k}}_1 = \hat{\mathbf{k}}_2 = \hat{\mathbf{k}}$, i.e.,

$$\tilde{\mathbf{G}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}; \hat{\mathbf{v}}) = \tilde{\mathbf{G}}(-\hat{\mathbf{k}}, -\hat{\mathbf{k}}; -\hat{\mathbf{v}}) = \tilde{\mathbf{G}}^T(-\hat{\mathbf{k}}, -\hat{\mathbf{k}}; -\hat{\mathbf{v}}) \tag{A10}$$

for which case

$$\tilde{\mathbf{G}} = (\hat{\alpha}\hat{\alpha}' + \hat{\delta}\hat{\delta})\cdot\tilde{\mathbf{g}}\cdot(\hat{\alpha}'\hat{\alpha} + \hat{\delta}\hat{\delta}),$$
$$\tilde{\mathbf{g}} = \tilde{\mathbf{g}}(\hat{\mathbf{k}}', \hat{\mathbf{k}}') \doteq \tilde{\mathbf{g}}(-\hat{\mathbf{k}}', -\hat{\mathbf{k}}').$$

For arbitrary directions, if $\tilde{\mathbf{g}}$ has inversion symmetry, i.e., if

$$\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_1'; p_1') = \tilde{\mathbf{g}}(-\hat{\mathbf{k}}_2', -\hat{\mathbf{k}}_1'; p_1') = \tilde{\mathbf{g}}^T(\hat{\mathbf{k}}_1', \hat{\mathbf{k}}_2'; p_1'), \tag{A11}$$

then

$$\tilde{\mathbf{G}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1; \hat{\mathbf{v}}) = \tilde{\mathbf{G}}(-\hat{\mathbf{k}}_2, -\hat{\mathbf{k}}_1; -\hat{\mathbf{v}})$$
$$= \tilde{\mathbf{p}}_2^r\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_1'; p_1')\cdot\tilde{p}_1. \tag{A12}$$

In general we may rewrite (A2) as

$$\tilde{\mathbf{G}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1; \hat{\mathbf{v}}) + \tilde{\mathbf{G}}^*(-\hat{\mathbf{k}}_2, -\hat{\mathbf{k}}_1; -\hat{\mathbf{v}})$$
$$= 2\mathfrak{M}[\tilde{p}_2^r\cdot\tilde{\mathbf{g}}^*(-\hat{\mathbf{k}}_2', -\hat{\mathbf{k}}_3'; p_1')\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}_3', \hat{\mathbf{k}}_1'; p_1')\cdot\tilde{p}_1], \tag{A13}$$

where we can insert $\tilde{\mathbf{p}}_3\cdot\tilde{\mathbf{p}}_3^r$ between the g's to show that the integrand has the structure $\tilde{\mathbf{G}}^*\cdot\tilde{\mathbf{G}}$ with p_1' instead of p_3' in $\tilde{\mathbf{g}}^*$. If $\hat{\mathbf{k}}_2 = \hat{\mathbf{k}}_1 = \hat{\mathbf{k}}$, then by (A10) the left side reduces to $2\mathrm{Re}\tilde{\mathbf{G}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}; \hat{\mathbf{v}})$ and we obtain (30) by forming $\hat{\mathbf{p}}\cdot\mathbf{G}\cdot\hat{\mathbf{p}}$. If the scatterer has inversion symmetry, then (A13) reduces to

$$-\mathrm{Re}\tilde{\mathbf{G}}(\hat{\mathbf{k}}_2, \hat{\mathbf{k}}_1; \hat{\mathbf{v}})$$
$$= \mathfrak{M}[\tilde{\mathbf{p}}_2^r\cdot\tilde{\mathbf{g}}^*(\hat{\mathbf{k}}_2', \hat{\mathbf{k}}_3'; p_1')\cdot\tilde{\mathbf{g}}(\hat{\mathbf{k}}_3', \hat{\mathbf{k}}_1'; p_1')\cdot\tilde{\mathbf{p}}_1].$$

---

* This work was supported in part by National Science Foundation Grants NSF-GP-8734 and 21052.

1 A. Einstein, Ann. Phys (Paris) 17, 891 (1905).

2 W. Pauli, *Theory of Relativity* (Pergamon, New York, 1958); A. Sommerfeld, *Electrodynamics* (Academic, New York, 1952).

3 L. Silberstein, *The Theory of Relativity* (Macmillan, London, 1924), p. 237.

4 V. Twersky, J. Math. Phy. 8, 589 (1967); see Report EDL-L30 (1965) Mountain View, Calif., for additional details.

5 V. Twersky, in *Electromagnetic Waves*, R. E. Langer, Ed. (U. of Wisconsin Press, Madison, 1962), pp. 361–89.

6 C. Yeh and K. F. Casey, Phys. Rev. 144, 665 (1966).

7 D. Censor, "Scattering in Velocity Dependent Systems," thesis, Technion-Israel Institute of Technology, Haifa, Israel,

1967 [Radio Sci., (to be published)]. This work also discusses measurement procedures and alternative interpretations.
8 S. W. Lee and R. Mittra, Can. J. Phys. **45**, 1999 (1967).
9 R. C. Restrick, Radio Sci. **3**, 1144 (1968).
10 Chen- To Tai, unpublished work cited by Restrick.
11 P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Chap. 13.
12 D. S. Saxon, Phys. Rev. **100**, 1771 (1955).
13 V. Twersky, J. Math. Phys, **3**, 700, 716 (1962).
14 J. E. Burke, D. Censor, and V. Twersky, J. Acoust. Soc. Am. **37**, 5 (1965).
15 J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill, New York, 1941).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Conservation of Energy and Momentum in Relativistic Electromagnetic Scattering*

Victor Twersky
Mathematics Department, University of Illinois, Chicago, Illinois 60680
(Received 8 December 1970)

In a previous paper we transformed the plane wave excitation $\Phi(\mathbf{r},t)$ for an obstacle moving with constant velocity in free space (Σ) to obtain $\Phi'(\mathbf{r}',t')$ in the scatterer's system (Σ'), and considered the scattered wave $\mathbf{U}'$ in Σ' and its transform $\mathbf{U}$ in Σ. The wave Φ has period T in t, and Φ' and U' have period T' in t'; the wave $\mathbf{U}$ is not periodic in $\mathbf{r}, t$, but in retarded $(\mathbf{R}, t)$ and present coordinates it has the period T_s equal to the dilation of T'. Now we transform t'-averages (over T') of quadratic functions of $\Phi' + \mathbf{U}'$ (the time-averaged energy density, the energy flux vector, and the momentum flux tensor) to obtain $\mathbf{r}, t$-dependent forms in Σ (which in $\mathbf{R}, t$ may be interpreted as t-averages over T_s). We consider the average power absorbed by the scatterer and the force that acts on it in Σ', and the theorems that relate these to the scattered and interference terms. Then we show how the known Σ' conservation theorems are exhibited in Σ, and determine in Σ the corresponding ($\mathbf{r}, t$-independent) power imparted to the scatterer and the force that acts on it, and the reradiated and interference terms. Since T_s is, in general, small enough to regard the present position as practically fixed in Σ, we also consider the corresponding differential reradiated cross section, etc.

INTRODUCTION

In a previous paper,[1] we applied Einstein's procedure[2] to the scattering of an electromagnetic wave Φ by an obstacle moving with constant velocity $\mathbf{v}$ in free space. The wave $\Phi(\mathbf{r}, t) = \hat{\mathbf{p}}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}$ in the observer's system Σ was transformed[2-4] to the scatterer's system Σ' as the incident wave $\Phi'(\mathbf{r}', t') = \hat{\mathbf{p}}'p'e^{i\mathbf{k}'\cdot\mathbf{r}'-i\omega' t'}$; then, the corresponding scattered wave $\mathbf{U}'(\mathbf{r}',t')$ was transformed to Σ as the required function $\mathbf{U}$. The function Φ has the period $T = 2\pi/\omega$ in t, and Φ' and $\mathbf{U}'$ have the period $T' = 2\pi/\omega'$ in t'. The wave $\mathbf{U}$ is not periodic in $\mathbf{r}, t$, but in retarded $(\mathbf{R},t)$ and present $(\mathbf{r}_s, t)$ coordinates, it has the period T_s equalling the dilation of T'.

For $r' \sim \infty$, the far-field $\mathbf{U}' \sim \mathbf{U}'_a$ is proportional to $\mathbf{G}' = \mathbf{g}(\hat{\mathbf{r}}')p'(\hat{\mathbf{k}}\cdot\hat{\mathbf{v}})$, where $\mathbf{g} = g_{\theta'}\hat{\boldsymbol{\theta}}' + g_{\varphi}\hat{\boldsymbol{\varphi}}$ is the scattering amplitude for the conventional problem in Σ'. Similarly for $R \sim \infty$, the corresponding function $\mathbf{U} \sim \mathbf{U}_a$ is proportional to $\mathbf{G}(\hat{\mathbf{R}}) = (g_{\theta'}\hat{\Theta} + g_{\varphi}\hat{\boldsymbol{\varphi}})p'(\hat{\mathbf{k}}\cdot\hat{\mathbf{v}})/p'(\hat{\mathbf{R}}\cdot\hat{\mathbf{v}})$, where $\hat{\mathbf{R}}, \hat{\Theta}, \hat{\boldsymbol{\varphi}}$ is the retarded basis. The result $\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}}) = \hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')$ interrelates the interference effects in the two systems.

Now we consider t'-averages (over T') of quadratic functions[5-8] of $\boldsymbol{\psi}' = \Phi' + \mathbf{U}'$: the time-averaged energy density (W'), energy flux vector ($\mathbf{S}'$), and momentum flux tensor ($\tilde{\mathbf{M}}'$). In Σ, in $\mathbf{r}, t$ coordinates, the analogs $W, \mathbf{S}$, and $\tilde{\mathbf{M}}$ depend in general on t; however, in $\mathbf{R}, t$ or $\mathbf{r}_s, t$ coordinates, the functions may be interpreted as t-averages over T_s. We then show how the known Σ' conservation theorems[8-12] are exhibited in Σ, and determine the average power (P_B) imparted to the scatterer and the force ($\mathbf{F}$) that acts on it in Σ, etc. (The interval T_s is, in general, small enough to regard the present position of the scatterer as practically fixed for far-field intensity measurements by a receiver with rest system Σ. Restrick[13] and Censor[14] interpret $\mathbf{S}$ as the limit of a t-average over an infinite interval.)

We discuss several different derivations of the results for P_B and $\mathbf{F}$. The first, and most direct, involves transformation from Σ' to Σ of the known densities in the scatterer's volume $\mathcal{V}'$. The second involves transformation of Σ' surface (A') integrals and facilities unambiguous resolution of interference terms, etc. Then we consider the quadratic functions directly in Σ, in order to clarify interrelations between different functions in the two systems.

We use the same notation and the same symbols as before.[1] We begin with a short statement of several key results discussed earlier in detail,[1] and then consider the quadratic functions.

1. FAR-FIELD SCATTERING

In Σ, we write the incident wave as[1]

$$\Phi = e^{i\nu}\hat{\mathbf{p}}, \quad \nu = \mathbf{k}\cdot\mathbf{r} - \omega t = k(\hat{\mathbf{k}}\cdot\mathbf{r} - ct),$$
$$\hat{\mathbf{p}} = (\hat{\boldsymbol{\alpha}}\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})\cdot\hat{\mathbf{p}}, \quad (1)$$

where $\hat{\mathbf{k}}, \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\delta}}$ form a special set in the spherical basis $\hat{\mathbf{r}}, \hat{\theta}, \hat{\varphi}$; we use $\hat{\mathbf{r}} = \hat{\mathbf{v}}\cos\theta + \hat{\boldsymbol{\rho}}(\varphi)\sin\theta$, etc. The transform in Σ' is [1-4]

$$\Phi' = e^{i\nu'}\hat{\mathbf{p}}'p', \quad \nu' = \mathbf{k}'\cdot\mathbf{r}' - \omega' t' = \nu,$$
$$\hat{\mathbf{p}}' = (\hat{\boldsymbol{\alpha}}'\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})\cdot\hat{\mathbf{p}}, \quad p' = \gamma(1 - \beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}}) = k'/k,$$
$$\hat{\mathbf{k}}' = \tilde{L}\cdot(\hat{\mathbf{k}} - \beta\hat{\mathbf{v}})/p', \quad \hat{\boldsymbol{\alpha}}' = \hat{\boldsymbol{\delta}} \times \hat{\mathbf{k}}',$$

1967 [Radio Sci., (to be published)]. This work also discusses measurement procedures and alternative interpretations.
[8] S. W. Lee and R. Mittra, Can. J. Phys. **45**, 1999 (1967).
[9] R. C. Restrick, Radio Sci. **3**, 1144 (1968).
[10] Chen- To Tai, unpublished work cited by Restrick.
[11] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Chap. 13.
[12] D. S. Saxon, Phys. Rev. **100**, 1771 (1955).
[13] V. Twersky, J. Math. Phys, **3**, 700, 716 (1962).
[14] J. E. Burke, D. Censor, and V. Twersky, J. Acoust. Soc. Am. **37**, 5 (1965).
[15] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill, New York, 1941).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Conservation of Energy and Momentum in Relativistic Electromagnetic Scattering*

Victor Twersky
Mathematics Department, University of Illinois, Chicago, Illinois 60680
(Received 8 December 1970)

In a previous paper we transformed the plane wave excitation $\Phi(\mathbf{r},t)$ for an obstacle moving with constant velocity in free space (Σ) to obtain $\Phi'(\mathbf{r}',t')$ in the scatterer's system (Σ'), and considered the scattered wave $\mathbf{U}'$ in Σ' and its transform $\mathbf{U}$ in Σ. The wave Φ has period T in t, and Φ' and U' have period T' in t'; the wave $\mathbf{U}$ is not periodic in $\mathbf{r}, t$, but in retarded $(\mathbf{R}, t)$ and present coordinates it has the period T_s equal to the dilation of T'. Now we transform t'-averages (over T') of quadratic functions of $\Phi' + \mathbf{U}'$ (the time-averaged energy density, the energy flux vector, and the momentum flux tensor) to obtain $\mathbf{r}, t$-dependent forms in Σ (which in $\mathbf{R}, t$ may be interpreted as t-averages over T_s). We consider the average power absorbed by the scatterer and the force that acts on it in Σ', and the theorems that relate these to the scattered and interference terms. Then we show how the known Σ' conservation theorems are exhibited in Σ, and determine in Σ the corresponding ($\mathbf{r}, t$-independent) power imparted to the scatterer and the force that acts on it, and the reradiated and interference terms. Since T_s is, in general, small enough to regard the present position as practically fixed in Σ, we also consider the corresponding differential reradiated cross section, etc.

INTRODUCTION

In a previous paper,[1] we applied Einstein's procedure[2] to the scattering of an electromagnetic wave Φ by an obstacle moving with constant velocity $\mathbf{v}$ in free space. The wave $\Phi(\mathbf{r}, t) = \hat{\mathbf{p}}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}$ in the observer's system Σ was transformed[2-4] to the scatterer's system Σ' as the incident wave $\Phi'(\mathbf{r}', t') = \hat{\mathbf{p}}'p'e^{i\mathbf{k}'\cdot\mathbf{r}'-i\omega' t'}$; then, the corresponding scattered wave $\mathbf{U}'(\mathbf{r}',t')$ was transformed to Σ as the required function $\mathbf{U}$. The function Φ has the period $T = 2\pi/\omega$ in t, and Φ' and $\mathbf{U}'$ have the period $T' = 2\pi/\omega'$ in t'. The wave $\mathbf{U}$ is not periodic in $\mathbf{r}, t$, but in retarded $(\mathbf{R},t)$ and present $(\mathbf{r}_s, t)$ coordinates, it has the period T_s equalling the dilation of T'.

For $r' \sim \infty$, the far-field $\mathbf{U}' \sim \mathbf{U}'_a$ is proportional to $\mathbf{G}' = \mathbf{g}(\hat{\mathbf{r}}')p'(\hat{\mathbf{k}}\cdot\hat{\mathbf{v}})$, where $\mathbf{g} = g_{\theta'}\hat{\boldsymbol{\theta}}' + g_\varphi\hat{\boldsymbol{\varphi}}$ is the scattering amplitude for the conventional problem in Σ'. Similarly for $R \sim \infty$, the corresponding function $\mathbf{U} \sim \mathbf{U}_a$ is proportional to $\mathbf{G}(\hat{\mathbf{R}}) = (g_{\theta'}\hat{\Theta} + g_\varphi\hat{\boldsymbol{\varphi}})p'(\hat{\mathbf{k}}\cdot\hat{\mathbf{v}})/p'(\hat{\mathbf{R}}\cdot\hat{\mathbf{v}})$, where $\hat{\mathbf{R}}, \hat{\Theta}, \hat{\boldsymbol{\varphi}}$ is the retarded basis. The result $\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}}) = \hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')$ interrelates the interference effects in the two systems.

Now we consider t'-averages (over T') of quadratic functions[5-8] of $\boldsymbol{\psi}' = \Phi' + \mathbf{U}'$: the time-averaged energy density (W'), energy flux vector $(\mathbf{S}')$, and momentum flux tensor $(\tilde{\mathbf{M}}')$. In Σ, in $\mathbf{r}, t$ coordinates, the analogs $W, \mathbf{S}$, and $\tilde{\mathbf{M}}$ depend in general on t; however, in $\mathbf{R}, t$ or $\mathbf{r}_s, t$ coordinates, the functions may be interpreted as t-averages over T_s. We then show how the known Σ' conservation theorems[8-12] are exhibited in Σ, and determine the average power (P_B) imparted to the scatterer and the force $(\mathbf{F})$ that acts on it in Σ, etc. (The interval T_s is, in general, small enough to regard the present position of the scatterer as practically fixed for far-field intensity measurements by a receiver with rest system Σ. Restrick[13] and Censor[14] interpret $\mathbf{S}$ as the limit of a t-average over an infinite interval.)

We discuss several different derivations of the results for P_B and $\mathbf{F}$. The first, and most direct, involves transformation from Σ' to Σ of the known densities in the scatterer's volume $\mathcal{V}'$. The second involves transformation of Σ' surface (A') integrals and facilities unambiguous resolution of interference terms, etc. Then we consider the quadratic functions directly in Σ, in order to clarify interrelations between different functions in the two systems.

We use the same notation and the same symbols as before.[1] We begin with a short statement of several key results discussed earlier in detail,[1] and then consider the quadratic functions.

1. FAR-FIELD SCATTERING

In Σ, we write the incident wave as[1]

$$\Phi = e^{i\nu}\hat{\mathbf{p}}, \quad \nu = \mathbf{k}\cdot\mathbf{r} - \omega t = k(\hat{\mathbf{k}}\cdot\mathbf{r} - ct),$$
$$\hat{\mathbf{p}} = (\hat{\boldsymbol{\alpha}}\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})\cdot\hat{\mathbf{p}}, \quad (1)$$

where $\hat{\mathbf{k}}, \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\delta}}$ form a special set in the spherical basis $\hat{\mathbf{r}}, \hat{\theta}, \hat{\varphi}$; we use $\hat{\mathbf{r}} = \hat{\mathbf{v}}\cos\theta + \hat{\boldsymbol{\rho}}(\varphi)\sin\theta$, etc. The transform in Σ' is [1-4]

$$\Phi' = e^{i\nu'}\hat{\mathbf{p}}'p', \quad \nu' = \mathbf{k}'\cdot\mathbf{r}' - \omega' t' = \nu,$$
$$\hat{\mathbf{p}}' = (\hat{\boldsymbol{\alpha}}'\hat{\boldsymbol{\alpha}} + \hat{\boldsymbol{\delta}}\hat{\boldsymbol{\delta}})\cdot\hat{\mathbf{p}}, \quad p' = \gamma(1 - \beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}}) = k'/k,$$
$$\hat{\mathbf{k}}' = \tilde{L}\cdot(\hat{\mathbf{k}} - \beta\hat{\mathbf{v}})/p', \quad \hat{\boldsymbol{\alpha}}' = \hat{\boldsymbol{\delta}} \times \hat{\mathbf{k}}',$$

$$\tilde{\mathbf{L}} = \gamma\hat{\mathbf{v}}\hat{\mathbf{v}} + (\tilde{\mathbf{I}} - \hat{\mathbf{v}}\hat{\mathbf{v}}),$$
$$\beta = v/c, \quad \gamma = (1-\beta^2)^{-1/2}, \tag{2}$$

with $\hat{\mathbf{k}}'$, $\hat{\alpha}'$, $\hat{\delta}$ as the corresponding set in $\hat{\mathbf{r}}'$, $\hat{\theta}'$, $\hat{\varphi}$. We have $\hat{\mathbf{k}}\cdot\hat{\mathbf{v}} = \cos\alpha$, etc., so that $p' = \gamma(1-\beta\cos\alpha) = 1/\gamma\,(1+\beta\cos\alpha')$, etc.

The corresponding scattered wave in Σ' for $r' \sim \infty$ is

$$\mathbf{U}' \sim \mathbf{U}'_a = e^{i\nu'_s} p' \mathbf{g}(\hat{\mathbf{r}}')/ik'r', \quad \nu'_s = k'r' - \omega' t',$$
$$\mathbf{g}(\hat{\mathbf{r}}') = (\hat{\theta}'\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\mathbf{g}(\hat{\mathbf{r}}'), \tag{3}$$

where $\mathbf{g}(\hat{\mathbf{r}}') = \mathbf{g}(\hat{\mathbf{r}}', \hat{\mathbf{k}}' : \hat{\mathbf{p}}')$ is the conventional scattering amplitude. (The more usual normalization corresponds to $\mathbf{g}/ik' = \mathbf{f}$.) Its transform in Σ is[1]

$$\mathbf{U} \sim \mathbf{U}_a = e^{i\nu_s}\mathbf{G}(\hat{\mathbf{R}})/ik'r',$$
$$\mathbf{G} = p'p_s(\hat{\Theta}\hat{\theta}' + \hat{\varphi}\hat{\varphi})\cdot\mathbf{g}(\hat{\mathbf{r}}'), \quad p_s = \gamma(1+\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{r}}')$$
$$\nu_s = \nu'_s = p'p_s(k\hat{\mathbf{R}}\cdot\mathbf{r} - \omega t) = p'(kR - \omega t)/\gamma,$$
$$\hat{\mathbf{R}} = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{r}}' + \beta\hat{\mathbf{v}})/p_s, \tag{4}$$

with $\hat{\mathbf{R}}, \hat{\Theta}, \hat{\varphi}$ as the retarded basis, and $\mathbf{R}, t$ as the retarded coordinates. For brevity, we write the relativistic scattering amplitude $\mathbf{G}(\hat{\mathbf{R}}, \hat{\mathbf{k}} : \hat{\mathbf{p}}; \hat{\mathbf{v}})$ as $\mathbf{G}(\hat{\mathbf{R}})$. We have

$$\mathbf{r}' = \tilde{\mathbf{L}}\cdot(\mathbf{R} - R\beta\hat{\mathbf{v}}) = \tilde{\mathbf{L}}\cdot\mathbf{r}_s, \quad r' = R/p_s = r_s/q,$$
$$q = 1/\gamma(1-\beta^2\sin^2\theta_s)^{1/2},$$
$$\hat{\mathbf{r}}'\cdot\hat{\mathbf{v}} = \cos\theta' = \gamma p_s(\cos\Theta - \beta) = \gamma q\cos\theta_s,$$
$$p_s = \gamma(1+\beta\cos\theta') = 1/\gamma(1-\beta\cos\Theta), \tag{5}$$

where $\hat{\mathbf{r}}_s, \hat{\theta}_s, \hat{\varphi}$ is the present (simultaneous) basis, and $\mathbf{r}_s, t$ are the present coordinates. Equation (4) corresponds to $R \sim r_s \sim \infty$. For forward scattering in Σ', we have $\hat{\mathbf{r}}' = \hat{\mathbf{k}}'$ and $\hat{\mathbf{R}} = \hat{\mathbf{k}}$; for this case, $p'p_s = 1$, and[1]

$$\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}}) = \hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') \tag{6}$$

enables us to interrelate the interference effects in the two systems.

The mates to Φ and $\mathbf{U}$, and their transforms, are given by

$$\Phi_M = \hat{\mathbf{k}}\times\Phi, \quad \Phi'_M = \hat{\mathbf{k}}'\times\Phi',$$
$$\mathbf{U}'_{Ma} = \hat{\mathbf{r}}'\times\mathbf{U}'_a, \quad \mathbf{U}_{Ma} = \hat{\mathbf{R}}\times\mathbf{U}_a$$

such that $\partial_t \mathbf{U}_M = -c\nabla\times\mathbf{U}$, etc. For t'-periodic fields in $\mathbf{r}', t'$, we have $\mathbf{U}'_M = \nabla'\times\mathbf{U}'/ik'$, etc. We take $\Phi = \mathbf{E}_0$ as the original electric field, so that $\mathbf{H}_0 = \Phi_M(\epsilon_0/\mu_0)^{1/2}$; similarly, $\mathbf{U} = \mathbf{E}_s$ is the scattered electric field and $\mathbf{U}_M = \mathbf{H}_s(\mu_0/\epsilon_0)^{1/2}$ is the normalized scattered magnetic field. Thus, $\Psi = \Phi + \mathbf{U} = \mathbf{E}_0 + \mathbf{E}_s = \mathbf{E}$ is the electric field in Σ, etc.

In retarded or present coordinates, $\mathbf{U}_a$ of (4) is a periodic function of t with period $T_s = 2\pi\gamma/\omega'$; this interval is the dilation of the t'-period $T' = 2\pi/\omega'$ of Φ' and $\mathbf{U}'$, and it is also simply related to the original period $T = 2\pi/\omega$. Thus,

$$T_s = \gamma T' = \gamma T/p' = T/(1-\beta\cos\alpha). \tag{7}$$

Since $\mathbf{U}$ differs from $\mathbf{U}_a$ in that $\mathbf{G}$ is replaced[1] by $\tilde{\mathfrak{D}}\cdot\mathbf{G} = [\tilde{\mathbf{I}} + (i/2k'r')\tilde{\mathbf{D}} + \cdots]\cdot\mathbf{G}$, with $\tilde{\mathbf{D}}$ as a Beltrami differential operator on the angles,[10] $\mathbf{U}(\mathbf{R}, t)$ also has t-period T_s; similarly for $\mathbf{U}_M$ in terms of $\tilde{\mathfrak{D}}\cdot(\hat{\mathbf{R}}\times\mathbf{G})$. We also refer Φ to the retarded event $\mathbf{r}_0, t_0$ [with $\mathbf{r}_0 = \mathbf{v}t_0 = \mathbf{v}(t - R/c)$] by rewriting ν of (1) as $\nu = \mathbf{k}\cdot(\mathbf{r}_0 + \mathbf{R}) - \omega(t_0 + R/c)$ $R/c) = \nu_0 + kR(\hat{\mathbf{k}}\cdot\hat{\mathbf{R}} - 1)$; using $\nu_0 = \nu_s$ as discussed before,[1] we express Φ in retarded coordinates as

$$\Phi(\mathbf{R}, t) = e^{i\nu_s + i(\mathbf{k}\cdot\mathbf{R} - kR)}, \quad \nu_s = (1-\beta\cos\alpha)(kR - \omega t), \tag{8}$$

with ν_s as in (4). In present coordinates, we have

$$\Phi[\mathbf{r}_s, t] = e^{i\mathbf{k}\cdot\mathbf{r}_s - i\omega(1-\beta\cos\alpha)t}$$

In Σ', we factor the fields and write

$$\Phi' = e^{-i\omega' t'}p'\boldsymbol{\phi}, \quad \boldsymbol{\phi} = \hat{\mathbf{p}}' e^{i\mathbf{k}'\cdot\mathbf{r}'}, \quad \mathbf{U}' = e^{-i\omega' t'}p'\mathbf{u},$$
$$\boldsymbol{\phi} + \mathbf{u} = \boldsymbol{\psi}, \quad \mathbf{u} \sim e^{ik'r'}\mathbf{g}/ik'r' \tag{9}$$

where $\psi(\mathbf{r}'; \hat{\mathbf{k}}' : \hat{\mathbf{p}}')$ is the usual t'-independent solution of the reduced wave equation for real k'. The scattering amplitude $\mathbf{g}$ may be represented as an integral[11,1] over the scatterer's surface $\mathcal{A}'$:

$$\mathbf{g}(\hat{\mathbf{r}}') = \frac{-k'^2}{4\pi}\int[(\tilde{\phi}\times\hat{\mathbf{n}}')\cdot\mathbf{u}_M + \tilde{\phi}_M\cdot(\mathbf{u}\times\hat{\mathbf{n}}')]\,d\mathcal{A}'$$
$$\tilde{\phi}(-\hat{\mathbf{r}}') = (\hat{\theta}'\hat{\theta}' + \hat{\varphi}\hat{\varphi})\,e^{-ik'\hat{\mathbf{r}}'\cdot\mathbf{r}''},$$
$$\mathbf{u}_M = \nabla''\times\mathbf{u}/ik', \quad \tilde{\phi}_M = \hat{\mathbf{r}}'\times\tilde{\phi}. \tag{10}$$

We use $d\mathcal{A}' = \hat{\mathbf{n}}' d\mathcal{A}'(\mathbf{r}'')$ with $\hat{\mathbf{n}}'$ as the outward normal (and we may replace $\mathcal{A}'$ by any surface A' inclosing the scatterer, in the volume V' external to the scatterer's volume $\mathcal{V}'$). In the forward direction $\hat{\mathbf{r}}' = \hat{\mathbf{k}}'$, in terms of $\phi(-\hat{\mathbf{k}}') = \phi^*(\hat{\mathbf{k}}')$,

$$\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') = \frac{k'^2}{4\pi}\int[\boldsymbol{\phi}^*(\hat{\mathbf{k}}')\times\mathbf{u}_M - \mathbf{u}\times\boldsymbol{\phi}^*_M(\hat{\mathbf{k}}')]\cdot d\mathbf{A}' \tag{11}$$

2. ENERGY AND MOMENTUM

The fields are periodic in Σ' and we may average products over one cycle T' in t' to obtain the usual[8] quadratic functions: the time-averaged energy density

$$W' = \tfrac{1}{4}(\epsilon_0|\mathbf{E}'|^2 + \mu_0|\mathbf{H}'|^2) = \tfrac{1}{2}W_0(|\Psi'|^2 + |\Psi'_M|^2),$$
$$W_0 = \tfrac{1}{2}\epsilon_0; \tag{12}$$

the Poynting flux $\mathbf{S}'$ and momentum density $\mathbf{N}'$ vectors

$$\mathbf{S}' = c^2\mathbf{N}' = \tfrac{1}{2}\,\mathrm{Re}\,(\mathbf{E}'\times\mathbf{H}'^*) = S_0\,\mathrm{Re}\,(\Psi'\times\Psi'^*_M),$$
$$S_0 = \tfrac{1}{2}\epsilon_0 c = W_0 c; \tag{13}$$

and the momentum flux dyadic

$$\mathbf{M}' = -\tfrac{1}{2}\mathrm{Re}(\epsilon_0\mathbf{E}'\mathbf{E}'^* + \mu_0\mathbf{H}'\mathbf{H}'^*) + \tilde{\mathbf{I}}W' = -W_0\mathrm{Re}(\mathbf{\Psi}'\mathbf{\Psi}'^* + \Psi_M'\Psi_M'^*) + \tilde{\mathbf{I}}W'. \quad (14)$$

The square of the dimension of E is implicit in the definition of W_0, etc.

Transforming (12)–(14) to Σ, we have the analogs[5-7]

$$W = \gamma^2[(W' + \mathbf{v}\cdot\mathbf{N}') + \mathbf{v}\cdot(\mathbf{S}' + \tilde{\mathbf{M}}\cdot\mathbf{v})/c^2], \quad (15)$$

$$\mathbf{S} = \gamma\tilde{\mathbf{L}}\cdot[(\mathbf{S}' + \mathbf{v}W') + (\hat{\mathbf{M}}' + \mathbf{v}\mathbf{N}')\cdot\mathbf{v}],$$
$$\mathbf{N} = \gamma\tilde{\mathbf{L}}\cdot[(\mathbf{N}' + \mathbf{v}W'/c^2) + (\tilde{\mathbf{M}}' + \mathbf{v}\mathbf{S}'/c^2)\cdot\mathbf{v}/c^2], \quad (16)$$

$$\tilde{\mathbf{M}} = \tilde{\mathbf{L}}\cdot[(\tilde{\mathbf{M}}' + \mathbf{v}\mathbf{N}') + (\mathbf{S}'\mathbf{v} + W'\mathbf{v}\mathbf{v})/c^2]\cdot\tilde{\mathbf{L}}, \quad (17)$$

which depend on t in $\mathbf{r}, t$ (but in $\mathbf{R}, t$ correspond to t-averages over T_s). By superposition,

$$W - \mathbf{v}\cdot\mathbf{S}/c^2 = W' + \mathbf{v}\cdot\mathbf{N}',$$
$$W - \mathbf{v}\cdot\mathbf{N} = W' + \mathbf{v}\cdot\mathbf{S}'/c^2, \quad (18)$$

$$\mathbf{S} - W\mathbf{v} = \gamma\tilde{\mathbf{L}}^{-1}\cdot(\mathbf{S}' + \tilde{\mathbf{M}}'\cdot\mathbf{v}),$$
$$\mathbf{S} - \tilde{\mathbf{M}}\cdot\mathbf{v} = \tilde{\mathbf{L}}\cdot(\mathbf{S}' + W'\mathbf{v})/\gamma, \quad (19)$$

$$\tilde{\mathbf{M}} - \mathbf{S}\mathbf{v}/c^2 = \tilde{\mathbf{L}}\cdot(\tilde{\mathbf{M}}' + \mathbf{v}\mathbf{N}')\cdot\tilde{\mathbf{L}}^{-1},$$
$$\tilde{\mathbf{M}} - \mathbf{v}\mathbf{N} = \tilde{\mathbf{L}}^{-1}\cdot(\tilde{\mathbf{M}}' + \mathbf{S}'\mathbf{v}/c^2)\cdot\tilde{\mathbf{L}}. \quad (20)$$

We keep $\mathbf{S}$ and $\mathbf{N}$ distinct to facilitate interpretation.

We have $\mathbf{E}' = \mathbf{\Psi}' = \mathbf{\Phi}' + \mathbf{U}' = \mathbf{E}_0' + \mathbf{E}_s'$, etc., and $W' = W_0' + W_I' + W_s'$, etc. The incident (W_0') and scattered (W_s') energy densities are

$$W_0' = \tfrac{1}{2}W_0(|\mathbf{\Phi}'|^2 + |\mathbf{\Phi}_M'|^2) = W_0|\mathbf{\Phi}'|^2 = W_0 p'^2 \quad (21)$$

$$W_s' = \tfrac{1}{2}W_0(|\mathbf{U}'|^2 + |\mathbf{U}_M'|^2) \sim W_0|\mathbf{U}_a'|^2 = W_0'|\mathbf{g}(\hat{\mathbf{r}}')|^2|D|^2 = W_{sa}', \quad D = 1/ik'r'. \quad (22)$$

The interference term is

$$W_I' = W_0\,\mathrm{Re}(\mathbf{\Phi}'^*\cdot\mathbf{U}' + \mathbf{\Phi}_M'^*\cdot\mathbf{U}_M') \sim W_0'\,\mathrm{Re}\{e^{ik'r' - i\mathbf{k}'\cdot\mathbf{r}'}[\hat{\mathbf{p}}'\cdot\mathbf{g} + (\hat{\mathbf{k}}'\times\hat{\mathbf{p}}')\cdot(\hat{\mathbf{r}}'\times\mathbf{g})]D\} = W_{Ia}', \quad (23)$$

and the phase of the asymptotic form is stationary at $\hat{\mathbf{r}}' = \hat{\mathbf{k}}', -\hat{\mathbf{k}}'$; the stationary value of W_{Ia}' is $2W_0'\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')D$ for the first and zero for the second. (We use $\hat{\mathbf{k}}'\cdot\mathbf{g}(\pm\hat{\mathbf{k}}') = 0$, etc.)

The incident ($\mathbf{S}_0'$) and scattered ($\mathbf{S}_s'$) fluxes satisfy

$$\mathbf{S}_0' = S_0\,\mathrm{Re}(\mathbf{\Phi}'^*\times\mathbf{\Phi}_M') = \hat{\mathbf{k}}'S_0', \qquad S_0' = S_0 p'^2, \quad (24)$$

$$\mathbf{S}_s' = S_0\,\mathrm{Re}(\mathbf{U}'^*\times\mathbf{U}_M) \sim \hat{\mathbf{r}}'S_0'|\mathbf{g}(\hat{\mathbf{r}}')|^2|D|^2 = \mathbf{S}_{sa}', \quad (25)$$

The total power reradiated from the scatterer's surface $\mathcal{A}'$ is

$$P_s' = \int\mathbf{S}_s'\cdot d\mathcal{A}' = \int\mathbf{S}_s'\cdot d\mathbf{A}' = S_0'\sigma_s', \quad (26)$$

with σ_s' as the scattering cross section; we used $\nabla'\cdot\mathbf{S}_s' = 0$ in V' to replace $\mathcal{A}'$ by A'. Taking $d\mathbf{A}' = \hat{\mathbf{r}}'r'^2 d\Omega(\hat{\mathbf{r}}')$ with $r' \sim \infty$, (henceforth A_∞'),

$$\sigma_s' = b\mathfrak{M}[|g(\hat{\mathbf{r}}')|^2], \quad \mathfrak{M} = (1/4\pi)\int d\Omega(\hat{\mathbf{r}}'), \quad b = 4\pi/k'^2, \quad (27)$$

where $\mathfrak{M}$ indicates the mean over all values of $\hat{\mathbf{r}}'$.

The interference of the incident and scattered waves is shown by

$$\mathbf{S}_I' = S_0\,\mathrm{Re}(\mathbf{\Phi}'^*\times\mathbf{U}_M' - \mathbf{U}'\times\mathbf{\Phi}_M'^*), \quad (28)$$

and from (11), the power diverted from the incident wave by interference is

$$P_I' = \int\mathbf{S}_I'\cdot d\mathbf{A}' = S_0' b\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}'). \quad (29)$$

This result may also be obtained from the asymptotic form

$$\mathbf{S}_I' \sim S_0'\,\mathrm{Re}\{e^{ik'r - i\mathbf{k}'\cdot\mathbf{r}'}[\hat{\mathbf{p}}'\times(\hat{\mathbf{r}}'\times\mathbf{g}) + \mathbf{g}\times(\hat{\mathbf{k}}'\times\hat{\mathbf{p}}')]D\} = \mathbf{S}_{Ia}', \quad (30)$$

which reduces to $\mathbf{S}_{Ia}' = S_0' 2\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')\hat{\mathbf{k}}'D, 0$ at the stationary points $\hat{\mathbf{r}}' = \hat{\mathbf{k}}', -\hat{\mathbf{k}}'$. Thus, evaluation of $\int\mathbf{S}_{Ia}'\cdot d\mathbf{A}'$ by the method of stationary phase,

$$\int e^{ik'r'f(\theta',\varphi)}\frac{\mathfrak{F}(\theta',\varphi)}{ik'r'}r'^2 d\theta' d\varphi \sim \frac{2\pi}{k'^2}\sum_m \frac{e^{ik'r'f_m}\mathfrak{F}_m}{[\partial_{\theta'}^2 f_m \partial_\varphi^2 f_m - (\partial_{\theta'}\partial_\varphi f_m)^2]^{1/2}},$$

also yields (29). Here $f = 1 - \hat{\mathbf{k}}'\cdot\hat{\mathbf{r}}'$, and we sum over the set (m) of stationary values.

The net flux into the scatterer's surface, the power absorbed in $\mathcal{V}'$, equals

$$P_A' = -\int\mathbf{S}'\cdot d\mathcal{A}' = S_0'\sigma_A', \quad (31)$$

where σ_A' is the absorption cross section. Since $\nabla'\cdot\mathbf{S}' = 0$ in V', we also have

$$\int\mathbf{S}'\cdot d\mathcal{A}' = \int\mathbf{S}_I'\cdot d\mathbf{A}' + \int\mathbf{S}_S'\cdot d\mathbf{A}' = P_I + P_S = S_0'[b\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}'(\hat{\mathbf{k}}') + \sigma_S'], \quad (32)$$

where we used $\int\mathbf{S}_0'\cdot d\mathbf{A}' = 0$, and (26) and (29). From (31) and (32) we obtain the usual energy theorem[9,10] in the form

$$P_A' + P_S' = P_T' = -P_I', \quad \sigma_A' + \sigma_S' = \sigma_T' = -b\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}'), \quad P' = S_0'\sigma', \quad (33)$$

where σ_T' is the total cross section, and $P_T' = -P_I'$ is the energy diverted from the incident wave by interference with the scattered wave, and either absorbed or reradiated by the obstacle.

Similarly, for the components of the momentum flux tensor,

$$\tilde{\mathbf{M}}_0' = -W_0|\Phi'|^2[\hat{\mathbf{p}}'\hat{\mathbf{p}}' + (\hat{\mathbf{k}}'\times\hat{\mathbf{p}}')(\hat{\mathbf{k}}'\times\hat{\mathbf{p}}') - \tilde{\mathbf{I}}] = W_0'\hat{\mathbf{k}}'\hat{\mathbf{k}}' = \mathbf{S}_0'\hat{\mathbf{k}}'/c, \quad (34)$$

$$\tilde{\mathbf{M}}_S' \sim -W_0|\mathbf{U}_a'|^2[\hat{\mathbf{g}}'\hat{\mathbf{g}}' + (\hat{\mathbf{r}}'\times\hat{\mathbf{g}}')(\hat{\mathbf{r}}'\times\hat{\mathbf{g}}') - \tilde{\mathbf{I}}] = W_{Sa}'\hat{\mathbf{r}}'\hat{\mathbf{r}}' = \mathbf{S}_{Sa}'\hat{\mathbf{r}}'/c, \quad (35)$$

$$\tilde{\mathbf{M}}_I'\cdot\hat{\mathbf{k}}' = W_0\,\mathrm{Re}[\mathbf{U}'\times(\hat{\mathbf{k}}'\times\Phi')^* + \mathbf{U}_M'\times(\hat{\mathbf{k}}'\times\Phi_M')^*] = W_0(\mathbf{U}'\times\Phi_M'^* + \Phi'^*\times\mathbf{U}_M') = \mathbf{S}_I'/c,$$

$$\tilde{\mathbf{M}}_I'\cdot\hat{\mathbf{r}}' = -W_0\,\mathrm{Re}\{[\Phi'^*\mathbf{U}'\cdot\hat{\mathbf{r}}' + \Phi^*\times(\hat{\mathbf{r}}'\times\mathbf{U}')] - [\Phi_M'^*\mathbf{U}_M'\cdot\hat{\mathbf{r}}' + \Phi_M'^*\times(\hat{\mathbf{r}}'\times\mathbf{U}_M)]\} \sim \mathbf{S}_I'/c. \quad (36)$$

The analog of (26) is the force

$$\mathbf{F}_S' = \int\tilde{M}_S'\cdot d\mathbf{\alpha}' = W_0'b\mathfrak{M}[|\mathbf{g}(\hat{\mathbf{r}}')|^2\hat{\mathbf{r}}'] = W_0'\sigma_s'\langle\hat{\mathbf{r}}'\rangle = P_s'\langle\hat{\mathbf{r}}'\rangle/c,$$

$$\langle\hat{\mathbf{r}}'\rangle = \int|g(\hat{\mathbf{r}}')|^2\hat{\mathbf{r}}'d\Omega(\hat{\mathbf{r}}')/\int|g(\hat{\mathbf{r}}')|^2d\Omega(\hat{\mathbf{r}}') = b\mathfrak{M}[|\mathbf{g}|^2\hat{\mathbf{r}}']/\sigma_s', \quad (37)$$

where we used $\nabla'\cdot\tilde{\mathbf{M}}_s' = 0$ in V'. The analog of (29),

$$\mathbf{F}_I' = \int\tilde{\mathbf{M}}_I'\cdot d\mathbf{\alpha}' = W_0'b\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')\hat{\mathbf{k}}' = P_I'\hat{\mathbf{k}}'/c, \quad (38)$$

gives the momentum diverted from Φ' by interference with $\mathbf{U}'$.

Since $\nabla'\cdot\mathbf{M}' = 0$ in the volume external to the scatterer, the radiation force on the obstacle [the analog of (31)] is

$$\mathbf{F}' = -\int\tilde{\mathbf{M}}'\cdot d\mathbf{\alpha}' = W_0'\boldsymbol{\sigma}' \quad (39)$$

where $\boldsymbol{\sigma}'$ is a directed cross section for force. In terms of (37) and (38), we also have

$$\int\tilde{\mathbf{M}}\cdot d\mathbf{\alpha}' = \int\tilde{\mathbf{M}}_I'\cdot d\mathbf{\alpha}' + \int\tilde{\mathbf{M}}_S'\cdot d\mathbf{\alpha}' = \mathbf{F}_I' + \mathbf{F}_S' = W_0'[b\,\mathrm{Re}\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')\hat{\mathbf{k}} + \sigma_s'\langle\hat{\mathbf{r}}'\rangle]. \quad (40)$$

From (39) and (40),

$$\mathbf{F}' + \mathbf{F}_S' = \mathbf{F}_T' = -\mathbf{F}_I',$$
$$\boldsymbol{\sigma}' + \sigma_S'\langle\hat{\mathbf{r}}'\rangle = \boldsymbol{\sigma}_T' = -b\,\mathrm{Re}\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')\hat{\mathbf{k}}' = \sigma_T'\hat{\mathbf{k}}';$$
$$\boldsymbol{\sigma}' = \sigma_T'\hat{\mathbf{k}}' - \sigma_s'\langle\hat{\mathbf{r}}'\rangle, \quad (41)$$

where $\mathbf{F}_T' = -\mathbf{F}_I'$, the momentum diverted from the incident wave by interference with the scattered wave, equals that imparted to the obstacle plus that reradiated. For a spherically symmetrical scatterer, the radiation pressure is specified by

$$\boldsymbol{\sigma}' = \sigma'\hat{\mathbf{k}}',$$
$$\sigma' = \sigma_T' - \sigma_s'\langle\hat{\mathbf{k}}'\cdot\hat{\mathbf{r}}'\rangle = \sigma_A' + \sigma_s'\langle 1 - \hat{\mathbf{k}}'\cdot\hat{\mathbf{r}}'\rangle \quad (42)$$

as discussed by Debye,[11] and van de Hulst.[12]

We may write the absorbed power as an integral over the scatterer's volume ($\mathcal{V}'$)

$$P_A' = -\int\mathbf{S}'\cdot d\mathbf{\alpha}' = -\int\nabla'\cdot\mathbf{S}'d\mathcal{V}' = \int Q'd\mathcal{V}', \qquad \nabla'\cdot\mathbf{S}' = -Q', \quad (43)$$

where $Q'(\mathbf{r}')$ is the power loss density within the scatterer. Similarly for the force on the scatterer

$$\mathbf{F}' = -\int\tilde{\mathbf{M}}'\cdot d\mathbf{\alpha}' = -\int\nabla'\cdot\tilde{\mathbf{M}}'d\mathcal{V}' = \int\mathbf{f}'d\mathcal{V}', \qquad \nabla'\cdot\tilde{\mathbf{M}}' = -\mathbf{f}', \quad (44)$$

with $\mathbf{f}'(\mathbf{r}')$ as the internal force density. The divergence relations are the usual ones for the t'-independent problem. The densities transform as[2-5]

$$\mathbf{f} = \tilde{\mathbf{L}}\cdot\mathbf{f}' + \gamma\mathbf{v}Q'/c^2 = \tilde{\mathbf{L}}\cdot(\mathbf{f}' + \mathbf{v}Q'/c^2),$$
$$Q = Q'/\gamma; \qquad Q + \mathbf{v}\cdot\mathbf{f} = \gamma(Q' + \mathbf{v}\cdot\mathbf{f}'), \quad (45)$$

where we used the result for Q corresponding to heat; $\mathbf{v}\cdot\mathbf{f}$ is the work per unit volume. From the above and the relations

$$dV = dV'/\gamma, \qquad d\mathbf{A} = \tilde{\mathbf{L}}\cdot d\mathbf{A}'/\gamma, \quad (46)$$

we determine the absorbed power P_A and force $\mathbf{F}$ in Σ.

In Σ, the corresponding force on the scatterer is

$$\mathbf{F} = \int\mathbf{f}d\mathcal{V} = \gamma^{-1}\int(\mathbf{f}' + \mathbf{v}Q'/c^2)\cdot\tilde{\mathbf{L}}d\mathcal{V}' = -\gamma^{-1}\int d\mathbf{\alpha}'\cdot(\tilde{\mathbf{M}}' + \mathbf{S}'\mathbf{v}/c^2)\cdot\tilde{\mathbf{L}} = -\int d\mathbf{\alpha}\cdot(\tilde{\mathbf{M}} - \mathbf{v}\mathbf{N}), \quad (47)$$

where we used (43)-(46), and finally (20). Thus the force on the scatterer depends on both the momentum flux tensor and the momentum density vector. Similarly, the corresponding absorbed power is

$$P_A = \int Qd\mathcal{V} = \gamma^{-2}\int Q'd\mathcal{V}' = -\gamma^{-2}\int\mathbf{S}'\cdot d\mathbf{\alpha}' = -\int d\mathbf{\alpha}\cdot[\mathbf{S} - \mathbf{v}W - (\tilde{\mathbf{M}} - \mathbf{v}\mathbf{N})\cdot\mathbf{v}], \quad (48)$$

where the final form follows from (16). Since the mechanical power that the field spends on the moving scatterer is

$$P_M = \mathbf{v}\cdot\mathbf{F} = \int\mathbf{v}\cdot\mathbf{f}\,d\mathcal{V} = -\int d\mathbf{\alpha}\cdot(\tilde{\mathbf{M}} - \mathbf{v}\mathbf{N})\cdot\mathbf{v}, \quad (49)$$

the total power imparted to the scattering body

$$P_B = P_A + P_M = \int(Q + \mathbf{v}\cdot\mathbf{f})d\mathcal{V} = \int(Q' + \mathbf{v}\cdot\mathbf{f}')d\mathcal{V} = -\int(\mathbf{S}' + \mathbf{v}\cdot\tilde{\mathbf{M}})\cdot d\mathbf{\alpha}' = -\int(\mathbf{S} - \mathbf{v}W)\cdot d\mathbf{\alpha} \quad (50)$$

depends only on the energy flux and energy density.

Rewriting the last form of (47) as an integral over $\mathcal{V}$,

$$\mathbf{F} = \int\mathbf{f}d\mathcal{V} = -\int\nabla\cdot(\tilde{\mathbf{M}} - \mathbf{v}\mathbf{N})d\mathcal{V}, \quad (51)$$

we have, within $\mathcal{V}$,

$$-\mathbf{f} = \nabla\cdot\tilde{\mathbf{M}} - \nabla\cdot\mathbf{v}\mathbf{N} = \nabla\cdot\tilde{\mathbf{M}} + \partial_t\mathbf{N}, \quad (52)$$

where $\nabla\cdot\mathbf{v}\mathbf{N} = \mathbf{v}\cdot\nabla\mathbf{N} = -\partial_t\mathbf{N}$ follows from $\gamma(\mathbf{v}\cdot\nabla + \partial_t)\mathbf{N} = \partial_{t'}\mathbf{N} = 0$. Outside the scatterer's volume,

$$\nabla\cdot(\tilde{\mathbf{M}} - \mathbf{v}\mathbf{N}) = 0. \tag{53}$$

Similarly, from (50) in the form

$$P_B = \int (Q + \mathbf{v}\cdot\mathbf{f})d\mathcal{V} = -\int \nabla\cdot(\mathbf{S} - \mathbf{v}W)d\mathcal{V}, \tag{54}$$

within $\mathcal{V}$,

$$-Q - \mathbf{v}\cdot\mathbf{f} = \nabla\cdot\mathbf{S} - \nabla\cdot\mathbf{v}W = \nabla\cdot\mathbf{S} + \partial_t W \tag{55}$$

and outside $\mathcal{V}$,

$$\nabla\cdot(\mathbf{S} - \mathbf{v}W) = 0. \tag{56}$$

The forms of (52) and (55) in $-\mathbf{v}\cdot\nabla = \partial_t$, the usual ones[8] for the $\mathbf{r}, t$-dependent problem in Σ, may be taken as the starting ones for the development.

We determine $\mathbf{F}$ and P_B initially by two procedures based on the results obtained in Σ'. Then we consider W, $\mathbf{S}$ and $\tilde{\mathbf{M}}$ in Σ and discuss derivations based on evaluating the Σ integrals in (47) and (50).

The most direct procedure for determining $\mathbf{F}$ and P_B etc., and the corresponding cross sections $\boldsymbol{\sigma} = \mathbf{F}/W_0$, $\sigma_B = P_B/S_0$, etc., is to compare the $\mathcal{V}'$ integrals of (47) and (50) with those in (43) and (44). Thus,

$$\mathbf{F} = \tilde{\mathbf{L}}\cdot(\mathbf{F}' + \mathbf{v}P'_A/c^2)/\gamma = \tilde{\mathbf{L}}\cdot\mathbf{F}'/\gamma + \mathbf{v}P'_A/c^2 = W_0\boldsymbol{\sigma}, \tag{57}$$

$$P_A = P'_A/\gamma^2 = S_0\sigma_A, \tag{58}$$

$$P_M = \mathbf{v}\cdot\mathbf{F} = \mathbf{v}\cdot\mathbf{F}' + \beta^2 P'_A = S_0\sigma_M, \tag{59}$$

$$P_B = P_A + P_M = P'_A + \mathbf{v}\cdot\mathbf{F}' = S_0\sigma_B. \tag{60}$$

The last form (60) is the simplest to interpret. In Σ, the power P_B imparted to the moving scatterer is the electromagnetic power P'_A it absorbs in its rest system plus the work done on it by the rest system electromagnetic force $\mathbf{F}'$. However, the power P_A of (58) absorbed in Σ is the relativistic transformation of the power P'_A absorbed in Σ'. The first form (57) says that the force $\mathbf{F}$ that acts on the scatterer in Σ consists of the distorted rest system electromagnetic force $\mathbf{F}'$ plus a force arising from motion and the inertial effect (P'_A/c^2) of the absorbed energy; both forces contribute to the work done on the scatterer in Σ, i.e., to P_M of (59). If $P'_A = 0$, the scatterer is lossless; the results simplify to $\mathbf{F} = \tilde{\mathbf{L}}\cdot\mathbf{F}'/\gamma$, and $P_B = P_M = \mathbf{v}\cdot\mathbf{F}' = \mathbf{v}\cdot\mathbf{F}$.

We construct the cross sections in Σ by substitution. The simplest form is (58). Substituting from (31)–(33), we obtain

$$P_A = S_0\sigma_A = S'_0\sigma'_A/\gamma^2,$$
$$\sigma_A = (1-\beta\cos\alpha)^2\sigma'_A = (1-\beta\cos\alpha)^2(\sigma'_T - \sigma'_S). \tag{61}$$

Next we consider (57) in terms of (41) and (33),

$$\begin{aligned}\mathbf{F} = W_0\boldsymbol{\sigma} &= W'_0\tilde{\mathbf{L}}\cdot(\boldsymbol{\sigma}' + \hat{\mathbf{v}}\beta\sigma'_A)/\gamma \\ &= W'_0\tilde{\mathbf{L}}\cdot[\sigma'_T(\hat{\mathbf{k}}' + \beta\hat{\mathbf{v}}) - \sigma'_S\langle\hat{\mathbf{r}}' + \beta\hat{\mathbf{v}}\rangle] \\ &= W'_0[\sigma'_T\hat{\mathbf{k}}/p' - \sigma'_S\langle\hat{\mathbf{R}}p_s\rangle]/\gamma \\ &= W_0 p'^2[\sigma'_T\hat{\mathbf{k}}(1+\beta\cos\alpha') - \sigma'_S\langle\hat{\mathbf{R}}(1+\beta\cos\theta')\rangle],\end{aligned}$$

$$\begin{aligned}\boldsymbol{\sigma} &= p'^2\sigma'_T\hat{\mathbf{k}}(1+\beta\cos\alpha') - p'^2\sigma'_S\langle\hat{\mathbf{R}}(1+\beta\cos\theta')\rangle \\ &= \sigma'_T(1-\beta\cos\alpha)\hat{\mathbf{k}} - p'^2\sigma'_S\langle\hat{\mathbf{R}}(1+\beta\cos\theta')\rangle,\end{aligned} \tag{62}$$

where $\hat{\mathbf{R}}(1+\beta\cos\theta') = \tilde{\mathbf{L}}\cdot(\hat{\mathbf{r}}' + \beta\hat{\mathbf{v}})/\gamma = \hat{\mathbf{v}}(\cos\theta' + \beta) + \hat{\boldsymbol{\rho}}(\sin\theta')/\gamma$ with $\hat{\boldsymbol{\rho}} = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi$. We obtain (59) from (62):

$$P_M = S_0\sigma_M = \mathbf{v}\cdot\mathbf{F} = S_0\beta\hat{\mathbf{v}}\cdot\boldsymbol{\sigma}$$
$$\begin{aligned}\sigma_M &= \beta p'^2\sigma'_T(\beta + \cos\alpha') - \beta p'^2\sigma'_S\langle\beta + \cos\theta'\rangle \\ &= \beta\sigma'_T(1-\beta\cos\alpha)\cos\alpha - \beta p'^2\sigma'_S\langle\beta + \cos\theta'\rangle.\end{aligned} \tag{63}$$

Finally from (61) and (63), or more directly from (31) and (41), we express (60) as

$$P_B = S_0\sigma_B = S_0(\sigma_A + \sigma_M) = S_0 p'^2(\sigma'_A + \beta\hat{\mathbf{v}}\cdot\boldsymbol{\sigma}'),$$
$$\begin{aligned}\sigma_B &= p'^2\sigma'_T(1+\beta\cos\alpha') - p'^2\sigma'_S\langle 1+\beta\cos\theta'\rangle \\ &= \sigma'_T(1-\beta\cos\alpha) - p'^2\sigma'_S\langle 1+\beta\cos\theta'\rangle.\end{aligned} \tag{64}$$

If the scatterer is lossless, then $\sigma_B = \sigma_M = p'^2\beta\sigma'_S\langle\cos\alpha' - \cos\theta'\rangle$; see Restrick[13] and Censor[14] for different developments.

From (33) and (41), we have

$$\sigma'_A = \sigma'_T - \sigma'_S, \quad \boldsymbol{\sigma}' = \sigma'_T\hat{\mathbf{k}}' - \sigma'_S\langle\hat{\mathbf{r}}'\rangle, \tag{65}$$

and we see that (64) and (63) are similarly related. By comparison, we identify the total cross section in Σ as

$$\sigma_T = p'^2\sigma'_T(1+\beta\cos\alpha') = \sigma'_T(1-\beta\cos\alpha), \tag{66}$$

and the reradiation cross section as

$$\begin{aligned}\sigma_R &= p'^2\sigma'_S\langle 1+\beta\cos\theta'\rangle \\ &= p'^2 b\mathfrak{M}[|\mathbf{g}(\hat{\mathbf{r}}')|^2(1+\beta\cos\theta')] \\ &= k^{-2}\int|\mathbf{g}(\hat{\mathbf{r}}')|^2(1+\beta\cos\theta')d\Omega(\hat{\mathbf{r}}'),\end{aligned} \tag{67}$$

and introduce

$$\begin{aligned}\langle\langle\hat{\mathbf{R}}\rangle\rangle &= \mathfrak{M}[|\mathbf{g}|^2\hat{\mathbf{R}}(1+\beta\cos\theta')]/\mathfrak{M}[|\mathbf{g}|^2(1+\beta\cos\theta')] \\ &= b\mathfrak{M}[|\mathbf{g}|^2\hat{\mathbf{R}}(1+\beta\cos\theta')]/\sigma_R\end{aligned} \tag{68}$$

to exhibit the same structure as (65):

$$\sigma_B = \sigma_T - \sigma_R, \quad \boldsymbol{\sigma} = \sigma_T\hat{\mathbf{k}} - \sigma_R\langle\langle\hat{\mathbf{R}}\rangle\rangle. \tag{69}$$

Soon we derive the components directly.

We make the interference effects explicit by using (33) in terms of (6):

$$\sigma'_T = -b\,\mathrm{Re}\,\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}') = -b\,\mathrm{Re}\,\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}}). \tag{70}$$

Thus, although we are simply substituting Σ' results, the interference of $\boldsymbol{\Phi}$ and $\mathbf{U}$ in Σ is shown by the last form. In particular,

$$\sigma_B + \sigma_R = \sigma_T = \sigma'_T(1-\beta\cos\alpha)$$
$$= -(1-\beta\cos\alpha)b\ \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}}),$$
$$P_B + P_R = P_T = -P_I. \tag{71}$$

Essentially as for (33) in Σ', in Σ the function P_T is the total power derived from the incident wave $\mathbf{\Phi}$ by interference with the scattered wave $\mathbf{U}$ and either spent (as absorbed or mechanical power) or reradiated by the obstacle. Similarly, we rewrite (62) in the form (41) as

$$\sigma + \sigma_R\langle\!\langle\hat{\mathbf{R}}\rangle\!\rangle = \sigma_T\hat{\mathbf{k}} = \sigma'_T(1-\beta\cos\alpha)\hat{\mathbf{k}}$$
$$= -(1-\beta\cos\alpha)b\ \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}})\hat{\mathbf{k}},$$
$$\mathbf{F} + \mathbf{F}_R = \mathbf{F}_T = -\mathbf{F}_I \tag{72}$$

and interpret the result essentially as for (41). From (7), the factor $1-\beta\cos\alpha$ in (72) equals T/T_S, the ratio of the incident and dilated periods.

Now we rederive our results by using the surface integrals in Σ'. This enables us to evaluate the reradiated and interference terms separately, and gives directly the decompositions of (71) and (72).

Since $\nabla'\cdot\mathbf{S}' = 0$ and $\nabla'\cdot\tilde{\mathbf{M}}' = 0$ in V', we also have $\nabla'\cdot(\mathbf{S}' + \mathbf{v}\cdot\tilde{\mathbf{M}}') = 0$ in V', and may therefore replace the $\mathcal{A}'$-surface integral for P_B in (50) by one over any surface A' inclosing the scatterer. Proceeding essentially as for (31)-(33), we write

$$P_B = -\int(\mathbf{S}' + \mathbf{v}\cdot\tilde{\mathbf{M}}')\cdot d\mathbf{A}'$$
$$= -P_I - P_R = P_T - P_R. \tag{73}$$

For P_R, we use $\mathbf{S}'_S$ of (25) and $\tilde{\mathbf{M}}'_S$ of (35) and proceed as for (26); thus

$$P_R = \int(\mathbf{S}'_S + \mathbf{v}\cdot\tilde{\mathbf{M}}'_S)\cdot d\mathbf{A}'$$
$$= S'_0\sigma'_S\langle 1+\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{r}}'\rangle = S_0\sigma_R, \tag{74}$$

with σ_R as in (67). Similarly, from $\mathbf{S}'_I$ of (30) and $\tilde{\mathbf{M}}'_I$ of (36),

$$P_I = \int(\mathbf{S}'_I + \mathbf{v}\cdot\tilde{\mathbf{M}}'_I)\cdot d\mathbf{A}' = S'_0 b(1+\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}}')\ \mathrm{Re}\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')$$
$$= S_0(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}})b\ \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}}), \tag{75}$$

$$P_T = -P_I = S'_0(1+\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}}')\sigma'_T$$
$$= S_0(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}})\sigma'_T = S_0\sigma_T. \tag{76}$$

We follow essentially the same procedure for the force functions in terms of the Σ'-surface integral in (47). Since $\nabla'\cdot(\tilde{\mathbf{M}}' + \mathbf{S}'\mathbf{v}/c^2) = 0$, we proceed essentially as for (39)-(41). Thus

$$\mathbf{F} = -\gamma^{-1}\int d\mathbf{A}'\cdot(\tilde{\mathbf{M}}' + \mathbf{S}'\mathbf{v}/c^2)\cdot\tilde{\mathbf{L}}$$
$$= -\mathbf{F}_I - \mathbf{F}_R = \mathbf{F}_T - \mathbf{F}_R. \tag{77}$$

From (25) and (35),

$$\mathbf{F}_R = \gamma^{-1}\tilde{\mathbf{L}}\cdot\int(\tilde{\mathbf{M}}'_S + \mathbf{v}\mathbf{S}'_S/c^2)\cdot d\mathbf{A}'$$
$$= W'_0\sigma'_S\langle\hat{\mathbf{r}}' + \beta\hat{\mathbf{v}}\rangle\cdot\tilde{\mathbf{L}}/\gamma$$
$$= W_0 p'^2\sigma'_S\langle\hat{\mathbf{R}}(1+\beta\cos\theta')\rangle = W_0\sigma_R\langle\!\langle\hat{\mathbf{R}}\rangle\!\rangle, \tag{78}$$

and from (30) and (36)

$$\mathbf{F}_I = \gamma^{-1}\mathbf{L}\cdot\int(\tilde{\mathbf{M}}'_I + \mathbf{v}\mathbf{S}'_I/c^2)\cdot d\mathbf{A}'$$
$$= W'_0 b\ \mathrm{Re}\hat{\mathbf{p}}'\cdot\mathbf{g}(\hat{\mathbf{k}}')(\hat{\mathbf{k}}' + \beta\hat{\mathbf{v}})/\gamma$$
$$= W_0(1-\beta\cos\alpha)b\ \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}})\hat{\mathbf{k}}, \tag{79}$$

$$\mathbf{F}_T = -\mathbf{F}_I = W_0(1-\beta\cos\alpha)\sigma'_T\hat{\mathbf{k}} = W_0\sigma_T\hat{\mathbf{k}}. \tag{80}$$

Now we rederive our results by working with the quadratic functions in Σ, i.e., by using the $\mathcal{A}$-surface integrals in (47) and (50). This exhibits the physical content that the Σ' procedures have left implicit.

In Σ, with $\mathbf{\Psi} = \mathbf{\Phi} + \mathbf{U} = \mathbf{E}_0 + \mathbf{E}_S = \mathbf{E}$, etc., in terms of (1) and (4), we have the analogs of (21)-(23):

$$W_0 = \tfrac{1}{4}\epsilon_0(|\mathbf{\Phi}|^2 + |\mathbf{\Phi}_M|^2) = \tfrac{1}{2}\epsilon_0, \tag{81}$$

$$W_S \sim W_0|\mathbf{G}(\hat{\mathbf{R}})|^2|D|^2 = W_0|p'p_S\mathbf{g}(\hat{\mathbf{r}}')|^2|D|^2 = W_{Sa},$$
$$D = 1/ik'r' = p_S/p'ikR, \tag{82}$$

$$W_I \sim W_0\ \mathrm{Re}\,\{e^{ikR-i\mathbf{k}\cdot\mathbf{R}}[\hat{\mathbf{p}}\cdot\mathbf{G} + (\hat{\mathbf{k}}\times\hat{\mathbf{p}})\cdot(\hat{\mathbf{R}}\times\mathbf{G})]D\} = W_{Ia} \tag{83}$$

where $W_{Sa} = p_S^2 W'_{Sa}$. We use $\mathbf{\Phi}^*$ as given in (8) to cancel $e^{i\nu_S}$ of $\mathbf{U}$ in W_{Ia}; the result is the full analog of (23) in terms of the corresponding Σ quantities. In particular, at $\hat{\mathbf{R}} = \hat{\mathbf{k}}, -\hat{\mathbf{k}}$ we get $W_{Ia} = 2W_0\ \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}})D, 0$; the first value differs from the corresponding ($\hat{\mathbf{r}}' = \hat{\mathbf{k}}'$) result for (23) in containing W_0 instead of $W'_0 = W_0 p'^2$, and in that we now work with $D = 1/ikRp'^2$. Similarly the analogs of (24), (25), and (30) are

$$\mathbf{S}_0 = c^2\mathbf{N}_0 = \tfrac{1}{2}\epsilon_0 c\hat{\mathbf{k}} = S_0\hat{\mathbf{k}}, \tag{84}$$

$$\mathbf{S}_S = c^2\mathbf{N}_S \sim S_0|\mathbf{G}|^2|D|^2\hat{\mathbf{R}}$$
$$= S_0|p'p_S\mathbf{g}|^2|D|^2\hat{\mathbf{R}} = \mathbf{S}_{Sa}, \tag{85}$$

$$\mathbf{S}_T = c^2\mathbf{N}_I \sim S_0\ \mathrm{Re}\{e^{ikR-i\mathbf{k}\cdot\mathbf{R}}[\hat{\mathbf{p}}\times(\hat{\mathbf{R}}\times\mathbf{G})$$
$$+\mathbf{G}\times(\hat{\mathbf{k}}\times\hat{\mathbf{p}})]D\} = \mathbf{S}_{Ia} \tag{86}$$

where $\mathbf{S}_{Sa} = p_S^2\mathbf{S}'_{Sa}$. If $\hat{\mathbf{R}} = \hat{\mathbf{k}}, -\hat{\mathbf{k}}$ then $\mathbf{S}_{Ia} = 2S_0\ \mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}})\hat{\mathbf{k}}D, 0$. The first differs from the corresponding ($\hat{\mathbf{r}}' = \hat{\mathbf{k}}'$) result for (30) in containing $S_0\hat{\mathbf{k}}$ instead of $S'_0\hat{\mathbf{k}}'$. Finally, the analogs of (34)-(36), are

$$\tilde{\mathbf{M}}_0 = \tfrac{1}{2}\epsilon_0\hat{\mathbf{k}}\hat{\mathbf{k}} = W_0\hat{\mathbf{k}}\hat{\mathbf{k}}, \tag{87}$$

$$\tilde{\mathbf{M}}_S \sim W_0|\mathbf{G}|^2|D|^2\hat{\mathbf{R}}\hat{\mathbf{R}} = \mathbf{S}_{Sa}\hat{\mathbf{R}}/c, \tag{88}$$

$$\tilde{\mathbf{M}}_I\cdot\hat{\mathbf{k}} \sim \tilde{\mathbf{M}}_I\cdot\hat{\mathbf{R}} \sim \mathbf{S}_{Ia}/c. \tag{89}$$

The original procedure (31)-(33) for P'_A in Σ' was based on $\nabla'\cdot\mathbf{S}' = 0$ in V'. We can parallel this procedure in Σ for P_B of (50), since by (56), $\nabla\cdot(\mathbf{S}-\mathbf{v}W)=0$ in V. Thus, the analog of the sequence (31)–(33) is

$$P_B = -\int(\mathbf{S}-\mathbf{v}W)\cdot d\mathbf{\alpha} = -\int(\mathbf{S}-\mathbf{v}W)\cdot d\mathbf{A} = -P_I - P_R = P_T - P_R, \quad (90)$$

with corresponding cross sections given by P/S_0. In particular, in terms of W_S of (82) and $\mathbf{S}_S$ of (85),

$$P_R = \int(\mathbf{S}_S-\mathbf{v}W_S)\cdot d\mathbf{\alpha} = \int(\mathbf{S}_S-\mathbf{v}W_S)\cdot d\mathbf{A} = S_0\int\frac{p_s^2|\mathbf{g}(\hat{\mathbf{r}}')|^2}{k^2\gamma'^2}(\hat{\mathbf{R}}-\beta\hat{\mathbf{v}})\cdot d\mathbf{A}, \quad (91)$$

where A is any distant closed surface around the scatterer. If we take A as A_∞ in $\mathbf{R}$, then since $d\Omega(\hat{\mathbf{R}}) = d\Omega(\hat{\mathbf{r}}')(\partial_\theta \cos\Theta)/\partial_{\theta'} \cos\theta' = d\Omega(\hat{\mathbf{r}}')/p_s^2$, and $R=r'p_s$, we have $d\mathbf{A}=\mathbf{R}R^2d\Omega(\mathbf{R}) = \hat{\mathbf{R}}r'^2d\Omega(\hat{\mathbf{r}}')$; thus,

$$P_R = (S_0/k^2)\int|\mathbf{g}|^2p_s^2(\hat{\mathbf{R}}-\beta\hat{\mathbf{v}})\cdot\hat{\mathbf{R}}d\Omega(\hat{\mathbf{r}}') = (S_0/k^2)\int|\mathbf{g}|^2p_s^2(1-\beta\cos\Theta)d\Omega(\hat{\mathbf{r}}') = S_0\sigma_R$$

which, since $p_s^2(1-\beta\cos\Theta) = p_s/\gamma = (1+\beta\cos\theta')$ is the result given before in (67) and (74). The same result follows if we take A as A_∞ in $\mathbf{r}_s$ and use $d\Omega(\hat{\mathbf{r}}_s) = d\Omega(\hat{\mathbf{r}}')(\partial_\theta \cos\theta_S)/\partial_{\theta'}\cos\theta' = d\Omega(\hat{\mathbf{r}}')/\gamma q^3$ and $r_s = r'q$ as in (5) to obtain $d\mathbf{A} = \hat{\mathbf{r}}_s r_s^2 d\Omega(\hat{\mathbf{r}}_s) = \hat{\mathbf{r}}_s r'^2 d\Omega(\mathbf{r}')/\gamma q$; substituting into (91), and noting that $\hat{\mathbf{R}}-\beta\hat{\mathbf{v}} = \hat{\mathbf{r}}_s q/p_S$, we again obtain (74). Most simply, we use $p_s(\hat{\mathbf{R}}-\beta\hat{\mathbf{v}}) = \hat{\mathbf{r}}'\cdot\tilde{\mathbf{L}}^{-1}$ of (5) to write $p_s^2(\hat{\mathbf{R}}-\beta\hat{\mathbf{v}}) = \gamma(1+\beta\cos\theta')\hat{\mathbf{r}}'\cdot\tilde{\mathbf{L}}^{-1}$ in (91); taking $\gamma\tilde{\mathbf{L}}^{-1}\cdot d\mathbf{A} = d\mathbf{A}'$ with A' as A'_∞ gives (74).

In general, T_s is small enough for the implicit slow t-variation of W_{Sa} and $\mathbf{S}_{Sa}$ in $\mathbf{r}, t$ to be neglecneglected for practical purposes. We may identify

$$\Delta P_{Ra} = (S_0/k^2)\int_{\Delta_S}|\mathbf{g}(\hat{\mathbf{r}}')|^2(1+\beta\cos\theta')d\Omega(\hat{\mathbf{r}}'), \quad \Delta_s = \Delta\Omega(\hat{\mathbf{r}}_s), \quad (92)$$

with the flux through the directed aperture $\Delta\mathbf{A}(\mathbf{r}_S)$ of a fixed receiver in Σ pointing at the scatterer's present position $\mathbf{v}t$. If we replace Δ_S by $\Delta = \Delta\Omega(\hat{\mathbf{R}})$, the form corresponds to the flux through the directed aperture $\Delta\mathbf{A}(\hat{\mathbf{R}})$ pointing at the scatterer's retarded position $\hat{\mathbf{v}}(vt-\beta R) = \mathbf{v}t_0$. The corresponding differential cross sections are

$$d\sigma_R(\hat{\mathbf{R}})/d\Omega(\hat{\mathbf{R}}) = p_s^3|\mathbf{g}|^2/k^2\gamma$$
$$d\sigma_R(\hat{\mathbf{r}}_s)/d\Omega(\hat{\mathbf{r}}_s) = p_s q^3|\mathbf{g}|^2/k^2. \quad (93)$$

The distant Poynting flux through $\Delta\mathbf{A}(\hat{\mathbf{R}})$ is

$$\Delta P_{Sa} = (S_0/k^2)\int_\Delta p_s^2|\mathbf{g}(\hat{\mathbf{r}}')|^2 d\Omega(\hat{\mathbf{r}}') = (S_0/k^2)\gamma^2\int_\Delta(1+\beta\cos\theta')^2|\mathbf{g}(\hat{\mathbf{r}}')|^2d\Omega(\hat{\mathbf{r}}'),$$
$$d\sigma_s(\hat{\mathbf{R}})/d\Omega(\hat{\mathbf{R}}) = p_s^4|\mathbf{g}|^2/k^2 \quad (94)$$

but since $\nabla\cdot\mathbf{S}_S\neq 0$, in general, (94) is not a fundamental differential flux measure in Σ, e.g., if we use $\Delta\mathbf{A}(\hat{\mathbf{r}}_s)$, the integrand becomes $p_s^2|\mathbf{g}|^2\mathbf{R}\cdot\hat{\mathbf{r}}_s/\gamma q = |\mathbf{g}|^2(p_s/\gamma q)^2 = |\mathbf{g}|^2(1+\beta\cos\theta')/(1-\beta\cos\theta')$ with corresponding $d\sigma_s(\hat{\mathbf{r}}_s)/d\Omega(\hat{\mathbf{r}}_s) = p_s^2q|\mathbf{g}|^2/k^2\gamma$. Sommerfeld[4] converts the differential form in (94) to the first form in (93) for the case of a radiating accelerated electron by introducing $\partial t/\partial t_0 = 1-\beta\cos\Theta$, i.e., he replaces $\hat{\mathbf{R}}\cdot\mathbf{S}_{Sa}$ by $\hat{\mathbf{R}}\cdot\mathbf{S}_{Sa}\partial t/\partial t_0 = \hat{\mathbf{R}}\cdot\mathbf{S}_{Sa}(1-\beta\cos\Theta) = S_{Sa}\hat{\mathbf{R}}\cdot(\hat{\mathbf{R}}-\beta\hat{\mathbf{v}})$, which equals $(\mathbf{S}_{Sa}-\mathbf{v}W_{Sa})\cdot\hat{\mathbf{R}}$. However, since $\nabla\cdot(\mathbf{S}_S-\mathbf{v}W_S)=0$ in V, we would use the second form in (91), i.e., $\int(\mathbf{S}_S-\mathbf{v}W_S)\cdot d\mathbf{A}$ for all distances. This indicates directly that (93) is the fundamental differential reradiated flux measure in Σ.

For the interference term, from W_I of (78) and $\mathbf{S}_I$ of (86), we obtain

$$\begin{aligned}P_I &= \int(\mathbf{S}_I-\mathbf{v}W_I)\cdot d\mathbf{A}\\ &= S_0\,\mathrm{Re}\int De^{ikR-i\mathbf{k}\cdot\mathbf{R}}\{[\hat{p}\times(\hat{\mathbf{R}}\times\mathbf{G}) + \mathbf{G}\times(\hat{\mathbf{k}}\times\hat{\mathbf{p}})]\\ &\quad - \hat{\mathbf{v}}\beta[\hat{\mathbf{p}}\cdot\mathbf{G} + (\hat{\mathbf{k}}\times\hat{\mathbf{p}})\cdot(\hat{\mathbf{R}}\times\mathbf{G})]\}\cdot d\mathbf{A}(\hat{\mathbf{R}})\\ &= S_0 b[\mathrm{Re}\;\hat{\mathbf{p}}\cdot\mathrm{G}(\hat{\mathbf{k}})\hat{\mathbf{k}} - \hat{\mathbf{v}}\beta\;\mathrm{Re}\;\hat{\mathbf{p}}\cdot\mathrm{G}(\hat{\mathbf{k}})]\cdot\mathbf{k}\\ &= S_0 b\;\mathrm{Re}\;\hat{\mathbf{p}}\cdot\mathrm{G}(\hat{\mathbf{k}})(1-\beta\hat{\mathbf{v}}\cdot\hat{\mathbf{k}})\end{aligned} \quad (95)$$

which, since $\hat{\mathbf{p}}\cdot G(\hat{\mathbf{k}}) = \hat{\mathbf{p}}'\cdot g(\hat{\mathbf{k}}')$ is the same as in (71) and (75).

The same development carries over for the force. Thus the original procedure (39)-(41) for $\mathbf{F}'$ in Σ', based on $\nabla'\cdot\mathbf{M}'=0$ in V', applies in Σ to $\mathbf{F}$ of (47), since by (53), $\nabla\cdot(\tilde{\mathbf{M}}-\mathbf{vN})=0$ in V. Thus,

$$\mathbf{F} = -\int(\tilde{\mathbf{M}}-\mathbf{Nv})\cdot d\mathbf{\alpha} = W_0\sigma = -\mathbf{F}_I - \mathbf{F}_R = \mathbf{F}_T - \mathbf{F}_R \quad (96)$$

with corresponding cross sections given by $\mathbf{F}/W_0$. In terms of $\tilde{\mathbf{M}}_S$ of (88) and $\mathbf{N}_S$ of (85)

$$\mathbf{F}_R = \int(\tilde{\mathbf{M}}_S-\mathbf{N}_S\mathbf{v})\cdot d\mathbf{\alpha} = \int(\tilde{\mathbf{M}}_S-\mathbf{N}_S\mathbf{v})\cdot d\mathbf{A} = W_0\int\frac{p_s^2|g(\hat{\mathbf{r}}')|^2}{k^2\gamma'^2}(\hat{\mathbf{R}}\hat{\mathbf{R}}-\beta\hat{\mathbf{R}}\hat{\mathbf{v}})\cdot d\mathbf{A} \quad (97)$$

and proceeding as for (92) we obtain

$$\begin{aligned}\mathbf{F}_R &= (W_0/k^2)\int|\mathbf{g}|^2p_s^2\hat{\mathbf{R}}(\hat{\mathbf{R}}-\beta\hat{\mathbf{v}})\cdot\hat{\mathbf{R}}d\Omega(\hat{\mathbf{r}}')\\ &= (W_0/k^2)\int|\mathbf{g}|^2p_s^2\hat{\mathbf{R}}(1-\beta\cos\Theta)d\Omega(\hat{\mathbf{r}}')\\ &= W_0\sigma_R\langle\!\langle\hat{\mathbf{R}}\rangle\!\rangle\end{aligned} \quad (98)$$

as in (69) and (78). Similarly, in terms of (89) and (86),

$$\begin{aligned}\mathbf{F}_I &= \int(\tilde{\mathbf{M}}_I-\mathbf{N}_I\mathbf{v})\cdot d\mathbf{A}\\ &= \mathrm{Re}\int De^{ikR-i\mathbf{k}\cdot\mathbf{R}}[\mathbf{S}_{Ia}\hat{\mathbf{R}} - \beta\mathbf{S}_{Ia}\hat{\mathbf{v}}]\cdot d\mathbf{A}(\hat{\mathbf{R}})/c\\ &= W_0 b\hat{\mathbf{k}}\;\mathrm{Re}\hat{\mathbf{p}}\cdot\mathbf{G}(\hat{\mathbf{k}})(\hat{\mathbf{k}}-\beta\hat{\mathbf{v}})\cdot\hat{\mathbf{k}}\\ &= W_0 b(1-\beta\cos\alpha)\;\mathrm{Re}\hat{\mathbf{p}}\cdot G(\hat{\mathbf{k}})\hat{\mathbf{k}}\end{aligned} \quad (99)$$

as in (72) and (79).

The present results also apply to arbitrary cylinders and slabs in terms of the representations for the fields given in the earlier paper[1] (which includes ΔP_R and ΔP_S for the three sets of scatterers) with $\mathfrak{M}$ equal to $(1/2\pi)\int d\theta'$ for the cylinder, and to the mean of the forward space and back space values for the slab. For the cylinder, we use $D_2 = (2/\pi k'r')^{1/2} e^{-i\pi/4}$, $b_2 = 4/k'$; and for the slab $D_1 = 1, b_1 = 2$. Although U for the cylinder is not periodic in R, t, its complete asymptotic expansion has period T_s, so that the essentials of the present development carry over.

---

* This work was supported in part by National Science Foundation Grants NSF-GP-8734 and 21052.

1 V. Twersky, Relativistic Scattering of Electromagnetic Waves by Moving Obstacles, J. Math. Phys, 12, 2328 (1971).
2 A. Einstein, Ann. Phys. (paris) 17, 891 (1905).
3 W. Pauli, *Theory of Relativity* (Pergamon, New York, 1958).
4 A. Sommerfeld, *Electrodynamics* (Academic, New York, 1952).
5 M. Laue, *Das Relativitätsprinzip* (Friedr, Vieweg und Sohn, Braunschweig, 1911), p. 79.
6 L. Silberstein, *The Theory of Relativity* (Macmillan, London, 1924), p. 237.
7 P. Penfield, Jr. and H. A. Haus, *Electrodynamics of Moving Media* (MIT Press, Mass., 1967).
8 J. A. Stratton, Electromagnetic Theory (McGraw-Hill, New York, 1941).
9 D. S. Saxon, Phys. Rev. 100, 1771 (1955).
10 V. Twersky, J. Math. Phys. 8, 589 (1967); see Report EDL-L30 (1965), Mountain View, Calif., for additional results.
11 P. Debye, Ann. Physik 30, 57 (1909).
12 H. C. van de Hulst, *Light Scattering by Small Particles* (Wiley, New York, 1957), p.13.
13 R. C. Restrick, Radio Science 3, 1144 (1968).
14 D. Censor, Tel-Aviv U, Report No. ES 70-005, Ramat-Aviv, Israel, 1969 [Radio Sci., (to be published)]. This work also discusses measurement procedures and alternative developments.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

The Phase Shift. I. As a Bounded Functional

William M. Frank
U.S. Naval Ordnance Laboratory, White Oak Silver Spring, Maryland 20910
(Received 16 March 1971)

Classes of potentials are defined by the finiteness of certain norms. For potentials in any of these classes, the phase shift for any partial wave is shown to possess a norm-dependent bound as a function of energy. Two norms are adduced in which the phase shift is uniformly bounded for all energies. A number of theorems are proven concerning the high-energy behavior of the phase shifts corresponding to potentials in these classes.

I. INTRODUCTION

The present and the following two papers will investigate the "scattering functions" of potential theory, *viz.* the partial wave phase shift $\delta_l(k)$ at a fixed energy k^2 ($\hbar = 2m = 1$ units are used throughout) and the S-wave scattering length A as (nonlinear) functionals of a spherically symmetric potential $V(r)$. The over-all questions raised in these papers deal with the boundedness and continuity of the partial wave phase shift as they depend on the potential function $V(r)$. These considerations are of interest in view of a number of paradoxes[1] noted in the literature calling for a clarification of these fundamental questions. These investigations also bring to light an interesting topological structure governing the dependence of scattering functions on potentials. In particular they point to a Banach space of potentials (see following papers) in which the scattering functions are continuous and bounded functionals. Such a structure may serve as a useful theoretical tool. A number of inequalities, some of which may be new, are arrived at in the course of this investigation which are likely useful in other contexts.

The present paper will establish a lemma which shows how the scattering functions have absolute bounds related to certain norms of the potential functions. While phase shifts are always subject to a mod-π ambiguity, we adhere to the convention that they be continuous in k and vanish at all energies for zero coupling. The bounds established in these papers apply to the phase shifts defined by this convention. They are of interest for the purposes of analysis as will be seen in the following articles. Some results on the high-energy limit of the phase shifts are presented in a theorem. In the following articles, it is shown how these norms, when bounded, serve as moduli of continuity for the dependence of the phase shift on the potential. In a subsequent paper, continuity is investigated when the potentials are of unbounded norm as in the case of repulsive singular potentials. All theorems and proofs will be explicitly presented for the $l = 0$ case. The considerations in the case of other partial waves are almost identical, and the necessary modifications are presented in Appendix A.

II. SPACES OF POTENTIALS

We deal in the present papers with potentials which are spherically symmetric and which are L^1 over any closed finite subinterval of $[0, \infty)$ which excludes the origin. We thus do allow for singular behavior at $r = 0$. One might allow for non-L^1 singularities at finite nonvanishing r, but they are not of sufficient interest though certain aspects are touched upon in an accompanying paper. The potentials are assumed to be point functions as distinguished from distributions, though such generafor the fields given in the earlier paper[1] (which includes ΔP_R and ΔP_S for the three sets of scatterers) with $\mathfrak{M}$ equal to $(1/2\pi) \int d\theta'$ for the cylinder, and to the mean of the forward space and back space values for the slab. For the cylinder, we use $D_2 = (2/\pi k'r')^{1/2} e^{-i\pi/4}$, $b_2 = 4/k'$; and for the slab $D_1 = 1, b_1 = 2$. Although U for the cylinder is not periodic in R, t, its complete asymptotic expansion has period T_s, so that the essentials of the present development carry over.

* This work was supported in part by National Science Foundation Grants NSF-GP-8734 and 21052.

1 V. Twersky, Relativistic Scattering of Electromagnetic Waves by Moving Obstacles, J. Math. Phys, 12, 2328 (1971).
2 A. Einstein, Ann. Phys. (paris) 17, 891 (1905).
3 W. Pauli, *Theory of Relativity* (Pergamon, New York, 1958).
4 A. Sommerfeld, *Electrodynamics* (Academic, New York, 1952).
5 M. Laue, *Das Relativitätsprinzip* (Friedr, Vieweg und Sohn, Braunschweig, 1911), p. 79.
6 L. Silberstein, *The Theory of Relativity* (Macmillan, London, 1924), p. 237.
7 P. Penfield, Jr. and H. A. Haus, *Electrodynamics of Moving Media* (MIT Press, Mass., 1967).
8 J. A. Stratton, Electromagnetic Theory (McGraw-Hill, New York, 1941).
9 D. S. Saxon, Phys. Rev. 100, 1771 (1955).
10 V. Twersky, J. Math. Phys. 8, 589 (1967); see Report EDL-L30 (1965), Mountain View, Calif., for additional results.
11 P. Debye, Ann. Physik 30, 57 (1909).
12 H. C. van de Hulst, *Light Scattering by Small Particles* (Wiley, New York, 1957), p. 13.
13 R. C. Restrick, Radio Science 3, 1144 (1968).
14 D. Censor, Tel-Aviv U, Report No. ES 70-005, Ramat-Aviv, Israel, 1969 [Radio Sci., (to be published)]. This work also discusses measurement procedures and alternative developments.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

The Phase Shift. I. As a Bounded Functional

William M. Frank
U.S. Naval Ordnance Laboratory, White Oak Silver Spring, Maryland 20910
(Received 16 March 1971)

Classes of potentials are defined by the finiteness of certain norms. For potentials in any of these classes, the phase shift for any partial wave is shown to possess a norm-dependent bound as a function of energy. Two norms are adduced in which the phase shift is uniformly bounded for all energies. A number of theorems are proven concerning the high-energy behavior of the phase shifts corresponding to potentials in these classes.

I. INTRODUCTION

The present and the following two papers will investigate the "scattering functions" of potential theory, *viz.* the partial wave phase shift $\delta_l(k)$ at a fixed energy k^2 ($\hbar = 2m = 1$ units are used throughout) and the S-wave scattering length A as (nonlinear) functionals of a spherically symmetric potential $V(r)$. The over-all questions raised in these papers deal with the boundedness and continuity of the partial wave phase shift as they depend on the potential function $V(r)$. These considerations are of interest in view of a number of paradoxes[1] noted in the literature calling for a clarification of these fundamental questions. These investigations also bring to light an interesting topological structure governing the dependence of scattering functions on potentials. In particular they point to a Banach space of potentials (see following papers) in which the scattering functions are continuous and bounded functionals. Such a structure may serve as a useful theoretical tool. A number of inequalities, some of which may be new, are arrived at in the course of this investigation which are likely useful in other contexts.

The present paper will establish a lemma which shows how the scattering functions have absolute bounds related to certain norms of the potential functions. While phase shifts are always subject to a mod-π ambiguity, we adhere to the convention that they be continuous in k and vanish at all energies for zero coupling. The bounds established in these papers apply to the phase shifts defined by this convention. They are of interest for the purposes of analysis as will be seen in the following articles. Some results on the high-energy limit of the phase shifts are presented in a theorem. In the following articles, it is shown how these norms, when bounded, serve as moduli of continuity for the dependence of the phase shift on the potential. In a subsequent paper, continuity is investigated when the potentials are of unbounded norm as in the case of repulsive singular potentials. All theorems and proofs will be explicitly presented for the $l = 0$ case. The considerations in the case of other partial waves are almost identical, and the necessary modifications are presented in Appendix A.

II. SPACES OF POTENTIALS

We deal in the present papers with potentials which are spherically symmetric and which are L^1 over any closed finite subinterval of $[0, \infty)$ which excludes the origin. We thus do allow for singular behavior at $r = 0$. One might allow for non-L^1 singularities at finite nonvanishing r, but they are not of sufficient interest though certain aspects are touched upon in an accompanying paper. The potentials are assumed to be point functions as distinguished from distributions, though such generalization is presumably possible, and in fact the limit as δ-function potentials are approached will be considered in the following paper. In practice we shall have piecewise continuous potentials in mind.

We shall be interested in a number of classes of potentials in what follows. The class L^1 is the familiarly defined class of potentials $V(r)$ for which

$$\zeta[V] \equiv \int_0^\infty dr\,|V(r)| < \infty, \tag{1}$$

which quantity we call the "L^1 norm" of the potential. The class $L_+^{(1)}$ consists of potentials $V(r)$ such that

$$\omega_\beta[V] \equiv \int_0^\infty \frac{dr\,r\,|V(r)|}{1+\beta r} < \infty \tag{2}$$

for some fixed positive β. The validity of Eq. (2) for one positive value of β implies its validity for all positive β. This integral will be termed the "$L_+^{(1)}$ norm" of the potential (β dependence suppressed). Two special cases are of interest, $\beta = k$ (k^2 is the energy) and $\beta = 0$. The latter class will be termed the "$L^{(1)}$ class" and corresponds to potentials with finite first moment, i.e.,

$$\chi \equiv \chi[V] \equiv \int_0^\infty dr\, r\,|V(r)| < \infty. \tag{3}$$

$\chi[V]$ is termed the $L^{(1)}$ norm of $V(r)$. If

$$\tau \equiv \tau[V] \equiv \int_0^\infty dr\,|V(r)|^{1/2} < \infty, \tag{4}$$

$V(r)$ will be said to belong to the class $L^{(1/2)}$ and the quantity τ is the $L^{(1/2)}$ norm of $V(r)$. We define the class $\bar{L}^{(1/2)}$ of potentials $V(r)$ to be those for which there is a $\bar{V}(r)$, such that

$$\begin{aligned} &\text{(i)}\ \ |V(r)| \leqslant \bar{V}(r),\\ &\text{(ii)}\ \ \bar{V}(r+a) \leqslant \bar{V}(r) \text{ for any } a \geqslant 0,\\ &\text{(iii)}\ \ \int dr\,|\bar{V}(r)|^{1/2} < \infty. \end{aligned} \tag{5}$$

[In what follows, $\bar{V}(r)$ will always denote an appropriate bounding potential corresponding to an $\bar{L}^{1/2}$ potential $V(r)$ for which (i), (ii), and (iii) are true.] We also introduce the notation which we exemplify for the $L^{(1)}$ norm

$$\chi[V]_a^b \equiv \int_a^b dr\, r\,|V(r)|$$

so that $\chi[V] \equiv \chi[V]_0^\infty$.

The subsequent paper shows that the $L^1, L_+^{(1)}\ L^{(1)}$, and $L^{(1/2)}$ norms serve as moduli of continuity, respectively, for the scattering functions in the $L^1, L_+^{(1)}, L^{(1)}$, and $\bar{L}^{(1/2)}$ classes of potentials. The following inclusion relations apply to these classes:

$$\bar{L}^{(1/2)} \subset L^{(1)} \subset L_+^{(1)}, \qquad L^1 \subset L_+^{(1)}. \tag{6}$$

These relations follow from the evident inequalities

$$\omega_\beta[V] < \chi[V], \qquad \omega_\beta[V] < (1/\beta)\zeta[V],$$

and the inequality valid for $V(r) \in \bar{L}^{1/2}$ follows from

$$\begin{aligned}\chi[V] &\equiv \int_0^\infty dr\,r\,|V(r)| = \int_0^\infty dx \int_x^\infty dr\,|V(r)|\\ &\leqslant \int_0^\infty dx \int_x^\infty dr\,\bar{V}(r) \leqslant \int_0^\infty dx\,\bar{V}(x)^{1/2}\\ &\quad\times \int_0^\infty dr\,\bar{V}(r)^{1/2} \equiv \tau^2[\bar{V}].\end{aligned} \tag{7}$$

It should be noted that the norms $\omega_\beta[V], \chi[V]$, and $\tau[V]$ are dimensionless in the units $\hbar = 2m = 1$ with β of dimensions length^{-1}.

III. BOUNDS ON PHASE SHIFTS

In this paper, we show that these norms serve as moduli of boundedness for their respective classes in the sense that the phase shifts for potentials in each of these classes can be bounded for each k by a quantity which depends on the corresponding norms of these potentials.

An extremely useful tool in the ensuing discussion is the following intuitively obvious comparison lemma.[2]

Comparison lemma: If two potentials $V_1(r)$, $V_2(r)$ satisfy the ordering relation for all r,

$$V_1(r) \geqslant V_2(r),$$

then correspondingly for each real energy k^2,

$$-\delta_1(k) \geqslant -\delta_2(k).$$

The conceptual content of this lemma is quite obvious; if one potential is at least as attractive as another everywhere, its phase shift at any energy is at least as great. In this sense we shall speak of the phase shift as a "monotonic functional" of the potential. It therefore suffices in order to establish bounds on the scattering functions to establish them for appropriately stronger potentials. Our interest in particular will be in bounds which are uniform in k. Only S-wave results are explicitly presented. (See Appendix A for discussion of higher l values.)

We define the respective attractive and repulsive parts $V^-(r)$, $V^+(r)$ of a potential $V(r)$ by

$$V^\pm(r) = \tfrac{1}{2}[V(r) \pm |V(r)|]. \tag{8}$$

Boundedness lemma: (i) If $V(r) \in L^1$, its phase shift at any nonzero energy obeys the inequalities[2]

$$-\left\{kL + \frac{1}{k}\zeta[V^+]_L^\infty\right\} \leqslant \delta(k) \leqslant \frac{1}{k}\zeta[V^-]. \tag{9}$$

with L arbitrary nonnegative.

(ii) If $V(r) \in L^{(1)}$, its phase shift obeys the inequalities

$$-\left\{kL + 2\omega_k[V^+(r)]_L^\infty\right\} \leqslant \delta(k) \leqslant F\{\chi[V^-(r)]\}, \tag{10a}$$

$$-\left\{kL + \chi[V^+(r)]_L^\infty\right\} \leqslant \delta(k) \leqslant F\{\chi[|V^-(r)|]\}, \tag{10b}$$

for any $L \geq 0$. $F(\chi)$ is a specific monotonically increasing function of its argument [see Eq. (28)] which vanishes at $\chi = 0$. These bounds are uniform in k.

(iii) If $V(r) \in \overline{L}^{(1/2)}$, then Eq. (10b) is valid as well as the weaker inequality (L arbitrary)

$$-\left\{kL + \tau^2[\overline{V}]_L^\infty\right\} \leq \delta(k) \leq F\{\tau^2[V]\}. \tag{11}$$

Remark: It is clear that, in order to prove this lemma, one must work with expressions for the phase shift which define it by the previously stated convention which resolves the mod-π ambiguity. Such relations are provided by Eqs. (13) and (22).

Proof: We first note that the inequality, Eq. (11), applied to $\overline{L}^{(1/2)}$ potentials is an immediate consequence of Eq. (10b) for $L^{(1)}$ potentials, in view of Eq. (7). We also remark that the phase shift is finite for all k for all $L^{(1)}$ potentials. For $k=0$ this is a consequence of Levinson's theorem and the Bargmann–Schwinger inequality, Eq. (21a).[3] For $k \neq 0$, it is a consequence of the existence of the Jost function (see Appendix B) $f(k)$ (identical with the Jost solution at $r = 0$ in the S-wave case) and the fact that $f(k) \neq 0$ for real $k \neq 0$.[4] The phase shift is merely Im $\ln f(k)$.

From the comparison lemma, we readily conclude that

$$\delta(k, V^+) \leq \delta(k, V) \leq \delta(k, V^-) \tag{12}$$

(in an obvious notation). It suffices in establishing the theorem to prove the upper bound in Eqs. (9) and (10) for a purely attractive potential and the lower bound for a purely repulsive potential.

Let $V(r)$ be a purely repulsive potential, i.e., $V(r) \geq 0$. The variable phase equation[5] specifies the phase shift as

$$\begin{aligned}\delta(k) &= -\frac{1}{k}\int_0^\infty dr V(r)\sin^2[kr + \delta(r,k)]\\ &= -\frac{1}{k}\left(\int_0^L + \int_L^\infty\right)dr V(r)\sin^2[kr + \delta(r,k)]\\ &\equiv \delta_1(k) + \delta_2(k),\end{aligned} \tag{13}$$

where $\delta(r,k)$ is the phase shift for the potential truncated beyond r.[5] For purely repulsive potentials[6]

$$-kr \leq \delta(r,k) \leq 0. \tag{14}$$

In particular,

$$\delta_1(k) = \delta(L,k) \geq -kL. \tag{15}$$

If in $\delta_2(k)$ we employ the inequality $|\sin\theta| \leq 1$, we immediately find for L^1 potentials

$$\delta(k) \geq -\left\{kL + \frac{1}{k}\zeta[V]_L^\infty\right\}. \tag{16}$$

One may optimize this with respect to L. For $L^{(1)}$ potentials, we employ the alternative inequality

$$|\sin^2\theta| \leq |\sin\theta| \leq 2\theta/(1+\theta) \tag{17}$$

and one readily finds in view of Eq. (14)

$$\begin{aligned}|\delta_2(k)| &= \frac{1}{k}\int_L^\infty dr V(r)\sin^2[kr + \delta(r,k)]\\ &\leq 2\int_L^\infty \frac{dr\, r V(r)}{1+kr}\\ &= 2\omega_k[V]_L^\infty.\end{aligned} \tag{18}$$

Equations (15) and (18) together imply for the purely repulsive case the lower bound in Eq. (10a). The inequality $|\sin\theta| < \theta$ and Eq. (15) give Eq. (10b). By choosing $L = 0$, we find a bound uniform in k,

$$\delta(k) \geq -\chi[V^+]. \tag{19}$$

Through an alternative use of the inequality (17), one readily derives for purely repulsive potentials the inequality

$$\delta(k) \geq -4k\int_0^\infty \frac{dr\, r^2 V(r)}{(1+kr)^2}. \tag{20}$$

This inequality has not been emphasized in the lemma as it fails to have any counterpart in the attractive case, since the right-hand side is finite even for some singular potentials. Our object is to indicate the norms which serve as moduli of boundedness.

The bound we find for a purely attractive potential $V(r)$ is not quite as simple. For $k = 0$, however, simple expressions are possible in view of Levinson's theorem. If n_B denotes the number of bound states supported by the potential, one finds from the Bargmann–Schwinger inequality

$$\delta(0) = \pi n_B \leq \pi\int_0^\infty dr\, r|V(r)| = \pi\chi[V] \tag{21a}$$

for $L^{(1)}$ potentials. For $\overline{L}^{(1/2)}$ potentials one can, in fact, go beyond the implications of Eq. (7) by means of the inequality[7]

$$\frac{1}{\pi}\delta(0) = n_B \leq \frac{2}{\pi}\int_0^\infty dr|\overline{V}(r)|^{1/2} = \frac{2}{\pi}\tau[\overline{V}]. \tag{21b}$$

For $k \neq 0$, the upper bound in Eq. (9) is an immediate consequence of the variable phase equation. For nonzero energies, the proof of Eq. (10) is considerably more complicated. In this case, we show that a choice of radius $g > 1$ is possible, which will give $\delta(k, -g|V|)$ a uniform bound in k. We proceed from the following expression for the phase shift for a potential[8]

$$\delta(k) = k\int_0^\infty dr[|f(k,r)|^{-2} - 1], \tag{22}$$

where $f(k,r)$ is the Jost solution for that potential. We write

$$\delta(k) = k\int_{C_+} dr[|f(k,r)|^{-2} - 1] - k\int_{C_-} dr[1 - |f(k,r)|^{-2}] \equiv \delta_+(k) - \delta_-(k), \tag{23}$$

where C_+ is the subset of the positive r axis over which $|f(k,r)| \leq 1$ and C_- is the complementary subset. Clearly $\delta(k) \leq \delta_+(k)$. An upper bound to $\delta_+(k)$ can be found from a lower bound to $|f(k,r)|$. In Appendix B, we establish the upper bound to $|f(k,r)|$,

$$|f(k,r)| \equiv |f(k,r;g)| \leq \exp\{2g\omega_k[V]_r^\infty\}, \tag{24}$$

where a coupling constant $g > 0$ has been attached to the potential (eventually to take the value unity). (The g dependence will occasionally be suppressed in the notation.) A standard function theoretic result states[9] that, complementary to the upper bound in Eq. (24), one can find a related lower bound on $|f(k,r)|$ valid in the entire g plane exclusive of certain small neighborhoods of the zeros of $f(k,r)$. We shall use the following form of this result for the case $g = 1$, which we prove in Appendix C.

Result: For fixed k and r,

$$|f(k,r;1)| \geq \exp\{-\tfrac{2}{9}\pi^2[\tfrac{22}{3} + 8\ln(32g^3\chi^2)]\omega_k[V]_r^\infty\} \equiv \exp\{-\Lambda\omega_k[V]_r^\infty\}. \tag{25}$$

We find from Eqs. (23) and (25)

$$\delta(k) \leq \delta_+(k) \leq k\int_0^\infty dr\{\exp\{2\Lambda\omega_k[V]_r^\infty\} - 1\} = 2k\Lambda\int_0^\infty \frac{dr r^2|V(r)|}{1+kr}\exp\{2\Lambda\omega_k[V]_r^\infty\}. \leq 2\chi\Lambda\exp(2\chi\Lambda), \tag{26}$$

where an integration by parts has been done in Eq. (26). The integrated part vanishes at the upper limit since

$$\int_r^\infty \frac{ds s|V(s)|}{1+ks} \leq \frac{1}{1+kr}\int_r^\infty ds s|V(s)| = O\left(\frac{1}{r}\right), \tag{27}$$

which follows from $\chi[V] < \infty$. The quantity $\omega_k[V]$ appearing in Eq. (26) is replaced by $\chi[V]$ only because a finite $L^{(1)}$ norm is necessary for the integrals to converge. One thus verifies the upper bounds in Eq. (10),

$$F(\chi) = \chi(\rho + \sigma\ln\chi)\exp[\chi(\rho + \sigma\ln\chi)], \tag{28}$$

with ρ, σ defined in Eq. (C17). We note that $F(\chi)$ is a continuous monotonically increasing function of χ which goes to zero as $\chi \to 0$.

We note that this proof which was based on the representation of Eq. (22) for the phase shift cannot be repeated for the S-wave scattering length which is expressible analogously by[10]

$$A = \int_0^\infty dr[|f(0,r)|^{-2} - 1]. \tag{29}$$

Indeed the scattering length for attractive potentials is not a bounded functional in any of the norms, as it becomes infinite at every bound state threshold. The argument fails because the scattering length is not a monotonic functional of the potential. Bounds on the scattering length in the purely repulsive case can be inferred from the present approach, but this will be deferred to another treatment.

When the potential becomes singular in the sense that $\chi[V]_0^\alpha = \infty$ for any $\alpha > 0$, the upper bound in Eq. (10) fails to be finite, while the lower bound is generally finite, though it grows unbounded as $k \to \infty$.

IV. HIGH-ENERGY BEHAVIOR

The behavior of $\delta(k)$ for large k is described in the following theorem.

Theorem: (i) If, for some $\beta > 0, \omega_\beta[V] < \infty$, then $\delta(k) \to 0$ as $k \to \infty$.

(ii) If $r^2V(r) \to +\infty$ monotonically as $r \to 0$ and $\omega_\beta[V]_\alpha^\infty < \infty$ for all $\alpha > 0$, then $\delta(k) \to \infty$ as $k \to \infty$.

(iii) If, for some $\beta > 0$,

$$\omega_\beta[V^-] < \infty, \quad \omega_\beta[V^+]_\alpha^\infty < \infty \text{ for any } \alpha > 0, \tag{30}$$

then $\delta(k)/k \to 0$.

Proof: To prove (i), we appeal to the expression for $\delta(k)$ in Eq. (13), in particular, to the decomposition into $\delta_1(k)$ and $\delta_2(k)$ with L to be specified. We choose an $\epsilon > 0$. $\delta_1(k)$ is the phase shift for the potential $V(r)$ truncated beyond $r = L$. Now $F[\chi]$ of the lemma goes to zero continuously as $\chi \to 0$, and so does $\omega_\beta[V]_0^L$ as $L \to 0$. It follows from

$$\chi[V]_0^L \leq (1 + \beta L)\omega[V]_0^L \tag{31}$$

and the inequalities in Eqs. (10b) and (19) that, through choice of sufficiently small L, one can make $|\delta_1(k)| < \frac{1}{2}\epsilon$. For $\delta_2(k)$, one can write the inequality

$$|\delta_2(k)| \leq (1/k)(\beta + 1/L)\omega_\beta[V], \tag{32}$$

which, with L fixed, can be made smaller than $\frac{1}{2}\epsilon$ through choice of sufficiently large k. Since ϵ is arbitrary, one concludes that $\delta(k) \to 0$ as $k \to \infty$.

We now consider statement (ii). One considers only $V(r)$ purely repulsive in the neighborhood of $r = 0$, as the phase shift for a strongly attractive singular potential is essentially undefined. We again consider the decomposition into $\delta_1(k)$ and $\delta_2(k)$ of Eq. (13). It has been presumed that within some fixed finite neighborhood of $r = 0$, $r^2V(r)$ is positive and monotonically decreasing. Define r_l by the condition

$$r_l^2 V(r_l) = l(l+1). \tag{33}$$

Then $r_l \to 0$ as $l \to \infty$. In Eq. (13), choose $L = r_l$. For fixed l,

$$|\delta_2(k)| \leq \frac{1}{k}\int_{r_l}^{\infty} dr\,|V(r)| \leq \frac{1}{k}\left(\beta + \frac{1}{r_l}\right)\omega_\beta[V]_{r_l}^{\infty}, \quad (34)$$

which shows that $\delta_2(k) \to 0$ as $k \to \infty$. By comparison, one concludes from the monotonicity of $V(r)$ for small r for sufficiently large l that

$$\delta_1(k) \leq \delta(k; C_l), \quad (35)$$

where $\delta(k; C_l)$ is the phase shift corresponding to

$$C_l(r) \equiv [l(l+1)/r^2]\theta(r_l - r). \quad (36)$$

$\delta(k; C_l)$ is expressible by means of the $(l=0)$ variable phase expression in Eq. (13)

$$\begin{aligned}\delta(k; C_l) &= -[l(l+1)/k]\int_0^{r_l} dr r^{-2}\sin^2[kr + \delta(r,k;l)] \\ &= [l(l+1)/k]\int_0^{\infty} dr r^{-2}\sin^2[kr + \delta(r,k;l)] \\ &\quad + [l(l+1)/k]\int_{r_l}^{\infty} dr r^{-2}\sin^2[kr + \delta(r,k;l)] \\ &= -\tfrac{1}{2}l\pi + [l(l+1)/k]\int_{r_l}^{\infty} dr r^{-2} \\ &\quad \times \sin^2[kr + \delta(r,k;l)], \end{aligned} \quad (37)$$

where $\delta(r,k;l)$ is the variable phase function for the centrifugal potential $l(l+1)r^{-2}$. For fixed l, one readily sees that $\delta(k; C_l) \to -\frac{1}{2}l\pi$ as k diverges. Since l is arbitrary, one concludes from Eq. (35) that $\delta_1(k) \to -\infty$ as $k \to \infty$, from which follows the same for $\delta(k)$.

We now prove statement (iii) which is meant to apply to singular potentials, i.e., potentials for which $\chi[V] = \infty$. It follows by comparison from statement (i) and $\omega_\beta[V^-] < \infty$ that, in fact, $\delta(k) \leq 0$ as $\lim k \to \infty$. Choose an $\epsilon > 0$. Then if $L = \frac{1}{2}\epsilon$,

$$\delta_1(k)/k \geq -\tfrac{1}{2}\epsilon$$

from Eq. (15). For such an L, one can choose k so large that Eq. (18) implies $k^{-1}\delta_2(k) \geq \frac{1}{2}\epsilon$. The result follows from the arbitrariness of ϵ.

V. DISCUSSION

The upper bound in Eq. (10) is likely to be generous in view of the simpler form for $k = 0$, Eq. (21a), and the known bounds for potentials which have monotonicity properties.[11] One may speculate in view of Eq. (9), the $k = 0$ case and the results for the purely repulsive case, whether an upper bound with only polynomial growth in χ is possible for large χ. One should also note the inequality in Eq. (25) as an inequality on the modulus of the Jost solution, which is useful in later contexts. The boundedness lemma is a vital consideration in the arguments of the following paper.

APPENDIX A: HIGHER l VALUES

The boundedness lemma and high-energy theorem remain essentially valid for the lth partial phase shift with only minor modification of the reasoning or results. The upper bounds in Eqs. (9) and (10) are only changed by addition of $\frac{1}{2}l\pi$ to the right-hand side. The presence of the centrifugal barrier does not change the attractive part of the potential, while the "S-wave phase shift" for $V(r) - l(l+1)r^{-2}$ is $\frac{1}{2}l\pi$ less than the l partial wave phase shift. The lower bound can be studied by a parallel treatment to the $l = 0$ case. Again we may take $V(r)$ to be purely repulsive. The variable phase equation for the lth partial phase shift is[12]

$$\frac{d\delta_l}{dr}(r,k) = -\frac{1}{k}V(r)\hat{D}_l^2(kr)\sin^2[\hat{\delta}_l(kr) + \delta_l(r,k)], \quad (A1)$$

where $\hat{D}_l(x)$ and $\hat{\delta}_l(x)$ are defined in terms of the conventional spherical Bessel functions $j_l(x)$ and $n_l(x)$[13]:

$$\begin{aligned}\hat{D}_l(x) &= x[j_l^2(x) + n_l^2(x)]^{1/2} \\ \hat{\delta}_l(x) &= \arctan[j_l(x)/n_l(x)]. \end{aligned} \quad (A2)$$

$\hat{\delta}_l(x)$ is defined for all $x \geq 0$ by $\hat{\delta}_l(0) = 0$ (in the repulsive case) and $\delta_l(x)$ continuous. From (A1)

$$\begin{aligned}\delta_l(k) &= -(1/k)\int_0^{\infty} dr V(r)\hat{D}_l^2(kr) \\ &\quad \times \sin^2[\hat{\delta}_l(kr) + \delta_l(r,k)] \\ &= \delta_l(L,k) - (1/k)\int_L^{\infty} dr V(r)\hat{D}_l^2(kr) \\ &\quad \times \sin^2[\hat{\delta}_l(kr) + \delta_l(r,k)]. \end{aligned} \quad (A3)$$

We appeal to a number of relations. For purely repulsive $V(r)$,[14]

$$0 \leq \hat{\delta}_l(kr) + \delta_l(r,k) \leq \hat{\delta}_l(kr) \quad (A4)$$

and

$$\hat{\delta}_l(x) \leq x, \quad \hat{D}_l^2(x)\delta_l(x) \leq x, \quad (A5)$$

which follow from the monotonically decreasing character[15] of $\hat{D}_l(x)$, $\hat{D}_l(\infty) = 1$, and the relation[16]

$$\delta_l(x) = \int_0^x dy \hat{D}_l^{-2}(y). \quad (A6)$$

We conclude from Eqs. (A3)–(A5) that, for purely repulsive $V(r)$,

$$\delta_l(k) \geq -\{\hat{\delta}_l(kL) + 2\omega_k[V]_L^{\infty}\}, \quad (A7)$$

which is the appropriate inequality to appear in Eq. (10a) with $V^+(r)$ replacing $V(r)$ in the general case. Setting $L = 0$, we readily verify the lower bound in Eq. (9). We note the behavior[17] of $\hat{\delta}_l(x)$ for small and large x as

$$\hat{\delta}_l(x) \underset{x\sim 0}{\sim} \frac{x^{2l+1}}{(2l+1)!!(2l-1)!!}, \qquad \hat{\delta}_l(x) \underset{x\sim\infty}{\sim} x - \tfrac{1}{2}l\pi. \quad (A8)$$

Equation (10b) is proved in the same way to hold with $\hat{\delta}_l(kL)$ replacing kL. One derives analogously to Eq. (20) for purely repulsive potentials

$$\delta_l(k) \geq -4\int_0^\infty dr\, \frac{r\hat{\delta}_l(kr)V(r)}{[1+\hat{\delta}_l(kr)]^2}. \qquad \text{(A9)}$$

The theorem on the high-energy behavior applies to higher partial phase shifts, with essentially no change in the proof.

APPENDIX B: BOUNDS ON THE JOST SOLUTION

The Jost solution to the $l=0$ partial wave equation

$$\frac{d^2}{dr^2}f(k,r) + [k^2 - gV(r)]f(k,r) = 0, \qquad \text{(B1)}$$

satisfying the boundary condition for large r

$$f(k,r) \sim e^{-ikr},$$

also obeys the integral equation[18]

$$f(k,r) = e^{-ikr} + g\int_r^\infty dr'[\sin k(r-r')/k]V(r')f(k,r'). \qquad \text{(B2)}$$

This Volterra type integral equation allows the solution by iteration

$$f(k,r) = e^{-ikr} + \sum_{n=1}^\infty \left(\frac{g}{k}\right)^n \int_r^\infty dr_1 \cdots \times \int_{r_{n-1}}^\infty dr_n\, \sin k(r_n - r_{n-1}) \cdots$$

$$\sin k(r_2 - r_1)\, \sin k(r_1 - r) e^{-ikr_n} \cdot \prod_{j=1}^n V(r_j)$$

$$\equiv \sum_{n=1}^\infty g^n \phi_n(k,r). \qquad \text{(B3)}$$

Bounds are easily derived from this expression. If $V(r) \in L_+^{(1/2)}$ for k real, one readily finds from the inequality (17)

$$|\phi_n(k,r)| \leq 2^n \int_r^\infty dr_1 \cdots \int_{r_{n-1}}^\infty dr_n \prod \frac{r_j|V(r_j)|}{1+kr_j}$$

$$= \frac{1}{n!}\{2\omega_k[V]_r^\infty\}^n, \qquad \text{(B4)}$$

which implies

$$|f(k,r)| \leq \exp\{2|g|\omega_k[V]_r^\infty\}. \qquad \text{(B5)}$$

From $|\sin\theta| \leq \theta$, one immediately deduces that if $V(r) \in L^{(1)}$,

$$|f(k,r)| \leq \exp\{|g|\chi[V]_r^\infty\}. \qquad \text{(B6)}$$

Alternatively,[19] if $V(r) \in \overline{L}^{(1/2)}$,

$$|\phi_n(k,r)| \leq \int_r^\infty dr_1 \cdots \int_{r_{n-1}}^\infty dr_n (r_n - r_{n-1}) \cdots \times (r_2 - r_1)(r_1 - r)\prod_{j=1}^n |V(r_j)|$$

$$= \int_r^\infty dx_1 \int_{x_1}^\infty dr_1 \int_{r_1}^\infty dx_2 \int_{x_2}^\infty dr_2 \cdots \times \int_{x_{n-1}}^\infty dx_n \int_{x_n}^\infty dr_n \prod_{j=1}^n |V(r_j)|$$

$$\leq \int_r^\infty dx_1 \int_{x_1}^\infty dr_1 \cdots \int_{x_{n-1}} dx_n \times \int_{x_n}^\infty dr_n \prod_{j=1}^n |\overline{V}(r_j)\overline{V}(x_j)|^{1/2}$$

$$= \frac{1}{(2n)!}\{\tau[\overline{V}]_r^\infty\}^{2n}, \qquad \text{(B7)}$$

so that

$$|f(k,r)| \leq \cosh\{|g|^{1/2}\tau[\overline{V}]_r^\infty\}. \qquad \text{(B8)}$$

APPENDIX C: PROOF OF THE INEQUALITY OF EQ. (25)

We appeal to the representation of $f(k,r;g)$ as infinite product representation in terms of its zeros (in g). In general $f(k,r;g)$ may have exponential order as high as 1 in g,[20] and, therefore, $f(k,r;g)$ would have the infinite product representation

$$f(k,r;g) = e^{-ikr}\Pi(1 - g/g_n). \qquad \text{(C1)}$$

The dependence of g_n on k,r is suppressed, and the known value of $f(k,r;0)$ has been included. Equation (24) implies an inequality[21] on the number of zeros of $f(k,r;g)$ within a circle of radius g

$$n(g) \leq 4g\omega_k[V]_r^\infty \equiv 4g\omega_k(r), \qquad \text{(C2)}$$

which implies that

$$|g_n| \geq \frac{n}{4\omega_k(r)}. \qquad \text{(C3)}$$

The r dependence of the g_n is frequently suppressed in the notation. We consider[22]

$$|f(k,r;g)f(k,r;-g)|$$

$$= \left|\Pi\left(1 - \frac{g^2}{g_n^2}\right)\right| \geq \Pi\left[1 - \frac{g^2}{|g_n|^2}\right] \equiv \phi(g). \qquad \text{(C4)}$$

We shall find a lower bound to $\phi(g)$. $\phi(g)$ of course has its minima at its zeros. Since $\phi(g)$ clearly vanishes at $g = |g_n|$, we exclude each of these points together with a small neighborhood. We surround each point $g = g_n(r)$ by a circle of radius

$$|g - g_n(r)| = 2/3n^2, \qquad \text{(C5)}$$

and exclude the interior of the circle from the region for which we try to establish a lower bound to $\phi(g)$. The choice of radius of the disc is arbitrary, so long as the sum of the radii of the excluded circles is finite. We denote the g-plane with these r-dependent circles excluded by $G(r)$. The total diameter of the excluded circles is bounded by

$$\bar{g} \equiv \tfrac{4}{3}\sum_{n=1}^\infty n^{-2} = \tfrac{2}{9}\pi^2 > 1, \qquad \text{(C6)}$$

where Eq. (C3) has been used. We note that $\bar{g}$ as defined in Eq. (C6) serves as a k- and r-independent radius, for which for some value of $g \leq \bar{g}$, the inequality to be derived will be valid. For g general,

$$\ln|\phi(g)| = \sum_n \ln\left|1 - \frac{g^2}{|g_n|^2}\right|$$

$$= \sum_{|g_n|<2g} \ln\left|1 - \frac{g^2}{|g_n|^2}\right| + \sum_{|g_n|\geq 2g} \ln\left|1 - \frac{g^2}{|g_n|^2}\right|$$

$$\equiv L_1 + L_2. \tag{C7}$$

For $|g_n| < 2g$,

$$|g^2 - |g_n|^2| \geq \tfrac{3}{2}|g_n||g - |g_n|| \geq |g_n|/n^2, \tag{C8}$$

and therefore from Eq. (C3)

$$\ln\left|1 - \frac{g^2}{|g_n|^2}\right| \geq -\ln(n^2|g_n|) \geq -\ln(32g^3\chi^2), \tag{C9}$$

so that

$$L_1 = \sum_{|g_n|<2g} \ln\left|1 - \frac{g^2}{|g_n|^2}\right| \geq -n(2g)\ln(32g^3\chi^2) \geq -8g\ln(32g^3\chi^2)\omega_k(r). \tag{C10}$$

By employing the inequality $\ln(1-x) \geq -\frac{4}{3}x$ for $x \leq \frac{1}{4}$, we find

$$L_2 = \sum_{|g_n|>2g} \ln\left|1 - \frac{g^2}{|g_n|^2}\right| \geq -\tfrac{4}{3}g^2 \sum_{|g_n|\geq 2g} \frac{1}{|g_n|^2}. \tag{C11}$$

Now from Eq. (C3)

$$\sum_{|g_n|\geq 2g} \frac{1}{|g_n|^2} \leq \sum_{n=1}^{\infty} \min\left[\frac{1}{4g^2}, \frac{16\omega_k^2(r)}{n^2}\right]$$

$$= \frac{n(2g)}{4g^2} + 16\omega_k^2(r) \sum_{n\geq 8g\omega_k(r)} n^{-2}$$

$$< \frac{2\omega_k(r)}{g} + \frac{2\omega_k(r)}{g} = \frac{4\omega_k(r)}{g}, \tag{C12}$$

so that

$$L_2 \geq -\tfrac{16}{3}g\omega_k(r), \tag{C13}$$

and

$$\ln\phi(g) > -g[\tfrac{16}{3} + 8\ln(32g^3\chi^2)]\omega_k(r). \tag{C14}$$

Consequently for any g in $G(r)$ from Eqs. (24), (C4), (C10), and (C14),

$$|f(k,r;-g)| \geq \exp - g[\tfrac{22}{3} + 8\ln(32g^3\chi^2)]\omega_k(r). \tag{C15}$$

The quantity on the right is a monotonically decreasing function of g. This inequality remains valid if a value of g in $G(r)$ is replaced by $\bar{g}$ of Eq. (C6) which is a k and r independent. Thus one obtains the statement of Eq. (25). This leads through the steps in Eqs. (26) and (27) to the form of $F(\chi)$ presented in Eq. (28)

$$F(\chi) = \chi(\rho + \sigma\ln\chi)\exp[\chi(\rho + \sigma\ln\chi)], \tag{C16}$$

where

$$\rho = \tfrac{8}{9}\pi^2[\tfrac{11}{3} + 12\ln(\pi^2/9) + 32\ln 2], \sigma = 64\pi^2/9. \tag{C17}$$

We have not attempted to find the sharpest possible inequalities. We note that $|f(k,r;-g)| \to 1$ as $\omega_k(r) \to 0$, as is to be expected.

---

1 F. Calogero, Phys. Rev. 139, B602 (1965); E. M. Ferreira and F. F. Teixeira, J. Math. Phys. 7, 1207 (1965); H. Cornille, Nuovo Cimento 39, 557 (1965); R. Vasudevan, K. Venkatesan, and G. Jagannathan, Nuovo Cimento Suppl. 5, 621 (1967).

2 F. Calogero, *Variable Phase Approach to Potential Scattering* (Academic, New York, 1967), p. 14.

3 V. Bargmann, Proc. Nat. Acad. Sci. 38, 961 (1952); J. Schwinger, *ibid.* 47, 122 (1961).

4 R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), pp. 344–345.

5 F. Calogero, Ref. 2, Chap. 3, Eq. (15). This equation is interpreted on p. 13.

6 F. Calogero, Ref. 2, Chap. 4, Eq. (3).

7 F. Calogero, Commun. Math. Phys. 1, 80 (1967). The result with a larger constant can be found in W. M. Frank, J. Math. Phys. 8, 466 (1967), Eq. (40). See also, e.g., K. Chadan, Nuovo Cimento, 58A, 191 (1968).

8 Newton, Ref. 4, p. 349, Eq. (12.69).

9 E. C. Titchmarsh, *The Theory of Functions* (Oxford U.P., London, 1939), Sec. 8.71.

10 This is an immediate consequence of Eq. (22).

11 F. Calogero, Ref. 2, Chap. 7, Eqs. (13)–(19).

12 F. Calogero, Ref. 2, Chap. 3, Eq. (14b).

13 L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, (1955), 2nd ed., p. 77 and F. Calogero, Ref. 2, Appendix I, Eqs (10a)–(11b).

14 F. Calogero, Ref. 2, Chap. 4, Eq. (3).

15 F. Calogero, Ref. 2, p. 202.

16 F. Calogero, Ref. 2, Appendix I, Eq. (12).

17 F. Calogero, Ref. 2, p. 202

18 R. G. Newton, Ref. 4, p. 344, Eq. (12.16). The Jost solution defined in this book differs from the Jost convention. The quantity $f_-(k,r)$ corresponds to the conventional Jost solution.

19 I am indebted to D. J. Land for this demonstration. A somewhat cruder result can be found in W. M. Frank, Ref. 7, Eq. 15.

20 W. M. Frank, Ref. 7. The inequality (P6) of this paper saturates for a potential like $[r^2 \ln|r| \ln\ln^2|r|]^{-1}$.

21 See E. C. Titchmarsh, Ref. 9, Sec. 5.24.

22 This proof is modeled after Secs. 8.71, 8.75 of E. C. Titchmarsh.

A New Approximation Method for Wave Theories*

S. Persides
Department of Physics, University of Texas, Austin, Texas
(Received 4 December 1970)

The scalar field due to a bounded source and obeying the wave equation is analyzed. As a result of this, a set of rules is derived for solving a class of "wave theories," including electrodynamics and general relativity, by expanding the field in a power series of c^{-1} in null-spherical coordinates. The method is applied for the Maxwell equations to give all the well-known results without the use of Fourier analysis and Bessel functions.

1. INTRODUCTION

From the time when general relativity was introduced as a gravitational theory, the problem of expressing explicitly the gravitational field in terms of the source was recognized as a very important one. It is the purpose of this paper to set up a method for solving this problem.

Because of the complexity of the Einstein equations, an exact general solution, as in electrodynamics, does not seem possible. However, we ask for the next best answer: namely, a procedure which will enable us to express the metric tensor $g_{\mu\nu}$ explicitly in terms of the source at any desired accuracy.

Earlier investigations by Bondi, van der Burg, and Metzner[1] and Newman and Penrose[2] opened the way for the exact treatment of the far zone of a gravitational field produced by a bounded source. These and other similar works[3-6] employ characteristic or asymptotically[6] characteristic hypersurfaces and are based on the possibility of expanding the metric tensor in powers of r^{-1}, where r is an appropriately defined parameter which at infinity coincides with the radial coordinate. However, because of the expansion in powers of r^{-1}, only the far zone can be studied by this method.

For the near zone, different procedures have been used. Einstein, Infeld,[7] Hoffman, Fock,[8] and Chandrasekhar[9] have given a solution for the field inside and near the source. Also the reaction on the source due to the emission of gravitational waves has been derived by Chandrasekhar and Esposito.[10] The "near zone" approach assumes an expansion of the field in powers of c^{-1} (or v/c) and is not valid far from the source because, among other reasons, the metric tensor behaves as r^n ($n \geqslant 1$) at large distances.

Consequently, the problem of uniting the two procedures arises. In that direction, the coupling of the radiation to nonrelativistic sources has been studied by Burke[11] in the linearized version of general relativity using the method of matched asymptotic expansions. However, this method appears to be rather complicated, and in the author's opinion, it is questionable whether it can be applied effectively for higher approximations.

In this paper, we adopt a different approach to the problem of relating the gravitational field in the far zone to the source. We consider a class (not exactly defined) of "wave theories" with the scalar wave theory, classical electrodynamics, and general relativity among them. Each "wave theory" consists of a set of field equations, a source function (with one or more components), and a set of boundary conditions. Our objective is to find a set of "rules" for reducing the field equations to a set of linear equations which can be rather easily solved. The rules must be more or less the same for all the wave theories of the class. Hence, they must not depend on the field equations (linear or nonlinear), the source function (charge distribution or energy-momentum tensor), and the boundary conditions.

In Sec. 2 we will discover the rules by examining some properties of the scalar wave equation and its solutions.

In Sec. 3 the new method will be applied to the Maxwell equations to derive all the well-known results (with emphasis on the radiation) without any use of Fourier analysis, Bessel functions, and retarded potentials.

In Sec. 4 we will briefly examine the limitations, if any, of the method, and in Sec. 5 some concluding remarks will be made.

The application of the technique in general relativity, which is the purpose for developing the method, will be done in a future paper.

2. THE SCALAR WAVE FIELD

In flat space-time with signature -2, we consider a one-component field ψ satisfying everywhere the equation

$$\Box\Psi = -4\pi f(t, \mathbf{r}), \tag{1}$$

where

$$\Box\Psi \equiv b^{\mu\nu}\Psi_{;\mu\nu}, \quad \mu, \nu = 0, 1, 2, 3, \tag{2}$$

$b^{\mu\nu}$ is the contravariant metric tensor of the space, $f(t, \mathbf{r})$ a function of the time t and position $\mathbf{r}$ representing a bounded source ($f = 0$ outside an appropriate sphere), and the semicolon denotes covariant differentiation with respect to $b_{\mu\nu}$.

Assuming that

$$f(t, \mathbf{r}) = f(\mathbf{r})e^{-i\omega t}, \tag{3}$$

we have the general solution of Eq. (1) outside the source as a linear combination of

$$\psi_{lm} = h_l(kr)Y_{lm}(\theta, \varphi)e^{-i\omega t}. \tag{4}$$

Every $h_l(kr)$ contains[12] a factor e^{ikr} which can be combined with $e^{-i\omega t}$ to give $e^{-i\omega u}$, where $u = t - c^{-1}r$. The remaining part of $h_l(kr)$ is a polynomial of r^{-1} with coefficients, which are powers of c^{-1}. This is the only place where c appears in ψ_{lm}, and consequently, ψ_{lm} is of the form (with the indices l and m omitted)

$$\psi = \sum_n F_n(u, \mathbf{r}) c^{-n}. \tag{5}$$

Let our space–time be represented by a four-dimensional manifold M with coordinates[13] u, $\mathbf{r}$ (u ranges from $-\infty$ to $+\infty$ and $\mathbf{r}$ stands for x, y, z or r, θ, φ with the appropriate ranges). A one-parameter family of functions on M, $\Psi(u, \mathbf{r}; c)$, labeled by the parameter c, will be called a *u-type function* if, for fixed u and $\mathbf{r}$, Ψ is analytic in c^{-1}, i.e., if Ψ can be written in the form (5) [with $F_n(u, \mathbf{r})$ independent of c]. A c-dependent tensor field on M will be called a *u-type field* if each component of that field (in this coordinate system) is a u-type function.

The importance of the "u-type function" concept lies in the fact that a u-type function can represent time-dependent fields generated by a bounded source, governed by linear or nonlinear equations, and exhibiting radiation phenomena. The simplest scalar outgoing wave $r^{-1}e^{-i\omega u}$ is a u-type function. Any solution of the Bessel equation multiplied by $e^{-i\omega t}$ becomes a u-type function. In flat-space electrodynamics, let J^μ be a contravariant vector field on M whose components are independent of c in the coordinate system t, $\mathbf{r}$. We suppose in addition that J^μ has compact support on each $t = \text{const}$ hypersurface and $J^\mu{}_{;\mu} = 0$. Then for each c, there is a unique retarded solution of Maxwell's equations with source J^μ and which goes to zero at spatial infinity. This solution is a u-type function. Because of the expected similarity between electrodynamics and general relativity, we will assume in Einstein's theory that the gravitational field of a bounded source is a u-type function with u, r, θ, and φ appropriately[1,6] generalized.

If we now express the operator $\Box$ using coordinates u, r, θ, and φ as a power series of c^{-1}, then automatically $\Box\psi_{lm}$ will be a power series of c^{-1}, and since $\Box\psi_{lm} = 0$, we conclude that the coefficient of c^{-n} of $\Box\psi_{lm}$ will be zero for every n. The same conclusion could be reached if we had considered c^{-1} as an *independent variable* instead of a constant. It is important to notice that any sum of ψ_{lm} with respect to l and m, and any sum or integral with respect to ω (in case the source has a discrete or continuous spectrum) are also u-type functions. Hence, *the solution of (1) outside the source is a u-type function and c^{-1} can be considered as a variable independent of the coordinates or any other parameter of the problem.* We now consider the inhomogeneous Eq. (1). Let $f(t, \mathbf{r})$ be given by (3). We also assume that $f(\mathbf{r})$ does not contain c. The physically acceptable ($\sim r^{-1}$ for large r) exact solution is

$$\Psi = \sum_{l,m} \psi_{lm} Y_{lm}, \tag{6}$$

where

$$\psi_{lm} = ikh_l(kr)e^{-i\omega t}\int_0^r r'^2 j_l(kr')F_{lm}(r')dr' + ikj_l(kr)e^{-i\omega t}\int_r^\infty r'^2 h_l(kr')F_{lm}(r')dr' \tag{7}$$

and

$$F_{lm}(r) = \int Y^*_{lm} f(\mathbf{r}) d\Omega. \tag{8}$$

The function ψ_{lm} satisfies exactly a differential equation which written in coordinates u, r, θ, and φ becomes

$$\left(L - \frac{1}{c} M\right)\psi_{lm} = -F_{lm} r^2 e^{-i\omega t}, \tag{9}$$

where

$$L = r^2 \frac{\partial^2}{\partial r^2} + 2r\frac{\partial}{\partial r} - l(l+1) \tag{10}$$

and

$$M = 2r^2 \frac{\partial^2}{\partial u \partial r} + 2r\frac{\partial}{\partial u}. \tag{11}$$

In the above, ψ_{lm} is not a u-type function. However, we can consider it as a function of u, r, θ, and φ and expand it formally in powers of c^{-1}. The factor $e^{-i\omega t}$ of the first term of (7) combined with e^{ikr} of $h_l(kr)$ will give $e^{-i\omega u}$. The factor $e^{-i\omega t}$ of the second term will be expanded as

$$e^{-i\omega t} = e^{-i\omega u} \cdot e^{-ikr} = e^{-i\omega u}\left(1 - \frac{i\omega r}{c} - \frac{\omega^2 r^2}{c^2} \dots\right). \tag{12}$$

Finally, we expand the Bessel functions $h_l(kr)$ and $j_l(kr)$ and replace k by ω/c. Keeping only the two first powers of c^{-1}, we find

$$\psi_{lm} = \psi^{(0)}_{lm} + (1/c)\psi^{(1)}_{lm} + \Theta(c^{-2})$$

where

$$\psi^{(0)}_{lm} = \frac{e^{-i\omega u}}{2l+1}\left[r^{-l-1}\int_0^r r'^{l+2}F_{lm}(r')dr' + r^l\int_r^\infty r'^{-l+1}F_{lm}(r')dr'\right] \tag{13}$$

and

$$\psi^{(1)}_{lm} = -\frac{i\omega e^{-i\omega u}}{2l+1}\left[r^{-l}\int_0^r r'^{l+2}F_{lm}(r')dr' + r^{l+1}\int_r^\infty r'^{-l+1}F_{lm}(r')dr'\right]. \tag{14}$$

We now have the u-type function $\psi^{(0)}_{lm} + c^{-1}\psi^{(1)}_{lm}$, and multiplying by $L - c^{-1}M$, we find

$$\left(L - \frac{1}{c} M\right)\left(\psi^{(0)}_{lm} + \frac{1}{c}\psi^{(1)}_{lm}\right) = -F_{lm}(r) r^2 e^{-i\omega u}\left(1 - \frac{i\omega r}{c}\right). \tag{15}$$

But the right-hand side is the first two terms in the expansion of $-F_{lm} r^2 e^{-i\omega t}$ of (9). This means that, instead of solving (9) exactly, we could expand the source in powers of c^{-1} (in coordinates u, r, θ, φ), and solve the equation

$$L\psi^{(0)}_{lm} = -F_{lm}(r) r^2 e^{-i\omega u} \tag{16}$$

to find $\psi^{(0)}_{lm}$, then solve the equation

$$L\psi^{(1)}_{lm} = M\psi^{(0)}_{lm} + i\omega F_{lm}(r) r^3 e^{-i\omega u} \tag{17}$$

to find $\psi^{(1)}_{lm}$ and so on.

At this point, we are ready to state the general rules for any wave theory of the considered class:

1. *Write down the field equations in null-spherical coordinates*[13] *u, r, θ, and φ and expand*[14] *the source-function in powers of c^{-1}.*

2. *Replace c^{-1} by ϵ and consider ϵ as a variable independent of the coordinates or any other parameter of the problem.*

3. *Consider the field as a power series of ϵ and write down the field equations as a sequence of equations for the various coefficients of ϵ^n.*

4. *Solve each set of equations (each member of the sequence) from $n = 0$ up to any desired ϵ^n.*

The approximate solution of the original field equations comes from the expansion of the field in powers of ϵ by replacing ϵ with c^{-1}. Having the field as a power series of c^{-1}, we can expand the coefficient of c^{-n} in a power series of r^{-1}. In this respect, the method appears similar to the use of Liénard–Wiechert potentials and, of course, gives the same results as these potentials or any other method in electrodynamics. However, the Liénard–Wiechert potentials are solutions of the linear wave equation in flat space and do not employ expansion in powers of c^{-1}. Contrary to the Lienard–Wiechert potentials, the present approach, as stated by the four rules, is suitable for solving nonlinear field equations (the Einstein equations in general relativity).

Comparing now the above rules with those followed by Chandrasekhar,[9,10] we see that there is one essential difference: namely, the coordinate frame. In fact, Chandrasekhar uses coordinates t, r, θ, and φ and considers the field as a t-type function (defined accordingly as the u-type function). In the near zone, t and $u = t - rc^{-1}$ are approximately equal, so the field can be considered to be of u-type or t-type. Consequently, the new method is expected to give essentially the same results as the E.I.H. and post-Newtonian methods in the *near zone*. However, in the *far zone*, t and u are completely different and the field is a u-type function. Although this difference seems small, it is enough to make the present method valid at large distances, where the other methods of expansion do not apply and radiation phenomena dominate. The use of u instead of t distinguishes, in a way, two kinds of factors of c^{-1}: one coming from the expansion procedure (which is replaced by ϵ) and one which remains hidden in u and generates the retarded effects.

In Sec. 3, we will apply the rules on the Maxwell equations leaving the question of the validity of the approximation for Sec. 4.

3. THE ELECTROMAGNETIC FIELD

A. The Field Equations

The solution of the Maxwell equations using the new method will serve two purposes. First, it will inspire confidence in the new technique since the results can be compared with the known exact solutions. This is not possible in general relativity and there the method has to be trusted. Second, it will raise questions which can be answered rather easily in electrodynamics. Similar questions are expected in general relativity, and it will be better for us to be prepared since at that time our whole attention will be focused on overcoming other difficulties due to nonlinearity, physical interpretation, etc.

We can start from the covariant form of the field equations which contain the field tensor $F_{\mu\nu}$ and apply the rules. However, it is better to start from the equivalent set

$$\nabla_t \cdot \mathbf{E} = 4\pi\rho(t, r, \theta, \varphi), \tag{18}$$

$$\nabla_t \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \tag{19}$$

$$\nabla_t \cdot \mathbf{B} = 0, \tag{20}$$

$$\nabla_t \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J}(t, r, \theta, \varphi) + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}, \tag{21}$$

where ∇_t is the usual ∇ operator with the understanding that $\mathbf{E}$ and $\mathbf{B}$ are functions of the four independent variables t, r, θ, and φ. If we consider u, r, θ, and φ as the independent variables, then we must replace

$$\frac{\partial}{\partial t} \text{ by } \frac{\partial}{\partial u},$$

$$\frac{\partial}{\partial r} \text{ by } -\frac{1}{c}\frac{\partial}{\partial u} + \frac{\partial}{\partial r},$$

and leave $\partial/\partial\theta$ and $\partial/\partial\varphi$ as they are. These changes send

$$\nabla_t \cdot \mathbf{E} \text{ to } \nabla \cdot \mathbf{E} - (1/c)\hat{r}_0 \cdot \mathbf{E}_{,0}$$

and

$$\nabla_t \times \mathbf{E} \text{ to } \nabla \times \mathbf{E} + (1/c)\mathbf{E}_{,0} \times \hat{r}_0$$

and similarly for $\mathbf{B}$. The operator ∇ is given by the usual formula but with u, r, θ, and φ being the independent variables for $\mathbf{E}$, and $\hat{r}_0$ is the unit vector in the radial direction.

The sources of the field are described by $\rho(t, r, \theta, \varphi)$ and $\mathbf{J}(t, r, \theta, \varphi)$ which are considered known and do not contain c. To expand the source function, we write

$$\rho(t, r, \theta, \varphi) = \rho(u + (r/c), r, \theta, \varphi) = \rho(u + \epsilon r, r, \theta, \varphi) = \sum_{n=0}^{\infty} \frac{r^n \rho^{(n)}}{n!}\epsilon^n, \tag{22}$$

where ρ stands for $\rho(u, r, \theta, \varphi)$ [from $\rho(t, r, \theta, \varphi)$ by replacement of t by u] and $\rho^{(n)}$ the nth partial derivative of ρ with respect to u. Similarly,

$$\mathbf{J}(t, r, \theta, \varphi) = \sum_{n=0}^{\infty} \frac{r^n \mathbf{J}^{(n)}}{n!} \epsilon^n. \quad (23)$$

Obviously, the coefficients of ϵ^n in (22) and (23) do not contain ϵ (or c). Field Eqs. (18)–(21) are now

$$\nabla \cdot \mathbf{E} = 4\pi \sum_{n=0}^{\infty} \frac{r^n \rho^{(n)}}{n!} + \epsilon \mathbf{E}_{,0} \cdot \hat{r}_0, \quad (24)$$

$$\nabla \times \mathbf{E} = \epsilon \hat{r}_0 \times \mathbf{E}_{,0} - \epsilon \mathbf{B}_{,0}, \quad (25)$$

$$\nabla \cdot \mathbf{B} = \epsilon \mathbf{B}_{,0} \cdot \hat{r}_0, \quad (26)$$

$$\nabla \times \mathbf{B} = 4\pi \sum_{n=0}^{\infty} \frac{r^n \mathbf{J}^{(n)}}{n!} \epsilon^{n+1} + \epsilon \hat{r}_0 \times \mathbf{B}_{,0} + \epsilon \mathbf{E}_{,0}, \quad (27)$$

with commas denoting partial derivatives with respect to u, r, θ, φ. This completes the second step. We now assume that

$$\mathbf{E} = \sum_{n=0}^{\infty} \mathbf{E}_n \epsilon^n, \quad (28)$$

$$\mathbf{B} = \sum_{n=0}^{\infty} \mathbf{B}_n \epsilon^n, \quad (29)$$

and replacing $\mathbf{E}$ and $\mathbf{B}$ in Eqs. (24)–(27), we have, since ϵ is an independent variable,

$$\nabla \cdot \mathbf{E}_n = \frac{4\pi r^n \rho^{(n)}}{n!} + \mathbf{E}_{n-1,0} \cdot \hat{r}_0, \quad (30)$$

$$\nabla \times \mathbf{E}_n = \hat{r}_0 \times \mathbf{E}_{n-1,0} - \mathbf{B}_{n-1,0}, \quad (31)$$

$$\nabla \cdot \mathbf{B}_n = \mathbf{B}_{n-1,0} \cdot \hat{r}_0, \quad (32)$$

$$\nabla \times \mathbf{B}_n = \frac{4\pi r^{n-1} \mathbf{J}^{(n-1)}}{(n-1)!} + \hat{r}_0 \times \mathbf{B}_{n-1,0} + \mathbf{E}_{n-1,0}, \quad (33)$$

for $n = 0, 1, 2, \ldots \infty$ (we define $\mathbf{E}_{-1}$, $\mathbf{B}_{-1}$, and $\mathbf{J}^{(-1)}$ to be zero). This is a sequence of equations equivalent to the original field Eqs. (18)–(21). We see that the $(n-1)$ th approximation serves as a source (partly) of the nth approximation.

Taking the divergence of (33) (with n replaced by $n+1$), we easily find that

$$\rho^{(n+1)} + \nabla \cdot \mathbf{J}^{(n)} = 0 \quad (34)$$

for $n = 0, 1, \ldots, \infty$. This condition corresponds to the continuity equation.

B. The Superpotentials

We come now to the fourth step, namely, the solution of Eqs. (30)–(33). As these equations stand, an obvious answer is the following: If we know all the approximations up to and including the $(n-1)$ th, then Eqs. (30) and (31) [or Eqs. (32) and (33)] determine uniquely (with the boundary conditions) $\mathbf{E}_n$ (or $\mathbf{B}_n$) by specifying its divergence and curl.[15] However, we can do better than that because of the following theorem.

Theorem 1: There is a sequence of potentials Φ_n and $\mathbf{A}_n$, $n = 0, 1, 2 \ldots \infty$, such that

$$\mathbf{E}_n = -\nabla \Phi_n + \Phi_{n-1,0} \hat{r}_0 - \mathbf{A}_{n-1,0}, \quad (35)$$

$$\mathbf{B}_n = \nabla \times \mathbf{A}_n + \mathbf{A}_{n-1,0} \times \hat{r}_0 \quad (36)$$

(we define Φ_{-1} and $\mathbf{A}_{-1}$ to be zero).

Proof: We will prove the theorem by induction. In the zeroth approximation, $n = 0$, Eqs. (30)–(33) reduce to

$$\nabla \cdot \mathbf{E}_0 = 4\pi\rho, \quad (37)$$

$$\nabla \times \mathbf{E}_0 = 0, \quad (38)$$

$$\nabla \cdot \mathbf{B}_0 = 0, \quad (39)$$

$$\nabla \times \mathbf{B}_0 = 0, \quad (40)$$

with physically acceptable solution (falling off as r^{-1} for large r)

$$\mathbf{E}_0 = -\nabla \Phi_0, \quad (41)$$

$$\mathbf{B}_0 = 0, \quad (42)$$

where[16]

$$\Phi_0 = \int \frac{\rho(u, r', \theta', \varphi')}{|\mathbf{r} - \mathbf{r}'|} dV'. \quad (43)$$

Obviously, Eqs. (41) and (42) can be derived from (35) and (36) with Φ_0 given as above and $\mathbf{A}_0 = 0$. Hence, the theorem holds for $n = 0$.

We assume that it holds for a specific n, namely, that Eqs. (35) and (36) are true for a fixed n. We have

$$\hat{r}_0 \times \mathbf{E}_{n,0} - \mathbf{B}_{n,0} = -\hat{r}_0 \times \nabla \Phi_{n,0} - \nabla \times \mathbf{A}_{n,0} = \nabla \times [\Phi_{n,0} \hat{r}_0 - \mathbf{A}_{n,0}] \quad (44)$$

and

$$\mathbf{B}_{n,0} \cdot \hat{r}_0 = \hat{r}_0 \cdot \nabla \times \mathbf{A}_{n,0} = \nabla \cdot (\mathbf{A}_{n,0} \times \hat{r}_0). \quad (45)$$

Hence, the equations resulting from (31) and (32) with replacement of n by $n+1$ will be satisfied whatever the choice of Φ_{n+1} and $\mathbf{A}_{n+1}$ is. Hence, Φ_{n+1} and $\mathbf{A}_{n+1}$ must be chosen so that $\mathbf{E}_{n+1}$ and $\mathbf{B}_{n+1}$ satisfy Eqs. (30) and (33) after replacing $n+1$. This means that Φ_{n+1} and $\mathbf{A}_{n+1}$ must obey the equations

$$\nabla^2 \Phi_{n+1} = -\frac{4\pi r^{n+1} \rho^{(n+1)}}{(n+1)!} + 2\Phi_{n,01} + 2\frac{\Phi_{n,0}}{r} - \Phi_{n-1,00} - \nabla \cdot \mathbf{A}_{n,0} + \mathbf{A}_{n-1,00} \cdot \hat{r}_0 \quad (46)$$

and

$$\nabla \times (\nabla \times \mathbf{A}_{n+1}) = +\frac{4\pi r^n \mathbf{J}^{(n)}}{n!} - 2\mathbf{A}_{n,01} - \frac{2\mathbf{A}_{n,0}}{r} + (\nabla \cdot \mathbf{A}_{n,0}) \hat{r}_0 + \nabla(\hat{r}_0 \cdot \mathbf{A}_{n,0}) - (\mathbf{A}_{n-1,00} \cdot \hat{r}_0) \hat{r}_0 - \nabla \Phi_{n,0} + \Phi_{n-1,00} \hat{r}_0. \quad (47)$$

These equations have always a solution; so this completes the theorem.

Equations (46) and (47) do not specify uniquely Φ_{n+1} and $\mathbf{A}_{n+1}$. In what follows we assume the gauge condition

$$\nabla\cdot\mathbf{A}_n - \mathbf{A}_{n-1,0}\cdot\hat{r}_0 + \Phi_{n-1,0} = 0 \tag{48}$$

and we ask from Φ_n and $\mathbf{A}_n$ to fall off as r^{-1} at infinity. Because of (48), Eqs. (46) and (47) reduce to (replacing $n+1$ by n)

$$\nabla^2\Phi_n = -\frac{4\pi r^n \rho^{(n)}}{n!} + 2\frac{\Phi_{n-1,0}}{r} + 2\Phi_{n-1,01} \tag{49}$$

and

$$\nabla^2\mathbf{A}_n = -\frac{4\pi r^{n-1}\mathbf{J}^{(n-1)}}{(n-1)!} + 2\frac{\mathbf{A}_{n-1,0}}{r} + 2\mathbf{A}_{n-1,01}. \tag{50}$$

The above introduced potentials are nothing else than the expansions of the usual Φ and $\mathbf{A}$. Equation (48) corresponds to the Lorentz gauge. In this gauge Φ_n and $\mathbf{A}_n$ are uniquely[17] determined as the solutions of Eqs. (49) and (50) which have continuous second derivatives and fall off as r^{-1} for large r. We will call Φ_n and $\mathbf{A}_n$ *superpotentials* because Φ_{n-1} and $\mathbf{A}_{n-1}$ contribute as sources to Φ_n and $\mathbf{A}_n$, as the case is for the superpotentials of the Newtonian gravitational theory introduced by Chandrasekhar and Lebovitz.[18] There is, however, an essential difference. Although Φ_{n-1} and $\mathbf{A}_{n-1}$ are in general of order r^{-1} for large r, the combinations $r^{-1}\Phi_{n-1,0} + \Phi_{n-1,01}$ and $r^{-1}\mathbf{A}_{n-1,0} + \mathbf{A}_{n-1,01}$ are such that the right-hand sides of (49) and (50) are of order r^{-3}. And exactly because of this, a solution $\Phi_n = \mathcal{O}(r^{-1})$, $\mathbf{A}_n = \mathcal{O}(r^{-1})$ exists, contrary to the superpotentials of Chandrasekhar and Lebovitz.

At this point, it appears that determination of $\mathbf{E}_n$, $\mathbf{B}_n$, Φ_n, and $\mathbf{A}_n$ requires solution of all the approximations from $n = 0$ up to n and calculation of integrals over all space. However, the following theorem simplifies the situation.

Theorem 2: If Φ_n and $\mathbf{A}_n$ satisfy everywhere Eqs. (49) and (50), respectively, and are twice continuously differentiable and are of order r^{-1} as $r\to\infty$, then

$$\Phi_n = \frac{1}{n!}\int \rho^{(n)}\frac{(r - |\mathbf{r}-\mathbf{r}'|)^n}{|\mathbf{r}-\mathbf{r}'|}\,dV' \tag{51}$$

and

$$\mathbf{A}_n = \frac{1}{(n-1)!}\int \mathbf{J}^{(n-1)}\frac{(r - |\mathbf{r}-\mathbf{r}'|)^{n-1}}{|\mathbf{r}-\mathbf{r}'|}\,dV' \tag{52}$$

for $n = 0, 1, 2, \ldots \infty$.

Proof: We can verify by direct substitution (after some calculations) that Φ_n and $\mathbf{A}_n$, as given by (51) and (52), satisfy (49) and (50). Since the solutions of these equations are unique under the assumptions of Theorem 2,[17] Eqs. (51) and (52) give just these solutions.[19]

This theorem enables us to calculate the superpotentials for a fixed n directly from the source function. Then $\mathbf{E}_n$ and $\mathbf{B}_n$ can be derived from Eqs. (35) and (36).

C. The Radiation Zone

Far from the source, we can expand the field in powers of r^{-1} and write

$$X_n = X_n^1 r^{-1} + \mathcal{O}(r^{-2}), \tag{53}$$

where X_n stands for $\mathbf{E}_n$, $\mathbf{B}_n$, Φ_n, or $\mathbf{A}_n$. Since ∇ acting on X_n always gives terms of order r^{-2}, we have from (48)

$$\mathbf{A}_{n-1,0}\cdot\hat{r}_0 - \Phi_{n-1,0} = \mathcal{O}(r^{-2}), \tag{54}$$

and from (35) and (36), we conclude that

$$\mathbf{E}_n^1 = (\mathbf{A}_{n-1,0}^1\times\hat{r}_0)\times\hat{r}_0 \tag{55}$$

$$\mathbf{B}_n^1 = \mathbf{A}_{n-1,0}^1\times\hat{r}_0. \tag{56}$$

Since $\mathbf{A}_0^1 = 0$, $\mathbf{E}_n^1$ and $\mathbf{B}_n^1$ can be nonzero only for $n \geqslant 2$.

Calling

$$\cos\gamma = \hat{r}_0\cdot\hat{r}_0', \tag{57}$$

we have

$$\frac{(r - |\mathbf{r}-\mathbf{r}'|)^n}{|\mathbf{r}-\mathbf{r}'|} = \frac{r'^n\cos^n\gamma}{r} + \mathcal{O}\left(\frac{1}{r^2}\right), \tag{58}$$

and from (52),

$$\mathbf{A}_n^1 = \frac{1}{(n-1)!}\int \mathbf{J}^{(n-1)} r'^{n-1}\cos^{n-1}\gamma\, dV'. \tag{59}$$

Using the addition theorem for spherical harmonics, we get

$$\cos^n\gamma = \sum_{l,m}\frac{4\pi c_l^n}{2l+1}Y_{lm}^*(\theta',\varphi')Y_{lm}(\theta,\varphi), \tag{60}$$

where[20]

$$c_l^n = (2l+1)n!/(n-l)!!(n+l+1)!! \tag{61}$$

for $n-l$ even nonnegative and otherwise zero. Combining (59) and (60), we find $\mathbf{A}_n$ in the radiation zone to be

$$\mathbf{A}_n^1 = \frac{4\pi}{(n-1)!}\sum_{l,m}\frac{c_l^{n-1}}{2l+1}Y_{lm}(\theta,\varphi) \cdot\int r'^{n-1}\mathbf{J}^{(n-1)}Y_{lm}^*(\theta',\varphi')\,dV'. \tag{62}$$

The above expression for $\mathbf{A}_n^1$ and Eqs. (55) and (56) determine completely the radiation field in terms of the source.

For $n = 2$ a detailed calculation gives

$$\mathbf{B}_2^1 = \mathbf{D}_{,00}\times\hat{r}_0, \tag{63}$$

where

$$\mathbf{D} = \int \mathbf{r}'\rho\, dV'; \tag{64}$$

in other words, we have the *dipole radiation*.

For $n = 3$ we have

$$\mathbf{B}_3^1 = (\mathbf{m}_{,00} \times \hat{r}_0) \times \hat{r}_0 - (1/6)\hat{r}_0 \times \mathbf{Q}_{,000}, \quad (65)$$

where the vector **Q** has components along the x, y, z axes[21]

$$Q_\alpha = \sum_\beta Q_{\alpha\beta}\cdot(\hat{r}_0)_\beta, \quad \alpha, \beta = 1, 2, 3, \quad (66)$$

$$Q_{\alpha\beta} = \int (3x_\alpha x_\beta - r^2\delta_{\alpha\beta})\rho dV, \quad (67)$$

and

$$\mathbf{m} = \tfrac{1}{2}\int \mathbf{r}' \times \mathbf{J} dV, \quad (68)$$

namely, the *magnetic dipole* and *electric quadrupole radiation.*[22]

4. THE VALIDITY OF THE METHOD

In the E.I.H. and post-Newtonian methods,[7-11] the expansion in powers of c^{-1} has been based essentially on the assumption of slow motion and not too strong fields. Accordingly, the question is raised here whether there are similar limitations for the present method. Remarkably enough the answer is negative. In other words, *there is no limit on how close to the exact solution we can get.* Although Eqs. (63) and (65) are the dipole and quadrupole distributions only in the slow motion (wavelength large compared to the dimensions of the source) limit, the higher approximations ($n > 3$) will contribute more terms to the dipole and quadrupole radiation, so that at the limit $n \to \infty$ we have the exact multipoles.

To be more precise, let $\rho(t, \mathbf{r})$ and $\mathbf{J}(t, \mathbf{r})$ represent a bounded source and let the potentials $\Phi(t, \mathbf{r})$ and $\mathbf{A}(t, \mathbf{r})$ of the resulting electromagnetic field be given by the well-known retarded integrals

$$\Phi(t, \mathbf{r}) = \int \frac{[\rho(t, \mathbf{r}')]_{\text{ret}}}{|\mathbf{r} - \mathbf{r}'|} dV' \quad (69)$$

and

$$\mathbf{A}(t, \mathbf{r}) = \frac{1}{c}\int \frac{[\mathbf{J}(t, \mathbf{r}')]_{\text{ret}}}{|\mathbf{r} - \mathbf{r}'|} dV'. \quad (70)$$

This is the usual approach in electrodynamics.

If we follow the method of this paper and calculate Φ_n and $\mathbf{A}_n$ from (51) and (52), *then*

$$\Phi(t, \mathbf{r}) = \sum_{n=0}^{\infty} \Phi_n \epsilon^n \quad (71)$$

and

$$\mathbf{A}(t, \mathbf{r}) = \sum_{n=0}^{\infty} \mathbf{A}_n \epsilon^n. \quad (72)$$

Hence *the two series,*

$$\sum_{n=0}^{\infty} \Phi_n \epsilon^n \quad \text{and} \quad \sum_{n=0}^{\infty} \mathbf{A}_n \epsilon^n \quad (73)$$

converge at a point (t, r) *in the same way* (uniformly or otherwise) *as the integrals (69) and (70) do* (or diverge if the integrals (69) and (70) do so). In other words, the knowledge of Φ_n and $\mathbf{A}_n$ for all n is *equivalent* to the knowledge of the retarded potentials. The proof of (71) and (72) is straightforward, i.e.,

$$\begin{aligned}\sum_{n=0}^{\infty} \Phi_n \epsilon^n &= \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!}\int \rho^{(n)}(u, \mathbf{r}')\frac{(r - |\mathbf{r} - \mathbf{r}'|)^n}{|\mathbf{r} - \mathbf{r}'|} dV' \\ &= \int \frac{\rho(u + \epsilon r - \epsilon|\mathbf{r} - \mathbf{r}'|, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' \\ &= \int \frac{\rho(t - c^{-1}|\mathbf{r} - \mathbf{r}'|, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' \\ &= \int \frac{[\rho(t, \mathbf{r}')]_{\text{ret}}}{|\mathbf{r} - \mathbf{r}'|} dV' = \Phi(t, \mathbf{r}) \end{aligned} \quad (74)$$

and similarly for $\mathbf{A}(t, \mathbf{r})$.

Since the series (73) converge, we can represent $\Phi(t, \mathbf{r})$ and $\mathbf{A}(t, \mathbf{r})$ by taking a finite number of terms in (71) and (72). If we have slow motion ($v \ll c$), the first approximations are enough. If we have large velocities or strong fields, we have to take more terms.

In general relativity, difficulties will arise as a result of the nonlinearity of the original field equations. In fact, we do not expect to have general formulas for any n as in (51) and (52) or theorems similar to the theorems of Sec. 3, and the question of convergence of the expansion cannot be answered rigorously.

5. CONCLUSION

From the application of the new method in electrodynamics, it is reasonable to claim at this point that the presented method constitutes an alternative way to the usual procedures in attacking electromagnetic problems. Moreover, it can be said that this method is preferable when a Fourier analysis of the source is difficult or when the usual integrals involving Bessel functions are too complicated compared to those of Eqs. (51) and (52).

Since the method does not depend on the original field equations, we can use it to study the field produced by a bounded source in any theory which predicts wave phenomena in a locally Minkowskian space-time. In the wave theories examined in this paper (scalar waves and electrodynamics), it is perfectly reasonable and proper to specify first the sources and then attempt to solve for the fields. However, such a procedure is inappropriate for general relativity. Fortunately, the application of the introduced method requires only the form of the energy-momentum tensor (as for example for a source of perfect fluid) and not the exact behavior of the source. In this respect, the method is similar to the E.I.H. and post-Newtonian expansions.

In Sec. 3C, we demonstrated the procedure through which the field in the far zone can be related to the source. The expansion in powers of r^{-1} holds only in the far zone and, consequently, must follow the expansion in powers of c^{-1} which holds everywhere. In this respect, the present method provides the studies of the far zone[1-6] (which employ expansion in powers of r^{-1} only) with the missing part: the tools to calculate the field in the far zone (the news function, the Newman–Penrose constants, etc.) in terms of the source.

In a future paper, we will use the method in general relativity to relate the gravitational radiation to the source by giving an explicit expression of the news function[1] in terms of the density, pressure, and other characteristics of the source. This could open the way for the definition of gravitational multipole moments in terms of the source and the physical interpretation of the Newman–Penrose constants.

ACKNOWLEDGMENTS

I wish to thank Dr. Robert Geroch and the referee for suggesting some improvements in the presentation of the paper.

---

* Supported in part by the National Science Foundation (Grant No. GP-20033) and by the Center for Relativity Theory, University of Texas at Austin.

1 H. Bondi, M. G. J. van der Burg, and A. W. K. Metzner, Proc. Roy. Soc. (London) A **269**, 21 (1962).
2 E. T. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962); **4**, 998 (1962).
3 R. K. Sachs, Proc. Roy. Soc. (London) A **270**, 103 (1962).
4 E. T. Newman and T. W. J. Unti, J. Math. Phys. **3**, 891 (1962).
5 E. T. Newman and R. Penrose, Proc. Roy. Soc. (London) A **305**, 175 (1968).
6 S. Persides, Proc. Roy. Soc. (London) A **320**, 349 (1970).
7 See, for example, I. Infeld and J. Plebanski, *Motion and Relativity* (Pergamon, London, 1960).
8 V. Fock, *The Theory of Space, Time and Gravitation* (Pergamon, London, 1964), 2nd ed.
9 S. Chandrasekhar, Astrophys. J. **142**, 1488 (1965).
10 S. Chandrasekhar and F. Paul Esposito, Astrophys. J. **160**, 153 (1970).
11 W. Burke, J. Math. Phys. **12**, 401 (1971).
12 J. D. Jackson, *Classical Electrodynamics* (John Wiley, New York, 1962), p. 540. The notation of this reference will be followed concerning the Bessel functions, spherical harmonics, and generally the wave equation and the electromagnetic field.
13 In coordinates u, r, θ, φ, the flat-space metric $b_{\mu\nu}$ is $b_{00} = \epsilon^{-2}, b_{01} = \epsilon^{-1}, b_{22} = -r^2, b_{33} = -r^2 \sin^2\theta$ with the remaining $b_{\mu\nu}$ equal to zero ($\epsilon = c^{-1}$). In general relativity, asymptotically null-spherical coordinates can be used (see Ref. 6).
14 It is assumed that the source functions $f(t, \mathbf{r})$ and later $\rho(t, \mathbf{r})$ and $\mathbf{J}(t, \mathbf{r})$ do not contain c. Consequently, the expansion procedure is clearly demonstrated by (22).
15 G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers* (McGraw-Hill, New York, 1968), 2nd ed., p. 166.
16 Integrals with unspecified limits are taken over that part of space in which the integrand is not zero.
17 See, for example, Ref. 15, p. 524.
18 S. Chandrasekhar and N. Lebovitz, Astrophys. J. **135**, 238 (1962).
19 Again, the similarity is pointed out of Φ_n and $\mathbf{A}_n$, as expressed by Eqs. (51) and (52), with the superpotentials of the Newtonian Gravitation.
20 O. D. Kellog, *Foundations of Potential Theory* (Dover, New York, 1953), p. 132.
21 See Ref. 12, p. 275.
22 It must be emphasized that (63) and (65) give the dipole and quadrupole distribution only in the long wavelength approximation. The complete moments require the calculation of $\mathbf{A}_n^1$ for all n (see also Sec. 4).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

${}_3F_2$ Representations for Spin Projection Coefficients

Koichi Mano
Air Force Cambridge Research Laboratories, Bedford, Massachusetts 01730
(Received 18 February 1971)

It is shown that a variety of equivalent representations for the spin projection coefficient, given in terms of the generalized hypergeometric function with unit argument, ${}_3F_2[1]$, can be generated by applying Whipple's theory to the function.

I. INTRODUCTION

Apparently dissimilar representations for the spin projection coefficient (SPC) were obtained by Sasaki and Ohno[1] and by Smith.[2] Equality of these representations was proved by Smith and Harris[3] by rewriting them in terms of an ${}_3F_2$ series, after applying certain identities for binomial coefficients to the Smith representation.

The purpose of this paper is to show in some detail[4] that an application of the ${}_3F_2$ theory developed by Whipple[5] gives a variety of equivalent ${}_3F_2$ forms for SPC such that the equality mentioned above follows directly from the theory.

II. SOME ${}_3F_2$ FORMS FOR SPC

The SPC that may be defined by[3]

$$C_j(S, M, n) = (-1)^j (2S+1) \int_0^1 {}_2F_1\left[\begin{matrix} -S+M, 1+S+M; z \\ 1 \end{matrix}\right] \times z^j (1-z)^{n-j+M} dz \qquad (1)$$

can be calculated by expanding the ${}_2F_1$ and evaluating the first Eulerian integral that arises there, in the following form:

$$C^1 = (-1)^j \frac{2S+1}{n+M+1} \binom{n+M}{j}^{-1} \times {}_3F_2\left[\begin{matrix} -S+M, 1+S+M, j+1; 1 \\ 1, n+M+2 \end{matrix}\right],$$

$$n - j + M + 1 > 0. \qquad (2)$$

(the news function, the Newman–Penrose constants, etc.) in terms of the source.

In a future paper, we will use the method in general relativity to relate the gravitational radiation to the source by giving an explicit expression of the news function[1] in terms of the density, pressure, and other characteristics of the source. This could open the way for the definition of gravitational multipole moments in terms of the source and the physical interpretation of the Newman-Penrose constants.

ACKNOWLEDGMENTS

I wish to thank Dr. Robert Geroch and the referee for suggesting some improvements in the presentation of the paper.

* Supported in part by the National Science Foundation (Grant No. GP-20033) and by the Center for Relativity Theory, University of Texas at Austin.

1 H. Bondi, M. G. J. van der Burg, and A. W. K. Metzner, Proc. Roy. Soc. (London) A **269**, 21 (1962).
2 E. T. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962); **4**, 998 (1962).
3 R. K. Sachs, Proc. Roy. Soc. (London) A **270**, 103 (1962).
4 E. T. Newman and T. W. J. Unti, J. Math. Phys. **3**, 891 (1962).
5 E. T. Newman and R. Penrose, Proc. Roy. Soc. (London) A **305**, 175 (1968).
6 S. Persides, Proc. Roy. Soc. (London) A **320**, 349 (1970).
7 See, for example, I. Infeld and J. Plebanski, *Motion and Relativity* (Pergamon, London, 1960).
8 V. Fock, *The Theory of Space, Time and Gravitation* (Pergamon, London, 1964), 2nd ed.
9 S. Chandrasekhar, Astrophys. J. **142**, 1488 (1965).
10 S. Chandrasekhar and F. Paul Esposito, Astrophys. J. **160**, 153 (1970).
11 W. Burke, J. Math. Phys. **12**, 401 (1971).
12 J. D. Jackson, *Classical Electrodynamics* (John Wiley, New York, 1962), p. 540. The notation of this reference will be followed concerning the Bessel functions, spherical harmonics, and generally the wave equation and the electromagnetic field.
13 In coordinates u, r, θ, φ, the flat-space metric $b_{\mu\nu}$ is $b_{00} = \epsilon^{-2}, b_{01} = \epsilon^{-1}, b_{22} = -r^2, b_{33} = -r^2 \sin^2\theta$ with the remaining $b_{\mu\nu}$ equal to zero ($\epsilon = c^{-1}$). In general relativity, asymptotically null-spherical coordinates can be used (see Ref. 6).
14 It is assumed that the source functions $f(t, \mathbf{r})$ and later $\rho(t, \mathbf{r})$ and $\mathbf{J}(t, \mathbf{r})$ do not contain c. Consequently, the expansion procedure is clearly demonstrated by (22).
15 G. A. Korn and T. M. Korn, *Mathematical Handbook for Scientists and Engineers* (McGraw-Hill, New York, 1968), 2nd ed., p. 166.
16 Integrals with unspecified limits are taken over that part of space in which the integrand is not zero.
17 See, for example, Ref. 15, p. 524.
18 S. Chandrasekhar and N. Lebovitz, Astrophys. J. **135**, 238 (1962).
19 Again, the similarity is pointed out of Φ_n and $\mathbf{A}_n$, as expressed by Eqs. (51) and (52), with the superpotentials of the Newtonian Gravitation.
20 O. D. Kellog, *Foundations of Potential Theory* (Dover, New York, 1953), p. 132.
21 See Ref. 12, p. 275.
22 It must be emphasized that (63) and (65) give the dipole and quadrupole distribution only in the long wavelength approximation. The complete moments require the calculation of $\mathbf{A}_n^1$ for all n (see also Sec. 4).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

${}_3F_2$ Representations for Spin Projection Coefficients

Koichi Mano

Air Force Cambridge Research Laboratories, Bedford, Massachusetts 01730

(Received 18 February 1971)

It is shown that a variety of equivalent representations for the spin projection coefficient, given in terms of the generalized hypergeometric function with unit argument, ${}_3F_2[1]$, can be generated by applying Whipple's theory to the function.

I. INTRODUCTION

Apparently dissimilar representations for the spin projection coefficient (SPC) were obtained by Sasaki and Ohno[1] and by Smith.[2] Equality of these representations was proved by Smith and Harris[3] by rewriting them in terms of an ${}_3F_2$ series, after applying certain identities for binomial coefficients to the Smith representation.

The purpose of this paper is to show in some detail[4] that an application of the ${}_3F_2$ theory developed by Whipple[5] gives a variety of equivalent ${}_3F_2$ forms for SPC such that the equality mentioned above follows directly from the theory.

II. SOME ${}_3F_2$ FORMS FOR SPC

The SPC that may be defined by[3]

$$C_j(S, M, n) = (-1)^j(2S+1)\int_0^1 {}_2F_1\left[\begin{matrix}-S+M, 1+S+M; z\\ 1\end{matrix}\right] \times z^j(1-z)^{n-j+M}dz \quad (1)$$

can be calculated by expanding the ${}_2F_1$ and evaluating the first Eulerian integral that arises there, in the following form:

$$C^1 = (-1)^j \frac{2S+1}{n+M+1}\binom{n+M}{j}^{-1} \times {}_3F_2\left[\begin{matrix}-S+M, 1+S+M, j+1; 1\\ 1, n+M+2\end{matrix}\right],$$

$$n-j+M+1 > 0. \quad (2)$$

Our concern in this section is to point out that SPC may be represented by many other forms of ${}_3F_2$. Thus, the application to Eq. (1) of the two-term relations

$$ {}_2F_1[a,b;c;z] = (1-z)^{c-a-b}\,{}_2F_1[c-a,c-b;c;z] \quad (3)$$

$$ = (1-z)^{-a}\,{}_2F_1\left[a,c-b;c;\frac{z}{z-1}\right], \quad (4)$$

with $a=-S+M, b=1+S+M$, and $c=1$, gives rise, respectively, to[6]

$$C^2 = \frac{(-1)^j(2S+1)}{n-M+1}\binom{n-M}{j}^{-1} \times {}_3F_2\left[\begin{matrix}-S-M,1+S-M,j+1;1\\ 1,n-M+2\end{matrix}\right],$$
$$n-j-M+1>0, \quad (5)$$

$$C^3 = \frac{(-1)^j(2S+1)}{n+S+1}\binom{n+S}{j}^{-1} \times {}_3F_2\left[\begin{matrix}-S+M,-S-M,j+1;1\\ 1,j-n-S\end{matrix}\right],$$
$$n-j+M+1>0. \quad (6)$$

The re-expressed form of Eq. (6) [Eq. (19) of Ref. 3]

$$\frac{(-1)^j(2S+1)}{n+S+1}\sum_k(-1)^k\binom{S-M}{k}\binom{S+M}{k}\binom{n+S}{j+k}^{-1} \quad (7)$$

will be referred to here as the Smith representation for SPC. In passing, we note that the symmetry of $C_j(S,M,n)$ in M can be made explicit by the use of Eq. (3).

Similarly, the use of three-term relations,[7] such as

$$ {}_2F_1\left[\begin{matrix}a,b;z\\ c\end{matrix}\right] = \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}(-z)^{-a} \times {}_2F_1\left[\begin{matrix}a,1-c+a;\frac{1}{z}\\ 1-b+a\end{matrix}\right] + (a\leftrightarrow b),$$

whose second term on the right-hand side vanishes, leads to

$$C^4 = \frac{(-1)^{j+S-M}(2S+1)!(n-j+M)!(S-M+j)!}{(S+M)!(S-M)!(n+S+1)!} \times {}_3F_2\left[\begin{matrix}-S+M,-S+M,-n-S-1;1\\ -2S,-j-S+M\end{matrix}\right],$$
$$n-j+M+1>0. \quad (8)$$

Further, we note that some other means help us augment the number of ${}_3F_2$ forms for SPC. Thus, direct rewriting of Eqs. (22), (26), and (27) of Ref. 3 produces, respectively,

$$C^5 = \frac{(S+M)!(n-M)!}{(2S)!(n-S)!}\binom{S-M}{j}\binom{n-M}{j}^{-1} \times {}_3F_2\left[\begin{matrix}1+S-M,1+S-M,-n+S;1\\ 1+S-M-j,2S+2\end{matrix}\right],$$
$$S-M-j+1>0, \quad (9)$$

$$C^6 = \frac{(2S+1)(n+M)!(n-M)!}{(n+S+1)!(n-S)!}\binom{S-M}{j}\binom{n-M}{j}^{-1} \times {}_3F_2\left[\begin{matrix}1+S-M,-n+S,-j;1\\ -n-M,1+S-M-j\end{matrix}\right],$$
$$S-M-j+1>0, \quad (10)$$

$$C^7 = \frac{(-1)^j(2S+1)(n+M)!(n-M)!}{(n+S+1)!(n-S)!} \times \binom{n-S}{j}\binom{n+M}{j}^{-1}\binom{n-M}{j}^{-1} \times {}_3F_2\left[\begin{matrix}-S-M,-S+M,-j;1\\ 1,n-S-j+1\end{matrix}\right],$$
$$n-S-j+1>0. \quad (11)$$

Also, in general, we may expect to obtain new forms by summing in reverse order[8] the finite ${}_3F_2$ terms in C's found above.

At this point, it is appropriate to rewrite the Sasaki-Ohno representation [Eq. (3.17) of Ref. 1]

$$\frac{(2S+1)(S+M)!(n-j-M)!}{(S-M)!}\sum_k\frac{(-1)^k[\Gamma(S-M+k+1)]^2}{k!\,\Gamma(S-M+k-j+1)\Gamma(n-S-k+1)\Gamma(2S+k+2)} \quad (12)$$

in terms of a ${}_3F_2$, which can readily be found to coincide with C^5.

In the foregoing, we indicated that the SPC, $C_j(S,M,n)$, can be represented by various forms of ${}_3F_2$. Their equivalence is evident by retracing the ways through which they were found. Here, let us suppose instead that we are interested in proving the equivalence by regarding them as just given to us without reference to their origins. It can be done by utilizing appropriate two- and three-term ${}_3F_2$ relations such as[9]

$$ {}_3F_2\left[\begin{matrix}a,b,c;1\\ e,f\end{matrix}\right] = \frac{\Gamma[f,s]}{\Gamma[f-c,s+c]}\,{}_3F_2\left[\begin{matrix}e-a,e-b,c;1\\ e,s+c\end{matrix}\right], \quad (13)$$

where $\Gamma[a,b,\ldots] = \Gamma[a]\Gamma[b]\cdots$ and $s=e+f-a-b-c$. In proving the equality of a pair of C's, we may apply these relations in a variety of ways to obtain many multistep routes that connect the pair. In view of the fact that ${}_3F_2$'s thus obtained are all equivalent to each other, the procedure may lead to the possibility of finding an increasingly large number of $_3F_2$ forms for SPC, when combined with the symmetry of $C_j(S,M,n)$ in M as mentioned earlier.

Questions then arise as to whether one can make any statement regarding the number of equivalent $_3F_2$ forms that can represent $C_j(S,M,n)$ and also as to a systematic method, if any, by which these forms can be exhausted. A key to the solution of this problem can be found in Whipple's theory for $_3F_2$ that will be described next.

III. WHIPPLE'S THEORY

In order to systematically study the numerous two- and three-term $_3F_2$ relations found by Thomae,[10] such as those mentioned in Ref. 9, Whipple introduced functions F_p and F_n as follows.

Let r_i, $i = 0, 1, \ldots, 5$, be numbers such that $\sum_{i=0}^{5} r_i = 0$, and α and β are associated with them by $\alpha_{lmn} = \frac{1}{2} + r_l + r_m + r_n$ and $\beta_{mn} = 1 + r_m - r_n$. The functions are then defined by

$$F_p(u; v, w) = \frac{1}{\Gamma(\alpha_{xyz}, \beta_{vu}, \beta_{wu})} {}_3F_2\begin{bmatrix}\alpha_{vwx}, \alpha_{vwy}, \alpha_{vwz}; 1\\ \beta_{vu}, \beta_{wu}\end{bmatrix}, \tag{14}$$

$$F_n(u; v, w) = \frac{1}{\Gamma(\alpha_{uvw}, \beta_{uv}, \beta_{uw})} {}_3F_2\begin{bmatrix}\alpha_{uyz}, \alpha_{uzx}, \alpha_{uxy}; 1\\ \beta_{uv}, \beta_{uw}\end{bmatrix}. \tag{15}$$

Here $\{u, v, w\}$ and $\{x, y, z\}$ are cosets of each other relative to the set $\{i \mid 0 \le i \le 5\}$. The F_n function is derived from the corresponding F_p by changing the signs of all r's. Through permutation of suffixes u, v, and w, we can find 60 F_p's and 60 F_n's.

If we set $\alpha_{145} = a$, $\alpha_{245} = b$, $\alpha_{345} = c$, $\beta_{40} = e$, $\beta_{50} = f$, and $\alpha_{123} = s$, it can be shown that $F_p(0; 4, 5) \propto {}_3F_2[a, b, c; e, f; 1]$ and all of the F_p's and F_n's are expressible in appropriate $_3F_2$'s.

Whipple showed that ten of $F_p(u; v, w)$ with the same u are all equal and hence may be denoted $F_p(u)$, and similarly for $F_n(u)$.

When c, say, is a nonpositive integer $-m$, Whipple showed that the following relations obtain:

$$\begin{aligned}\Gamma(\alpha_{123}, \alpha_{124}, \alpha_{125})F_p(0) &= \Gamma(\alpha_{023}, \alpha_{024}, \alpha_{025})F_p(1)\\ &= \Gamma(\alpha_{013}, \alpha_{014}, \alpha_{015})F_p(2)\\ &= (-1)^m\Gamma(\alpha_{123}, \alpha_{023}, \alpha_{013})F_n(3)\\ &= (-1)^m\Gamma(\alpha_{124}, \alpha_{024}, \alpha_{014})F_n(4)\\ &= (-1)^m\Gamma(\alpha_{125}, \alpha_{025}, \alpha_{015})F_n(5).\end{aligned} \tag{16}$$

This means that altogether 60 of $_3F_2$'s in the collection of $F_p(0)$, $F_p(1)$, $F_p(2)$, $F_n(3)$, $F_n(4)$, and $F_n(5)$, called Set I, are mutually proportional. By reversing the signs of r's in Eq. (16), we obtain similar relations in which $F_n(0)$, $F_n(1)$, $F_n(2)$, $F_p(3)$, $F_p(4)$, and $F_p(5)$, called Set II, are involved.

Based on Whipple's theory, let us list 120 of the $_3F_2$'s, starting with $F_p(0; 4, 5) \propto {}_3F_2[a, b, c; e, f; 1]$ with $a = 1 + S + M$, $b = j + 1$, $c = -S + M$, $e = 1$, and $f = n + M + 2$. An inspection of the list reveals that $F_p(0; 2, 4) = F_p(4; 0, 2) \propto C^2$, $F_p(0; 4, 5) = F_p(4; 0, 5) \propto C^1$, $F_p(4; 0, 3) = F_p(0; 3, 4) \propto C^7$, $F_p(5; 0, 1) = F_p(5; 1, 4) \propto C^6$, $F_n(0; 1, 4) = F_n(4; 0, 1) \propto C^3$, $F_n(1; 3, 5) \propto C^5$, and $F_n(3; 1, 2) \propto C^4$.

For these representative C's, we observe that (i) $C^1 = C^2 = C^7 = F_p(0)$, (ii) $C^1 = C^3 = C^4$ from proportionality of members of Set I, and (iii) $C^3 = C^5 = C^6$ from the corresponding property for Set II. The fact that C^1, C^2, and C^7 appear concurrently in Sets I and II as $F_p(0)$ and $F_p(4)$, respectively, for example, leads us to conclude that 120 $_3F_2$'s that correspond to the totality of Sets I and II are in fact all proportional to each other.

This shows that one can generate a large number of equivalent $_3F_2$ forms for SPC by starting from C^1 that follows directly from Eq. (1). These forms include in particular C^5 and C^3 that correspond to the Sasaki–Ohno and the Smith representations, respectively. In the light of Whipple's theory, then, the equivalence of these representations is an immediate consequence of the theory.

Note that the present case of integer values for parameters a, b, c, e, and f represents a deviation from the general conditions assumed for the Whipple's theory. A consequence of this is that some of the 120 $_3F_2$'s are degenerate [e.g., $F_p(0; 2, 4) = F_p(4; 0, 2)$] or may not be defined, resulting in reduction of the total number of different $_3F_2$ forms for SPC.

Finally, we will make two remarks. The first is that each C is valid under a certain condition, such as $n - j + M + 1 > 0$ for C^1. Equivalence of a pair of C's implies, then, that it holds in the overlapping portion of the validity region for the two. The second refers to the utility of selecting the most convenient form for actual evaluation of SPC. In particular, selecting one with the form $_3F_2[0, \ldots; \ldots; 1]$ or $_3F_2[a, \ldots; a, \ldots; 1]$, if any, will obviously be desirable. In the latter case, it reduces to a $_2F_1$ for which Gauss' or Vandermonde's theorem may be available.

IV. CONCLUSION

It has been shown that numerous equivalent $_3F_2$ forms for SPC can be generated by the use of Whipple's theory. Included are those corresponding to the Sasaki–Ohno and the Smith representations. It has been shown, therefore, that the equivalence of the two representations is an immediate consequence of Whipple's theory, once they are reexpressed in terms of $_3F_2$.

1 F. Sasaki and K. Ohno, J. Math. Phys. **4**, 1140 (1663).
2 V. H. Smith, Jr., J. Chem. Phys. **41**, 277 (1964).
3 V. H. Smith, Jr. and F. E. Harris, J. Math. Phys. **10**, 771 (1969).
4 K. Mano, J. Chem. Phys. **52**, 2785 (1970).
5 F. J. W. Whipple, Proc. London Math. Soc. **23**, 104 (1925).
6 In Eq. (6), ${}_3F_2[-a,-b,c;e,-a-m;1]$ with $a = S - M, b = S + M, c = j + 1, e = 1$, and $m = n - j + M$ is meant for the sum from $k = 0$ to $k = \min(a, b)$ of $(-a)_k(-b)_k(c)_k/(e)_k (-a-m)_k k!$ for $a, m = 0, 1, 2, \ldots$. This is done in the same spirit by which ${}_2F_1[-m, b; -m-n; z]$ for $m, n = 0, 1, 2, \ldots$ is defined in A. Erdélyi et al., *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 1, p. 101, rather than a slightly different definition given in Y. L. Luke, *The Special Functions and Their Applications* (Academic, New York, 1969), Vol. 1, p. 41.
7 See, for example, pp. 105-108 of *Higher Transcendental Functions* in Ref. 6. Care is to be exercised in using these formulas in order not to obtain ambiguity or nonsense.
8 For this, see, for example, L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge U. P., Cambridge, 1966), p. 47.
9 Other useful formulas may be found on pp. 14, 15, 21, 85, 93, and 98 in W. N. Bailey, *Generalized Hypergeometric Series* (Stechert–Hafner, New York, 1964).
10 J. Thomae, J. Math. **87**, 26 (1879).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Operator Algebras and Axioms of Measurements

Etang Chen
Department of Mathematics, East Carolina University, Greenville, North Carolina 27834
(Received 27 January 1971)

The axioms of measurements introduced by Ludwig are formulated and studied in the framework of operator algebras. It is shown that a concrete C^*-algebra with identity satisfies the axiom of sensitivity increase of effects if and only if it is a von Neumann algebra; although a von Neumann algebra satisfies the axiom of decompossability of ensembles, however, the axiom of components of the mixtures of two ensembles is true only if a von Neumann algebra is a factor of type $I_n (n < +\infty)$. It is also verified that the set of decision effects, which is proved to be a subset of projections of a von Neumann algebra, has similar lattice structure of quantum mechanics, and its connection with quantum logic in the sense of Varadarjan is also figured out.

INTRODUCTION

The most remarkable structure of quantum mechanics is described by the Hilbert space, which has been widely studied and developed by both mathematicians and physicists to understand this fundamental structure of the whole theory. In a series of papers, Ludwig[1-5] introduced, from the physical point of view, an axiomatic system of measurements to characterize the structure of Hilbert space in quantum theory. Instead of *observables* and *states* in quantum mechanics, *effects* and *ensembles*, which are more general and abstract but still physically interpretable, have been assumed as starting point of the whole theory. From some physically heuristic aspects, a system of axioms of measurements is established in terms of effects and ensembles.[1,2] Some consequences from this axiomatic system have been investigated, in particular, a similar lattice structure of quantum system has been figured out.[4]

In this paper we shall study and formulate Ludwig's axioms in terms of operator algebras, especially, C^*-algebra and von Neumann algebra, which plays an important role in the algebraic approach of quantum field theory, quantum mechanics, and statistical physics.

Our first task is to investigate the validity of these axioms for operator algebras. We have shown that a concrete C^*-algebra with identity satisfies the axiom of sensitivity increase of effects if and only if it is a von Neumann algebra; the axiom of decompossability and relationships of effects holds for a von Neumann algebra; and the axiom of the components of the mixture of two ensembles is true only for a finite degree of freedom.

Like Ludwig,[1,2] we have also shown the existence of decision effects, which are now projections of a von Neumann algebra. We have proved that the set of decision effects is an orthocomplemented, completed lattice satisfying orthomodular condition. Furthermore, we find that the set of decision effects is a *logic* in the sense of Varadarajan,[6] and it can be a *standard logic* if a von Neumann algebra is discrete and finite.

Indeed, Ludwig's axioms are only restricted in the case of finite-dimensional Hilbert space. Hence, a further development of this theory to the infinite-dimensional case will be more interesting. This work may be considered as a tentative approach in this direction.

In Sec. 1 the axioms of measurements will be given only in mathematical forms, without any physical interpretations, which can be found very detailed in Refs. 1 and 2. Following that, Axioms 2–4 will be formulated in terms of operators and studied separately in the subsequent sections. Section 2 is the axiom of sensitivity increase of effects, and its validity for a concrete C^*-algebra (Theorem 2.1). Section 3 deals with the decision effects, its lattice structure is given (Theorem 3.10), and its connection with Varadarajan's approach is investigated (Theorem 3.12). Axiom 3 is studied in Sec. 4, a modified form is proposed (Axiom 3'), which will be more essential for a C^*-algebra. Section 5 deals with Axiom 4 and some properties of *extremal sets* (see definition in Sec. 1) are given. The main consequence of this axiom is the modularity of the standard logic (Theorem 5.6), which implies that this axiom is true only for the case of a finite degree of freedom. In Sec. 6, we give some examples

[1] F. Sasaki and K. Ohno, J. Math. Phys. 4, 1140 (1663).
[2] V. H. Smith, Jr., J. Chem. Phys. 41, 277 (1964).
[3] V. H. Smith, Jr. and F. E. Harris, J. Math. Phys. 10, 771 (1969).
[4] K. Mano, J. Chem. Phys. 52, 2785 (1970).
[5] F. J. W. Whipple, Proc. London Math. Soc. 23, 104 (1925).
[6] In Eq. (6), ${}_3F_2[-a,-b,c;e,-a-m;1]$ with $a=S-M, b=S+M, c=j+1, e=1$, and $m=n-j+M$ is meant for the sum from $k=0$ to $k=\min(a,b)$ of $(-a)_k(-b)_k(c)_k/(e)_k(-a-m)_k k!$ for $a, m = 0, 1, 2, \ldots$. This is done in the same spirit by which ${}_2F_1[-m,b;-m-n;z]$ for $m, n = 0, 1, 2, \ldots$ is defined in A. Erdélyi et al., *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 1, p. 101, rather than a slightly different definition given in Y. L. Luke, *The Special Functions and Their Applications* (Academic, New York, 1969), Vol. 1, p. 41.
[7] See, for example, pp. 105-108 of *Higher Transcendental Functions* in Ref. 6. Care is to be exercised in using these formulas in order not to obtain ambiguity or nonsense.
[8] For this, see, for example, L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge U. P., Cambridge, 1966), p. 47.
[9] Other useful formulas may be found on pp. 14, 15, 21, 85, 93, and 98 in W. N. Bailey, *Generalized Hypergeometric Series* (Stechert-Hafner, New York, 1964).
[10] J. Thomae, J. Math. 87, 26 (1879).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Operator Algebras and Axioms of Measurements

Etang Chen
Department of Mathematics, East Carolina University, Greenville, North Carolina 27834
(Received 27 January 1971)

The axioms of measurements introduced by Ludwig are formulated and studied in the framework of operator algebras. It is shown that a concrete C^*-algebra with identity satisfies the axiom of sensitivity increase of effects if and only if it is a von Neumann algebra; although a von Neumann algebra satisfies the axiom of decompossability of ensembles, however, the axiom of components of the mixtures of two ensembles is true only if a von Neumann algebra is a factor of type $I_n (n < +\infty)$. It is also verified that the set of decision effects, which is proved to be a subset of projections of a von Neumann algebra, has similar lattice structure of quantum mechanics, and its connection with quantum logic in the sense of Varadarjan is also figured out.

INTRODUCTION

The most remarkable structure of quantum mechanics is described by the Hilbert space, which has been widely studied and developed by both mathematicians and physicists to understand this fundamental structure of the whole theory. In a series of papers, Ludwig[1-5] introduced, from the physical point of view, an axiomatic system of measurements to characterize the structure of Hilbert space in quantum theory. Instead of *observables* and *states* in quantum mechanics, *effects* and *ensembles*, which are more general and abstract but still physically interpretable, have been assumed as starting point of the whole theory. From some physically heuristic aspects, a system of axioms of measurements is established in terms of effects and ensembles.[1,2] Some consequences from this axiomatic system have been investigated, in particular, a similar lattice structure of quantum system has been figured out.[4]

In this paper we shall study and formulate Ludwig's axioms in terms of operator algebras, especially, C^*-algebra and von Neumann algebra, which plays an important role in the algebraic approach of quantum field theory, quantum mechanics, and statistical physics.

Our first task is to investigate the validity of these axioms for operator algebras. We have shown that a concrete C^*-algebra with identity satisfies the axiom of sensitivity increase of effects if and only if it is a von Neumann algebra; the axiom of decompossability and relationships of effects holds for a von Neumann algebra; and the axiom of the components of the mixture of two ensembles is true only for a finite degree of freedom.

Like Ludwig,[1,2] we have also shown the existence of decision effects, which are now projections of a von Neumann algebra. We have proved that the set of decision effects is an orthocomplemented, completed lattice satisfying orthomodular condition. Furthermore, we find that the set of decision effects is a *logic* in the sense of Varadarajan,[6] and it can be a *standard logic* if a von Neumann algebra is discrete and finite.

Indeed, Ludwig's axioms are only restricted in the case of finite-dimensional Hilbert space. Hence, a further development of this theory to the infinite-dimensional case will be more interesting. This work may be considered as a tentative approach in this direction.

In Sec. 1 the axioms of measurements will be given only in mathematical forms, without any physical interpretations, which can be found very detailed in Refs. 1 and 2. Following that, Axioms 2–4 will be formulated in terms of operators and studied separately in the subsequent sections. Section 2 is the axiom of sensitivity increase of effects, and its validity for a concrete C^*-algebra (Theorem 2.1). Section 3 deals with the decision effects, its lattice structure is given (Theorem 3.10), and its connection with Varadarajan's approach is investigated (Theorem 3.12). Axiom 3 is studied in Sec. 4, a modified form is proposed (Axiom 3′), which will be more essential for a C^*-algebra. Section 5 deals with Axiom 4 and some properties of *extremal sets* (see definition in Sec. 1) are given. The main consequence of this axiom is the modularity of the standard logic (Theorem 5.6), which implies that this axiom is true only for the case of a finite degree of freedom. In Sec. 6, we give some examples of operator algebras in mathematical physics; some of them satisfy Axiom 2, but some of them do not.

1. LUDWIG'S AXIOMS OF MEASUREMENT

We give a brief summary of Ludwig's axioms without any specification about their physical backgrounds to which we refer.[1,2]

Let K and L be the sets of *ensembles* and *effects*, respectively. A map μ of $K \times L$ into $[0, 1]$ is defined such that

Axiom 1:

(a) $\mu(V_1, F) = \mu(V_2, F)$ for all $F \in L$ implies $V_1 = V_2$.

(b) $\mu(V, F_1) = \mu(V, F_2)$ for all $V \in K$ implies $F_1 = F_2$.

(c) There exists an element $0 \in L$ such that $\mu(V, 0) = 0$ for all $V \in K$.

(d) There exists an element F such that $\mu(V, F) = 1$ for all $V \in K$.

Let

$$X(F) = \sum_{i=1}^{n} a_i \mu(V_i, F)$$

for $V_i \in K$, with $a_i \in R$, then X is a linear functional of L. The real vector space generated by all X of L is denoted by B. K is a subset of B by setting $X(F) = \mu(V, F)$. B is a normed vector space, with a norm defined as

$$\|X\| = \sup\{|X(F)|; F \in L\} \quad \text{for all } X \in B.$$

Then μ can be extended to $B \times L$ by setting $X(F) = \mu(X, F)$. For a fixed F, $\mu(X, F) = X(F)$ can be considered as a linear functional of B; hence L can be identified as a subset of the dual space B' of B. The norm-closed convex hull of K in B is denoted by $\mathcal{K}$, and the norm-closed convex hull of L in B' is denoted by $\mathcal{L}$. B' is a partially ordered vector space with positive cone $C = \{Y \in B', \mu(V, Y) \geq 0$ for all $V \in \mathcal{K}\}$.

Furthermore, we denote by $L_0(k)$ and $K_0(\ell)$ the annihilators of $k \subseteq \mathcal{K}$ and $\ell \subseteq \mathcal{L}$, respectively, i.e.,

$$L_0(k) = \{F \in \mathcal{L}; \mu(V, F) = 0 \text{ for all } V \in k\},$$
$$K_0(\ell) = \{V \in \mathcal{K}; \mu(V, F) = 0 \text{ for all } F \in \ell\}.$$

In particular, the annihilator of a singleton $\{V\}$ [resp., $\{F\}$], is denoted by $L_0(V)$ [resp., $K_0(F)$]. Then the first axiom of measurement can be formulated.

Axiom 2 (the sensitivity increase of effects): For any $F_1, F_2 \in \mathcal{L}$ there exists an effect $F_3 \in \mathcal{L}$ such that $F_3 \geq F_1$, $F_3 \geq F_2$, and $K_0(F_3) \supseteq K_0(F_1) \cap K_0(F_2)$.

In Ref. 4 this axiom has been developed, for technical reasons, to an additional part. However, the above portion of this axiom is more interesting for our present study.

Given a nonempty convex subset M of B', a nonempty convex subset S of M is called an *extremal set* if for $Y_1, Y_2, Y_3 \in M$, $Y_1 = mY_2 + (1 - m)Y_2$, with $m \in (0, 1)$; then $Y_1 \in S$ implies $Y_2, Y_3 \in S$. For each $V \in \mathcal{K}$ the norm closure of the extremal set generated by V is denoted by $C(V)$. Indeed, $C(V)$ is the smallest norm-closed extremal set containing V. $C(V)$ has its very interesting physical backgrounds.[2] The next axiom of measurements concerns $C(V)$.

Axiom 3 (decompossability and relationship of effects): $L_0(V_1) = L_0(V_2)$ implies $C(V_1) = C(V_2)$ for all $V_1, V_2 \in \mathcal{K}$.

The last axiom of measurements is formulated about the mixture of two ensembles.

Axiom 4 (the components of the mixture of two ensembles): For all $V_1, V_2, V_3 \in \mathcal{K}$, $C(V_1) \cap C(V_2) = \emptyset$, $C(\frac{1}{2} V_1 + \frac{1}{2} V_2) \supseteq C(V_3) \neq \emptyset$, and $d(V_1, V_2) = 1$ implies $C(\frac{1}{2} V_1 + \frac{1}{2} V_3) \cap C(V_2) \neq \emptyset$ where $d(V_1, V_2) = \sup\{|\mu(V_1, F) - \mu(V_2, F)|; F \in \mathcal{L}\}$.

One of the most important consequences from these axioms is that each annihilator $L_0(k)$ has a unique maximal element E, called the *decision effect*.[1] The set of all decision effects forms a completed lattice with an orthocomplementation, which is the characteristic structure in quantum mechanics. Moreover, each $C(V)$ is lattice-theoretically isomorphic to a decision effect E.[3] Therefore, Axiom 4 can be formulated in a lattice-theoretical version. (In this paper the lattice-theoretical intersection and union will be denoted by $\wedge, \vee$; and $\cap, \cup$ denote the set-theoretical intersection and union.)

Axiom 4': $a \wedge b = 0$, $c \leq a \vee b$, $a \perp c$, and $(a \vee c) \wedge b = 0$ implies $c = 0$, where $C(V_1) = a$, $C(V_2) = b$, $C(V_3) = c$, and $d(V_1, V_2) = 1$ is equivalent to $a \perp c$, i.e., a and c are orthogonal. A detailed discussion of this axiom in lattice form is referred to in Ref. 4.

We shall use this lattice form to study its validity for operator algebras in Sec. 5.

It is easy to verify that Axiom 1 is true for C^*-algebras and von Neumann algebras whenever $\mathcal{L}$ and $\mathcal{K}$ are properly chosen. Hence, we start to study Axiom 2 in Sec. 2 and other axioms in the subsequent sections.

2. AXIOM OF SENSITIVITY INCREASE OF EFFECTS

Given a C^*-algebra $\mathfrak{A}$ with identity on a Hilbert space $\mathfrak{H}$. Let $\mathfrak{A}^+$ and $\mathfrak{A}_1$ be the positive cone and unit sphere of $\mathfrak{A}$, respectively. The von Neumann algebra generated by $\mathfrak{A}$ will be denoted by $\mathfrak{R}$.

In this section we assume the set of effects $\mathcal{L} = \mathfrak{A}^+ \cap \mathfrak{A}_1$, and the set of ensembles $\mathcal{K}$ is the set of vector states of $\mathfrak{A}$. Hence, each ensemble $V \in \mathcal{K}$ will be denoted by ω with $\|\omega\| = 1$, and $\omega(F) = (Fx, x)$ for $F \in \mathcal{L}$ and $x \in \mathfrak{H}$. As in Sec. 1, $L_0(\omega)$ [resp., $L_0(k)$] denotes the annihilator of $\omega \in \mathcal{K}$ [resp., $k \subseteq \mathcal{K}$] consisting of all those effects in $\mathcal{L}$

which vanish on ω [resp., each $\omega \in k$]. $K_0(F)$ and $K_0(l)$ denote the annihilators of $F \in \mathfrak{L}$ and $l \subseteq \mathfrak{L}$, respectively.

Axiom 2: For any $F_1, F_2 \in \mathfrak{L}$, there exists $F_3 \in \mathfrak{L}$ such that $F_3 \geq F_1$, $F_3 \geq F_2$, and $K_0(F_3) \supseteq K_0(F_1) \cap K_0(F_2)$.

This axiom has exactly the same form as in Sec. 1; however, $\mathfrak{L}$ and $\mathfrak{K}$ are now visualized as positive operators of unit sphere and vector state of $\mathfrak{A}$, respectively.

We call that a C^*-algebra $\mathfrak{A}$ with identity on a Hilbert space $\mathfrak{H}$, satisfies the axiom of sensitivity increase of effects whenever Axiom 2 holds for $\mathfrak{L}$.

The main result of this section is formulated as the following theorem.

Theorem 2.1: A C^*-algebra $\mathfrak{A}$ with identity on a Hilbert space $\mathfrak{H}$ satisfies the axiom of sensitivity increase of effects if and only if $\mathfrak{A} = \mathfrak{R}$, the von Neumann algebra generated by $\mathfrak{A}$.

We need some preliminary lemmas to show the necessary condition of the theorem. The first lemma is an equivalent form of Axiom 2.

Lemma 2.2 (Ludwig): $\mathfrak{L}$ satisfies Axiom 2 if and only if $L_0(k)$ for $k \subseteq \mathfrak{K}$ is a bounded, monotone-increasing directed sequence of $\mathfrak{L}$.

Proof (See Ref. 4.).
We shall show that each bounded, monotone-increasing directed sequence of $\mathfrak{L}$ appears in this way, whenever Axiom 2 holds for $\mathfrak{L}$.

Lemma 2.3: For each $F \in \mathfrak{L}$, $K_0(F)$ is nonempty if $\mathfrak{L}$ satisfies Axiom 2.

Proof: Suppose that $K_0(F_1) = \emptyset$ and $K_0(F_2) \neq \emptyset$ for some $F_1, F_2 \in \mathfrak{L}$. Then by the given assumption, there exists $F_3 \in \mathfrak{L}$ such that $F_3 \geq F_1$, $F_3 \geq F_2$, and $K_0(F_3) \supseteq K_0(F_1) \cap K_0(F_2) = K_0(F_2)$, which implies $F_3 \leq F_2$.

Lemma 2.4: Let $\mathfrak{F}$ be a bounded, monotone-increasing sequence of $\mathfrak{L}$. If $K_0(F) \neq \emptyset$ for each $F \in \mathfrak{L}$, then $\mathfrak{F} \subseteq L_0(k)$ for some nonvoid subset k of $\mathfrak{K}$.

Proof: Since $\mathfrak{F}$ is bounded, there is an effect $F_0 \in \mathfrak{L}$ such that $F_0 \geq F$ for all $F \in \mathfrak{F}$. Hence $K_0(F_0) \subseteq K_0(F)$ for all $F \in \mathfrak{F}$. Let $k = K_0(F_0)$, which is nonempty by assumption. Then, to each $\omega \in k$ we have $\omega(F) = 0$ for all $F \in \mathfrak{F}$, because $\omega \in K_0(F)$. Hence $\mathfrak{F} \subseteq L_0(k)$ for some nonvoid subset k of $\mathfrak{K}$.

Lemma 2.5: Let $\mathfrak{F}$ be a bounded, monotone-increasing directed sequence of $\mathfrak{L}$. If $\mathfrak{F} \subseteq L_0(k)$ for some nonvoid $k \subseteq \mathfrak{K}$, then the least upper bound (l.u.b.) of $\mathfrak{F}$ lies in $\mathfrak{A}$.

Proof: The existence of l.u.b. F_0 of $\mathfrak{F}$ is well known; indeed, F_0 belongs to the strong-closure of $\mathfrak{F}$ (Ref. 7, p. 331). Since $\mathfrak{F} \subseteq L_0(k)$, F_0 is also in the strong-closure (hence weak-closure) of $L_0(k)$. But, $L_0(k)$ is weakly closed, therefore F_0 is in $L_0(k)$, and hence in $\mathfrak{A}$.

We are now able to prove Theorem 2.1.

Proof of Theorem 2.1: Let $\mathfrak{F}$ be a bounded, monotone-increasing directed sequence of self-adjoint elements of $\mathfrak{A}$. Without loss of generality, we may assume $\mathfrak{F} \subseteq \mathfrak{L}$; viz. $0 \leq F \leq I$ for each $F \in \mathfrak{F}$.

If we consider $\mathfrak{A}$ is a subset of its double dual $\mathfrak{A}^{**}$, which is a von Neumann algebra,[8] then $\mathfrak{F}$ converges strongly to its l.u.b. F_0. Since $\mathfrak{A}$ satisfies the axiom of sensitivity increase of effects, it follows from Lemmas 2.3–2.5 that $F_0 \in \mathfrak{A}$. Therefore, the strong-limit of $\mathfrak{F}$ lies in $\mathfrak{A}$, then $\mathfrak{A} = \mathfrak{R}$ from Ref. 9.

Conversely, if $\mathfrak{A} = \mathfrak{R}$, let $F_1, F_2 \in \mathfrak{L}$, with corresponding spectral projections P_1, P_2. If we assume that $\omega_x(F_1) = 0$ [resp., $\omega_y(F_2) = 0$] for each $x \in P_1\mathfrak{H}$ (resp., $y \in P_2\mathfrak{H}$). Let $P\mathfrak{H} = P_1\mathfrak{H} \cap P_2\mathfrak{h}$, then $P \in \mathfrak{A}$, in fact $P \in \mathfrak{L}$, since $P_1, P_2 \in \mathfrak{A}$ and $P_1 \wedge P_2 \in \mathfrak{A}$. Therefore, there exists $F_3 \in \mathfrak{L}$, e.g., $F_3 = I - P$, such that $F_3 \geq F_1$, $F_3 \geq F_2$, and $\omega_x(F_3) = \omega_x(F_2) = \omega_x(F_1) = 0$ for each $x \in P\mathfrak{H}$; and the proof of theorem is complete.

3. THE LATTICE STRUCTURE OF DECISION EFFECTS

In Sec. 2 we have seen that the annihilator of $\phi \in \mathfrak{K}$ (resp., $k \subseteq \mathfrak{K}$) $L_0(\phi)$ [resp., $L_0(k)$] is a directed set whenever it satisfies the axiom of sensitivity increase of effects. It has been shown that in each directed set there exists a maximum element, which is called the *decision effect*.[1] The set of decision effect has very interesting lattice structures,[4] which fulfill the basic structures of quantum theory. This is the most attractive aspect in the whole theory of Ludwig's axioms. In this section we shall study decision effects in terms of operator algebra. We shall show that the decision effect is identified to the projection of a von Neumann algebra, and the set of all decision effects has also similar lattice structure which one can expect for a quantum system. At the end of this section we shall show some connection between decision effects and Varadarajan's approach of quantum logic.[6]

From Theorem 2.1, we may consider only the case of von Neumann algebra $\mathfrak{R}$. Hence, in this section we assume that the set of effects $\mathfrak{L}$ is the positive portion of unit sphere of $\mathfrak{R}$, i.e., $\mathfrak{L} = \mathfrak{R}^+ \cap \mathfrak{R}_1$, and the set of ensembles $\mathfrak{K}$ is the set of all positive normal states of $\mathfrak{R}$, i.e., $\mathfrak{K} = \mathfrak{R}_*^+ \cap \Omega$, where $\mathfrak{R}_*$ is the predual of $\mathfrak{R}$, and Ω the set of all normalized positive linear functional of $\mathfrak{R}$, for which $\|\phi\| = 1$ if $\phi \in \Omega$. We shall use hereafter $[\mathfrak{F}\mathfrak{M}]$ to denote the closure of the set of vectors

$\{Tx; T \in \mathfrak{F}, x \in \mathfrak{M}\}$, where $\mathfrak{F}$ is a family of operators of $\mathfrak{R}$ and $\mathfrak{M}$ a set of vectors in $\mathfrak{H}$. We denote by this same notation the orthogonal projection on that subspace. As usual way, $\mathfrak{B}(\mathfrak{H})$ denotes the set of all bounded operators on $\mathfrak{H}$

As in Sec. 1, let $L_0(k)$ be the annihilator of a subset k of $\mathcal{K}$, i.e., $L_0(k) = \{T \in \mathcal{L}; \phi(T) = 0$ for all $\phi \in k\}$; and for a singleton $k = \{\phi\}$, we denote by $L_0(\phi)$ the annihilator of $\{\phi\}$.

For each $\phi \in \mathcal{K}$, there is a least projection $E_\phi \in \mathcal{L}$, called the *support* of ϕ, such that $L_0(\phi) = \mathfrak{R}(I - E_\phi)$ and $\phi(E_\phi) = \phi(I) = 1$ (Ref. 7, p. 61). Let $E = I - E_\phi$, then E is a projection of $\mathfrak{R}$, with $\mathfrak{R}E = L_0(\phi)$. For any $T \in L_0(\phi)$, one has $T = TE$, hence $T^* = (TE)^* = ET$, thus $T = TE = ET$, which implies $E \geq T$ for all $T \in L_0(\phi)$.[10] It is easy to see that $E \in L_0(\phi)$. Hence, we have verified that there is a maximum element in $L_0(\phi)$.

Lemma 3.1: For any $\phi \in \mathcal{K}$, if E_ϕ is the support of ϕ, then $E = I - E_\phi$ is the maximum element of $L_0(\phi)$.

To any arbitrary subset k of $\mathcal{K}$, one also can show the existence of a maximum element in $L_0(k)$.

Lemma 3.2: For any subset k of $\mathcal{K}$, there exists a maximum projection E in $L_0(k)$.

Proof: We follow a similar proof given in Ref. 7, p. 61. First, we note that $L_0(k)$ is ultraweakly closed, since it is weakly closed in $\mathfrak{R}_1$. To each $\phi \in k$, there is $x_i \in \mathfrak{H}$, with $\sum_{i=1}^{\infty} \|x_i\|^2 < +\infty$, such that $\phi = \sum_{i=1}^{\infty} \omega_{x_i}$. Hence, for each $T \in L_0(k)$, we have

$$\phi(T^2) = \sum_{i=1}^{\infty} \omega_{x_i}(T^2) = \sum_{i=1}^{\infty} \|Tx_i\|^2 \leq \sum_{i=1}^{\infty} \|T^{1/2}x_i\|^2 = \sum_{i=1}^{\infty} (Tx_i, x_i) = \phi(T) = 0;$$

And, by the Cauchy–Schwartz inequality,

$$|\phi(A^*T)|^2 \leq |\phi(A^*A)|\ |\phi(T^2)| = 0$$

for each $A \in \mathfrak{R}$, $T \in L_0(k)$, and $\phi \in k$. Therefore, $L_0(k)$ is an ultraweakly closed left ideal of $\mathfrak{R}$. Moreover, since $L_0(k)$ is self-adjoint $L_0(k)$ is also a two-side ideal of $\mathfrak{R}$. From Ref. 7, p. 45, there exists a projection $E \in \mathfrak{R}$ such that $L_0(k) = \mathfrak{R}E$ and $T = TE = ET$ for $T \in L_0(k)$. Hence, $E \geq T$ for all $T \in L_0(k)$.[10]

On the other hand,

$$L_0(k) = \bigcap_{\phi_i \in k} L_0(\phi_i),$$

and from Lemma 3.1, $L_0(\phi_i) = \mathfrak{R}E_i$, with the maximum element $E_i \in L_0(\phi_i)$. Hence we have $E = \wedge E_i$, where each E_i is corresponding to $L_0(\phi_i)$ for $\phi_i \in k$. Therefore, $E \leq E_i$ and $\phi_i(E) \leq \phi_i(E_i) = 0$ for all $\phi_i \in k$, which implies that $E \in L_0(k)$, and the proof of lemma is complete.

The maximum element in $L_0(k)$ is therefore a projection E in $\mathfrak{R}$, hence in $\mathcal{L}$. We call E the *decision effect*, and denote by $\mathcal{G}$ the set of all decision effects. In the rest of this section we shall study some lattice structures of $\mathcal{G}$ which are similar to Ludwig's results.[4]

We note that Lemmas 3.1 and 3.2 are different from Ludwig's results,[4] because there is no assumption about the axiom of sensitivity increase of effects, which is the main hypothesis for the existence of decision effects in Ludwig's work. Hence for a von Neumann algebra, the annihilators of k or $\{\phi\}$ always have decision effects, even when they are not directed sets.

The next lemma is a characterization of $L_0(k)$ for a von Neumann algebra, which is possible only for operator algebras.

Lemma 3.3: Let $L_0(k)$ be the annihilator of k, with decision effect E for any subset k of $\mathcal{K}$. Then

$$L_0(k) = E\mathcal{L}E.$$

Proof: For each $T \in \mathcal{L}$ and each $\phi \in k$, by Cauchy–Schwartz inequality, we have

$$|\phi(ETE)|^2 = |\phi((TE)^*E)|^2 \leq |\phi((TE)^*(TE))|\ |\phi(E^2)| = 0.$$

Then, $\phi(ETE) = 0$ for each $\phi \in k$; hence $ETE \in L_0(k)$. Conversely, let $T \in L_0(k)$, then $T \leq E$, hence $T = TE = ET = ETE$, so that $T \in E\mathcal{L}E$.

Another version of this lemma was given in Ref. 10. However, our proof is different, and we restrict only on $\mathcal{L}$ instead of on the whole positive cone of $\mathfrak{R}$.

We are now able to investigate the lattice structures of $\mathcal{G}$. Firstly, we shall show the existence of the least upper bound of any two decision effects, and the orthocomplementation on $\mathcal{G}$.

Lemma 3.4: If E_1 and E_2 are two decision effects in $\mathcal{G}$, then $E_1 \wedge E_2 \in \mathcal{G}$.

Proof: Let $L_0(k_1)$ [resp., $L_0(k_2)$] be the corresponding annihilators of E_1 (resp., E_2). Then $E_1E_2E_1 \in L_0(k_1)$ from Lemma 3.3, and the sequence $(E_1E_2E_1)^n$ converges strongly to $E_1 \wedge E_2$ as $n \to \infty$.[11] Since $L_0(k_1)$ is weakly closed, hence strongly closed, then $E_1 \wedge E_2 \in L_0(k_1)$. Similarly, $(E_2E_1E_2)^n$ converges strongly to $E_1 \wedge E_2$ and $E_1 \wedge E_2 \in L_0(k_2)$. Therefore,

$$E_1 \wedge E_2 \in L_0(k_1) \cap L_0(k_2) = L_0(k_1 \cup k_2) = L_0(k),$$

where $k = k_1 \cup k_2$. Finally, since $E_1 \geq T$ for all $T \in L_0(k_1) \cap L_0(k_2)$ and $E_2 \geq T$ for all $T \in L_0(k_1) \cap L_0(k_2)$, then $E_1 \wedge E_2 \geq T$ for all $T \in L_0(k_1) \cap L_0(k_2)$ from Ref. 6, p. 164. Therefore $E_1 \wedge E_2$ is the decision effect of $L_0(k) = L_0(k_1) \cap L_0(k_2)$ and $E_1 \wedge E_2 \in \mathcal{G}$.

A slight extension of this lemma will be given later to show the completeness of lattice $\mathcal{G}$. In the next lemmas we shall show the orthocomplementation of $\mathcal{G}$. It is well known that the orthocomplement of projection E is $I - E$, hence our next task is to show the following:

Lemma 3.5: If E is a decision effect in $\mathcal{G}$, then $I - E \in \mathcal{G}$.

Proof: Since E is a decision effect, without restriction of generality, we may assume $I - E = E_\phi$, the support of some $\phi \in \mathcal{K}$. Then $E_\phi = [\mathcal{R}'x_i]$ with $\phi = \sum_{i=1}^{\infty} \omega_{x_i}$ and $\sum_{i=1}^{\infty} \|x_i\|^2 = 1$ for $x_i \in \mathfrak{H}$. For $y_i \in (I - E_\phi)\mathfrak{H}$, we define $\psi = \sum_{i=1}^{\infty} \omega_{y_i}$, with $\sum_{i=1}^{\infty} \|y_i\|^2 = 1$; then $\psi(E) = \sum_{i=1}^{\infty} (Ey_i, y_i) = 1$. In fact, $E = [\mathcal{R}'y_i]$, i.e., E is the support of ψ. Hence, $I - E$ is the maximum element of $L_0(\psi)$ (Lemma 3.1), and $I - E \in \mathcal{G}$.

From Lemmas 3.4 and 3.5 we obtain the following result:

Lemma 3.6: $\mathcal{G}$ is a orthocomplemented lattice.

If E and F are two decision effects of $\mathcal{G}$, and $E \le F$, then $F(I - E) = (I - E)F$ and $F \wedge (I - E) = F - E$. Furthermore, $E(F - E) = (F - E)E$. Hence, $E \vee (F \wedge (I - E)) = E \vee (F - E) = E + (F - E) - E(F - E) = F$. Therefore, we have verified the following.

Lemma 3.7: $\mathcal{G}$ satisfies the orthomodular identity; for $E, F \in \mathcal{G}$

$$E \le F \quad \text{implies} \quad F = E\,(F \wedge (I - E)).$$

The other equivalent forms of orthomodularity will be given in Sec. 5, where the axiom of the components of two ensembles will be given so that $\mathcal{G}$ can be modular, which is true only in the case of finite-dimensional Hilbert space.

In the arguments of Lemma 3.2, we have seen that $L_0(k) = \mathcal{R}\,E$, $L_0(\phi_i) = \mathcal{R}\,E_i$ for all $\phi_i \in k$; hence $\mathcal{R}\,E = \mathcal{R}\,(\wedge\,E_i)$ and $E = \wedge\,E_i \in L_0(k)$ for all $\phi_i \in k$. Thus, $\wedge\,E_i \in \mathcal{G}$. A slight generalization of this statement enables us to prove the next result.

Lemma 3.8: Let E_i be the decision effect corresponding to $L_0(k_i)$ for any $i \in I$, then $\wedge\,E_i$ is the decision effect of $\bigcap_{i\in I} L_0(k_i)$.

Proof: We note that $\bigcap_{i\in I} L_0(k_i) = L_0(\bigcup_{i\in I} k_i)$. Moreover, $L_0(k_i)$ and $L_0(\bigcup_{i\in I} k_i)$ are ultraweakly closed two-side ideals of $\mathcal{R}$ (Lemma 3.2, then there exists maximum projections E_i and E, respectively, such that $L_0(k_i) = \mathcal{R}\,E_i$ and $L_0(\bigcup_{i\in I} k_i) = \mathcal{R}E$. Hence, $\mathcal{R}(\wedge_{i\in I} E_i) = \mathcal{R}E$, and $\wedge_{i\in I} E_i = E$. Indeed, $L_0(\bigcup_{i\in I} k_i)$ is a subset of $\mathcal{L}$ containing those operators T with $E_T \le E$, where E_T is the support of T.[12] Thus $T \le E_T \le E$ for all $T \in L_0(\bigcup_{i\in I} k_i)$, and $E = \wedge_{i\in I} E_i$ is the decision effect of $\bigcap_{i\in I} L_0(k_i)$.

The proof of the above lemma is different from Lemma 3.4, where we applied Varadarajan's lemma.[6] In fact one can easily extend Varadarajan's lemma to our form, which we give as follows.

Lemma 3.9 (Varadarjan): Let $S \in \mathcal{L}$, and $\{E_i\}_{i\in I}$ a set of projections on $\mathcal{R}$. If $S \le E_i$ for all $i \in I$, then $S \le \wedge_{i\in I} E_i$.

Proof: Since $S \le E_i$ for all $i \in I$ and $0 \le S \le I$, then $S = SE_i = E_i S$ for all $i \in I$,[10] which implies that S leaves $E_i\mathfrak{H}$ invariant for all $i \in I$. Hence S leaves $\bigcap_{i\in I} E_i\,\mathfrak{H}$ invariant, i.e., $Sx = S(\wedge\,E_i)x = (\wedge\,E_i)Sx$ for all $x \in \bigcap\,E_i\,\mathfrak{H}$ and all $i \in I$. Therefore, $S = S(\wedge\,E_i) = (\wedge\,E_i)S$, which implies that $S \le E_i$ for all $i \in I$.

We now summarize our results in the following theorem.

Theorem 3.10: $\mathcal{G}$ is a complete orthocomplemented lattice satisfying the orthomodular identity:

$$F \le F \quad \text{implies} \quad F = E\,(F \wedge (I - E))$$

for $E, F \in \mathcal{G}$.

A final remark about the lattice structure of $\mathcal{G}$ will be given here to compare with Varadarajan's approach.[6] Given a lattice $\mathcal{S}$ with zero element 0 and unit element e, $\mathcal{S}$ equipped with an orthocomplementation $x \to x^\perp$ is said to be a *logic*, if (i) for any countably infinite sequence $x_1, x_2, \cdots$ of elements of $\mathcal{S}$, $\vee_n x_n$ and $\wedge_n x_n$ exists in $\mathcal{S}$, (ii) if $x_1, x_2 \in \mathcal{S}$ and $x_1 < x_2$, there exists an element $x_3 \in \mathcal{S}$ such that $x_3 < x_1^\perp$ and $x_3 \vee x_1 = x_2$. Indeed, the existence of x_3 in (ii) is unique, one can show that $x_3 = x_1^\perp \wedge x_2$.[6] It is easy to verify that the set of all projections $\mathfrak{E}$ in a Hilbert space $\mathfrak{H}$ is a logic. We call $\mathfrak{E}$ the *standard logic*. A subset $\mathcal{S}$ of $\mathfrak{E}$ is a *sublogic* of the standard logic if $\mathcal{S}$ itself is a logic.

We now return to the set of decision effects $\mathcal{G}$. From Theorem 3.10, $\mathcal{G}$ is a complete orthocomplemented lattice with zero element 0 and unit element I. Obviously, $\mathcal{G}$ satisfies (i). If $E_1, E_2 \in \mathcal{G}$ and $E_1 \le E_2$, let $E_3 = (I - E) \wedge E_2$, which is an element of $\mathcal{G}$, hence (ii) also holds for $\mathcal{G}$. Therefore, we have the following consequence from the previous theorem.

Corollary 3.11: $\mathcal{G}$ is a logic, or more precisely, a sublogic of the standard logic.

We note that each $E \in \mathcal{G}$ can be identified as the support of some $\phi \in \mathcal{K}$, i.e., $E = [\mathcal{R}'x_i]$, with $\phi = \sum_{i=1}^{\infty} \omega_{x_i}$ and $\sum_{i=1}^{\infty} \|x_i\|^2 < +\infty$. On the other hand, let $\mathcal{S} = \{F \in \mathcal{R}; F = [\mathcal{R}'\mathfrak{M}] \text{ for } \mathfrak{M} \subseteq \mathfrak{H}\}$, then $\mathcal{S}$ is also a sublogic of $\mathfrak{E}$. We have the relation; $\mathcal{G} \subseteq \mathcal{S} \subseteq \mathfrak{E}$. However, if $\mathcal{G} = \mathcal{S} = \mathfrak{E}$, then $\mathcal{R} = \mathcal{B}(\mathfrak{H})$, hence $\mathcal{R}$ is a factor of type I. Conversely, if $\mathcal{R}$ is a factor of type I_n $(n < +\infty)$ on Hilbert space $\mathfrak{H}$, then the dimension of $\mathfrak{H}$ is $n < +\infty$. And, to any $F \in \mathcal{S}$, $F = [\mathcal{R}'\mathfrak{M}]$ for $\mathfrak{M} \subseteq \mathfrak{H}$. Since $\mathfrak{M}$ is finite-dimensional, we can define a positive normal state ϕ such that $\phi = \sum_{i=1}^{m} \omega_{x_i}$ with $x_i \in \mathfrak{M}$, $m \leq n$, then F is the support of ϕ. Therefore we have proved the following theorem.

Theorem 3.12: If $\mathcal{G}$ is a standard logic, then $\mathcal{R}$ is a factor of type I. Conversely, if $\mathcal{R}$ is a factor of type I_n ($n < +\infty$) then $\mathcal{G}$ is a standard logic.

4. AXIOM OF DECOMPOSSABILITY AND RELATIONSHIP OF EFFECTS

We defined extremal sets of $\mathcal{K}$ in Sec. 1, and formulated the axiom of decompossability of ensembles and relationship of effects. In this section we will formulate this axiom in terms of operator algebras and show that this axiom is always true for a von Neumann algebra.

First, we give a preliminary remark about the extremal set on a partially ordered vector space. Let X be a partially ordered Banach space and P the positive cone. Then a convex subset S of P is an extremal set of P if and only if S is a subcone of P such that for all $x, y \in P$, $x \in S$, and $y \leq x$ implies $y \in S$. An *order ideal* of X is a subspace J such that $x, y \in J$ implies $z \in J$ whenever $x \leq z \leq y$, $z \in X$. A subspace J is an order ideal if and only if $J \cap P$ is an extremal set of P.[10]

In the first part of this section we assume that $\mathcal{K} = \mathcal{R}_*^+$, the positive portion of predual $\mathfrak{R}_*$, and $\mathcal{L}$ is the same as in Sec. 3, although the set of effects will not be used explicitely in the subsequent discussion. The smallest norm-closed extremal set containing $\rho \in \mathcal{K}$ is denoted by $C(\rho)$, as in Sec. 1, then the axiom of decompossability of ensembles can be formulated as follows:

Axiom 3: For any $\rho, \tau \in \mathcal{K}$,

$$L_0(\rho) = L_0(\tau) \quad \text{implies} \quad C(\rho) = C(\tau).$$

If $B \in \mathcal{R}$ and $\phi \in \mathfrak{R}_*$, we define $B\phi$ and ϕB by

$$(B\phi)(T) = \phi(BT) \quad \text{and} \quad (\phi B)(T) = \phi(TB)$$

for $T \in \mathcal{R}$. In particular, $B^*\phi B$ is denoted by ϕ_B. With this notation, E_ϕ, the support of ϕ, is the smallest projection in $\mathcal{R}$ such that $\phi = \phi E_\phi = E_\phi \phi = \phi_{E_\phi}$. Then the smallest norm-closed extremal set containing $\rho \in \mathcal{K}$ can be characterized as $C(\rho) = \{\phi_{E_\rho}; \phi \in \mathcal{K}\}$, where E_ρ is the support of ρ.[10]

Let $\bar{\rho}$ be the smallest norm-closed order ideal in $\mathcal{R}_*^+$ containing ρ, then $\bar{\rho} = \{\phi \in \mathcal{K}; E_\phi \leq E_\rho\} = L_0(K_0(\rho))$, where E_ρ (resp., E_ϕ) is the support of ρ (resp., ϕ).[12] From the preliminary remark, it is easy to verify that $C(\rho)$ is also an order ideal containing ρ, hence $\bar{\rho} \subseteq C(\rho)$. If $\phi_{E_\rho} \in C(\rho)$ and the support of ϕ_{E_ρ} is F, then $E_\rho = [\mathcal{R}'x]$ with $\rho = \sum \omega_x$, $x \in \mathfrak{H}$, and $F = [\mathcal{R}'y]$, with $y \in E_\rho \mathfrak{H}$.

Therefore, $E_\rho F = E_\rho\, [\mathcal{R}'y] = [\mathcal{R}'y] = F$. Similarly, $FE_\rho = F$. Hence $E_\rho \geq F$ which implies $\phi_{E_\rho} \in \bar{\rho}$, and $C(\rho) \subseteq \bar{\rho}$. We have, therefore, the following lemma from Ref. 12.

Lemma 4.1: For $\rho \in \mathcal{K}$,

$$\begin{aligned} C(\rho) &= L_0(K_0(\rho)) \\ &= \{\phi \in \mathcal{K}; E_\phi \leq E_\rho\} \\ &= \{\phi_{E_\rho}; \phi \in \mathcal{K}\} \\ &= \bar{\rho}. \end{aligned}$$

Some further properties about norm-closed extremal sets will be given in Sec. 5. Axiom 3 is now trivial for a von Neumann algebra.

Corollary 4.2: Axiom 3 is true for a von Neumann algebra $\mathcal{R}$.

If we consider a C^*-algebra $\mathfrak{A}$ as a subalgebra of $\mathfrak{A}^{**}$, the double dual of $\mathfrak{A}$, which is again a von Neumann algebra, then $\mathfrak{A}^*$, the dual of $\mathfrak{A}$, coincide with the predual of $\mathfrak{A}^{**}$.[8] Hence, we may take $\mathcal{K}$ as $\mathfrak{A}_+^*$ the positive part of $\mathfrak{A}^*$, and Lemma 4.1 still holds. However, we shall modify Axiom 3 so that it will be more essential for a C^*-algebra.

A subset S of the dual $\mathfrak{A}^*$ of a C^* algebra $\mathfrak{A}$ is *invariant* if for all $\rho \in S$ and $T \in \mathfrak{A}$, ρ_T is in S, where $\rho_T(A) = \rho(T^*AT)$ for any $A \in \mathfrak{A}$. We denote by $\tilde{\rho}$ the smallest norm-closed invariant extremal set of $\mathcal{K}$ containing ρ, where $\mathcal{K} = \mathfrak{A}_+^*$ and $\mathcal{L} = \mathfrak{A}^+ \cap \mathfrak{A}_1$. Then we may enlarge $C(\rho)$ to $\tilde{\rho}$, and modify Axiom 3 to the following form.

Axiom 3′: For any $\rho, \tau \in \mathcal{K}$

$$L_0(\rho) = L_0(\phi) \quad \text{implies} \quad \tilde{\rho} = \tilde{\tau}.$$

Let π_ρ and π_τ denote representations of $\mathfrak{A}$ defined by ρ and τ on $\mathfrak{H}_\rho$ and $\mathfrak{H}_\tau$, respectively. Then $\tilde{\rho} = \tilde{\tau}$ implies π_ρ and π_τ are quasi-equivalent,[12] since $\tilde{\rho}$ and $\tilde{\tau}$ are also norm-closed invariant-order ideals in $\mathfrak{A}^*$. $L_0(\rho) = L_0(\tau)$ implies π_ρ and π_τ are weak-equivalent[13] (or physically equivalent.[14] Therefore Axiom 3′ claims that if π_ρ and π_τ are weak-equivalent then they are quasi-equivalent. This is not true in the case of C^*-algebras, but it holds for von Neumann algebras.[8]

5. AXIOM OF THE COMPONENTS OF THE MIXTURE OF TWO ENSEMBLES

As in Sec. 4, we assume $\mathcal{K} = \mathcal{R}_*^+$ and note that $C(\rho)$, the smallest norm-closed extremal set of $\mathcal{K}$ containing ρ, can be characterized by the support of ρ, E_ρ, viz. $C(\rho) = \{\phi \in \mathcal{K}; E_\phi \leq E_\rho\}$. Hence, we can study some properties of norm-closed extremal sets from their corresponding supports.

Lemma 5.1: $C(\rho) \subseteq C(\tau)$ if and only if $E_\rho \leq E_\tau$.

Proof: A straightforward verification.

Lemma 5.2: $C(\rho) \cap C(\tau) = \{\phi \in \mathcal{K}; E_\phi \leq E_\rho \wedge E_\tau\}$

Proof: Let $N = \{\phi \in \mathcal{K}; E_\phi \leq E_\rho \wedge E_\tau\}$. For each $\phi \in C(\rho) \cap C(\tau)$, $E_\phi \leq E_\rho$ and $E_\phi \leq E_\tau$; thus $E_\phi \leq E_\rho \wedge E_\tau$ and $\phi \in N$. Conversely, let $\phi \in N$, $E_\phi \leq E_\rho \wedge E_\tau$, then $E_\phi \leq E_\rho$ and $E_\phi \leq E_\tau$, so that $\phi \in C(\rho) \cap C(\tau)$.

A trivial corollary of this lemma: $C(\rho) \cap C(\tau) = \phi$ implies $E_\rho \wedge E_\tau = 0$.

For a subset k of $\mathcal{K}$, let $C(k)$ be the least norm-closed extremal set containing k. Then we can also characterize $C(k)$ in the following way.

Lemma 5.3:

$$C(k) = \{\phi \in \mathcal{K}; E_\phi \leq E_k\}$$

$$= \{\phi_{E_k}; \phi \in \mathcal{K}\},$$

where

$$E_k = \vee E_\rho \quad \text{for all } \rho \in k.$$

Proof: Since $C(k)$ is a norm-closed extremal set in $\mathcal{K}$, then $L_0(C(k))$ is an ultraweakly closed extremal set in $\mathcal{R}$. Hence there exists a unique projection E_k in $\mathcal{R}$ such that $L_0(C(k)) = \mathcal{R}(I - E_k)$. E_k is the least projection in $\mathcal{R}$ such that $\phi = E_k\phi = \phi E_k$ for each $\phi \in C(k)$. From a similar argument in Ref. 12, p. 405, $\phi \in \mathcal{K}$ lies in $C(k)$ if and only if $E_\phi \leq E_k$. The second part of the lemma follows directly from Lemma 3.9 of Ref. 10.

Furthermore, for any $\rho \in k, \rho \in C(k)$, then $E_\rho \leq E_k$, therefore $\vee E_\rho \leq E_k$ for all $\rho \in k$. On the other hand, since $\phi = \phi(\vee E_\rho) = (\vee E_\rho)\phi$ for each $\phi \in C(k)$ and $\rho \in k$, but E is the smallest projection with the same property, indeed E_k is the *support of* $C(k)$ (Ref. 10, p. 14), hence $\vee E_\rho \geq E_k$ for all $\rho \in k$. Therefore

$$E_\rho = \vee E_\rho \quad \text{for all } \rho \in k.$$

Corollary 5.4: If $\{E_\rho\}$ for all $\rho \in k$ are pairwire orthogonal, then

$$C(k) = \{\phi \in \mathcal{K}; E_\phi \leq \textstyle\sum_\rho E_\rho\}.$$

For the axiom of the components of the mixture of two ensembles, we are more interested in the case of $k = \{\rho, \tau\}$. If we denote $C(\{\rho, \tau\})$ by $C(\rho, \tau)$, then from the above lemma we have the following.

Corollary 5.5:

$$C(\rho, \tau) = C[m\rho + (1 - m)\tau],$$

where

$$m \in (0, 1).$$

Proof: We note that

$$C[m\rho + (1-m)\tau] = \{\phi \in \mathcal{K}; E_\phi \leq E_\omega\},$$

where $\omega = m\rho + (1 - m)\tau$. Since $\rho, \tau \in C(\rho, \tau)$, hence $\omega \in C(\rho, \tau)$ and $E_\omega \leq E_\rho \vee E_\tau$ from the above lemma. Therefore $C[m\rho + (1 - m)\tau] \subseteq C(\rho, \tau)$. Conversely, $\omega \in C[m\rho + (1 - m)\tau]$ implies that $\rho, \tau \in C[m\rho + (1 - m)\tau]$; hence $E_\rho \leq E_\omega$, $E_\tau \leq E_\omega$. Therefore, $E_\rho \vee E_\tau \leq E_\omega$, and $C(\rho, \tau) \subseteq C[m\rho + (1 - m)\tau]$.

From the above results, each $C(\rho)$ and $C(k)$ are characterized by projections E_ρ and E_k of $\mathcal{R}$, respectively; consequently, we can formulate this axiom in terms of decision effects defined in Sec. 3. As in Axiom 4′ in Sec. 1 we adopt the following lattice version.

Axiom 4: For each $E_1, E_2, E_3 \in \mathcal{G}$, if $E_1 \wedge E_2 = 0$, $E_3 \leq E_1 \vee E_2$, with $E_3 \perp E_1$ and $(E_1 \vee E_3) \wedge E_2 = 0$, then $E_3 = 0$.

As we have shown in Sec. 3, $\mathcal{G}$ satisfies the orthomodular condition. For $E_1, E_3 \in \mathcal{G}$

$$\text{if } E_1 \leq E_3, \text{ then } E_3 = E_1 \vee (E_3 \wedge (I - E_1)). \quad (1)$$

It is easy to show that this condition is equivalent to the following version of orthomodularity: For $E_1, E_2, E_3 \in \mathcal{G}$

$$\text{if } E_1 \leq E_3,\ E_1 \perp E_2, \text{ then } E_3 \wedge (E_1 \vee E_2) = E_1 \vee (E_3 \wedge E_2). \quad (2)$$

In fact, if we let $E_2 = I - E_1$, then (1) follows immediately from (2). Conversely, if $E_1 \leq E_3$ and $E_3 = E_1 \vee (E_3 \wedge (I - E_1))$, then $E_3 \wedge (E_1 \vee (I - E_1)) = E_1 \vee (E_3 \wedge (I - E_1))$, which implies (2) by setting $E_2 = I - E_1$.

Let $E_1 \vee E_2 = E_3$ in (2), then $E_3 \geq E_2$ and $E_3 \wedge E_2 = E_2$; (2) implies $E_3 = E_1 \vee E_2$. Hence we have another form of orthomodularity: For $E_1, E_3 \in \mathcal{G}$,

$$\text{if } E_1 \leq E_3, \text{ then there exists } E_2 \in \mathcal{G} \text{ such that } E_1 \perp E_2 \text{ and } E_3 = E_1 \vee E_2. \quad (3)$$

Obviously, (3) implies (2).

If we omit the orthogonal condition in (2), then we have the modularity; i.e., $E_1 \leq E_3$, then $E_3 \wedge (E_1 \vee E_2) = E_1 \vee (E_3 \wedge E_2)$. In general, $\mathcal{G}$ is not modular, unless $\mathcal{G}$ satisfies Axiom 4, which is the main purpose of axiom 4 in Ref. 4. We verify this result in the next theorem.

Theorem 5.6: The set of decision effects $\mathcal{G}$ is modular if and only if it satisfies Axiom 4.

Proof: Let $E_1, E_2, E_3 \in \mathcal{G}$, and $E_1 \wedge E_2 = 0$, $E_3 \leq E_1 \vee E_2$, with $E_1 \perp E_3$ and $(E_1 \vee E_3) \wedge E_2 = (E_1 + E_3) \wedge E_2 = 0$. Since $\mathcal{G}$ is modular, for $E_1 \leq E_1 + E_3$, we have $E_1 \vee (E_2 \wedge (E_1 + E_3)) = (E_1 + E_3) \wedge (E_1 \vee E_2)$. Hence

$$E_1 = (E_1 + E_3) \wedge (E_1 \vee E_2)$$
$$= E_1 \vee (E_3 \wedge (E_1 \vee E_2))$$
$$= E_1 \vee E_3 = E_1 + E_3,$$

which implies $E_3 = 0$.

Conversely, if $\mathcal{G}$ satisfies Axiom 4, since $\mathcal{G}$ is orthomodular, we can use (3). The modularity of $\mathcal{Y}$ follows from a similar argument given in Ref. 4.

It is well known that if the dimension of $\mathfrak{H}$ is infinite, then the standard logic (see Sec. 3) $\mathfrak{E}$ is not necessary modular. Therefore, from Theorem 3.12 we have a direct consequence of the above theorem.

Corollary 5. 7: $\mathcal{G}$ is modular only if $\mathfrak{R}$ is a factor of type I_n $(n < +\infty)$.

6. DISCUSSION

In the whole theory of Ludwig's formulation about axioms of measurements, the axiom of sensitivity increase of effects plays an important role. From the proof of Theorem 2.1 we note that this axiom holds for an operator algebra $\mathfrak{A}$ whenever $P_1 \wedge P_2$ lies in $\mathfrak{A}$ for any two projections P_1 and P_2 of $\mathfrak{A}$. Therefore, the projections of $\mathfrak{A}$ must be a lattice. The projections of a von Neumann algebra form a complete lattice. The other examples belonging to this category are AW^*-algebra[15] and JW-algebra.[16] An AW^*-algebra is a C^*-algebra such that (i) any set of orthogonal projections has a least upper bound, (ii) any maximal commutative self-adjoint subalgebra is generated by its projections. The set of all projections of an AW^*-algebra is also a complete lattice.[15] A JW-algebra is a weakly closed Jordan algebra of bounded self-adjoint operators. Its projections form a complete lattice with orthocomplementation and orthomodularity. Hence, a JW-algebra may be the most appropriate algebra for Ludwig's approach.

Another example satisfying this axiom is Σ^*-subalgebras of $\mathfrak{B}(\mathfrak{H})$.[17] A Σ^*-subalgebra of $\mathfrak{B}(\mathfrak{H})$ is a σ-closed C^*-subalgebra of $\mathfrak{B}(\mathfrak{H})$, which is also a von Neumann algebra as pointed out by Kadison in the Appendix of Ref. 17.

However, the quasilocal algebra of local observables in quantum field theory[14] can not satisfy the axiom of sensitivity increase of effects. Since its automorphisms will be inner, if it is a von Neumann algebra.[18] It is impossible for a quasilocal algebra, e.g., the automorphism induced by inhomogeneous Lorentz group is not inner.[14] Another example belonging to this category is the C^*-algebra of compact operators on separable Hilbert space.[18]

ACKNOWLEDGMENT

The author wishes to express his gratitude to Professor G. Ludwig and Dr. K. Kraus for encouragement and discussions during the early stage of this work in Marburg.

1 G. Ludwig, Z. Physik **181**, 233 (1964).
2 G. Ludwig Z. Naturforsch. **22a**, 1303 (1967).
3 G. Ludwig, Z. Naturforsch. **22a**, 1324 (1967).
4 G. Ludwig, Commun. Math. Phys. **4**, 331 (1967); **9**, 1 (1968).
5 G. Ludwig, Grundlegung Physikalischer Theorien, Speziell der Quantenmechanik, Teil I, (Universität Marburg, 1968) (unpublished).
6 V. S. Varadarajan, *Geometry of Quantum Theory* (Van Nostrand, Princeton, N.J., (1968), Vol. I.
7 J. Dixmier, *Les Algebres d'Operateurs dans l'Espace Hilbertien* (Gautheir-Villars, Paris, 1957).
8 J. Dixmier, *Les C*-algebres et Leurs Representations* (Gautheir-Villars. Paris, 1964).
9 R. V. Kadison, Ann. Math. **64**, 175 (1956).
10 R. T. Prosser, Mem. Am. Math. Soc. **45**, 1, (1963).
11 I. Halperin, Acta Sci. Math. **23**, 96 (1962).
12 E. G. Effros, Duke Math. J. **30**, 391 (1963).
13 J. M. G. Fell, Trans. Am. Math. Soc. **94**, 365 (1960).
14 R. Haag and D. Kastler, J. Math. Phys. **5**, 846 (1964).
15 I. Kaplansky, Ann. Math. **53**, 235 (1951).
16 D. M. Topping, Mem. Am. Math. **45** (1965).
17 E. D. Davis, Commun. Math. Phys. **8**, 147 (1968).
18 R. V. Kadison and J. R. Ringrose, Commun. Math. Phys. **4**, 32 (1967).

On Vacuum Space-Times Admitting a Null Killing Bivector

George C. Debney, Jr.
Department of Mathematics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061

(Received 5 March 1971)

Starting with a vacuum space-time ($R_{ab} = 0$) which admits a Killing vector field **K**, a study is made of the subclass where the Killing bivector (KBV) $K_{a;b}$ is null. Reference is made to an earlier paper [J. Math. Phys. 12, 1088 (1971)] by the author which established some of the general approach and formalism used here. All space-times with the property above turn out to be in the class of expansion-free radiation fields, which are necessarily algebraically special. Of these only Petrov types II, *D*, and *N* are allowed; furthermore, those of type *N* are the *pp* waves. A result obtained from applying this approach is that expansion-free radiation fields are the only vacuum space-times which admit a geodesic Killing vector field; that field is necessarily lightlike. Finally, since the spaces with symmetry studied by R. P. Kerr and the author [J. Math Phys. 11, 2807 (1970)] had nonzero expansion, the associated bivector to each of those symmetries must necessarily be nonnull.

1. INTRODUCTION

In a previous paper[1] a problem was formulated which was designed to classify certain vacuum space-times which admit a Killing vector field. The basic approach was to divide the problem into two basic parts: (1) those vacuum spaces which admit a nonnull Killing bivector and (2) those which admit a null Killing bivector.

After the formalism and the basic approach were developed,[1] the nonnull case was studied. Some general conclusions involving, first, geodesic Killing vectors and, second, hypersurface orthogonal Killing vectors were given through a study of the invariants made from the Riemann tensor and the nonnull Killing bivector.

This paper deals with the null Killing bivector cases which, by a theorem proved in Ref. 1, must necessarily concern only algebraically special spaces.

2. PRELIMINARIES AND FORMALISM

In Ref. 1 the formalism for a complex null tetrad $\{\mathbf{e}_a \mid a = 1,2,3,4\}$ with its dual $\{\epsilon^a \mid a = 1,2,3,4\}$ was developed. [$\mathbf{e}_1$ and $\mathbf{e}_2$ are complex conjugates; $\mathbf{e}_3$ and $\mathbf{e}_4$ are real; $\epsilon^a(\mathbf{e}_b) = \delta^a_b$.] Assuming that the metric tensor field $g = g_{\mu\nu}\, dx^\mu \otimes dx^\nu$ has signature $(+ + + -)$, the components $g_{ab} = g(\mathbf{e}_a, \mathbf{e}_b)$ can be put into the form

$$(g_{ab}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{2.1}$$

locally over the C^∞ Lorentz 4-manifold. The dual relationship between basis vectors $\{e^\mu_a \partial_\mu\}$ and $\{\epsilon^a_\mu dx^\mu\}$ is also expressed by $e^\mu_a \epsilon^b_\mu = \delta^a_b$ and $e^\mu_a \epsilon^a_\nu = \delta^\mu_\nu$ (Greek indices $\mu, \nu, \ldots$ on a kernel letter represent components of a tensor with respect to some local coordinate system $\{x^\mu\}$; latin indices $a, b, \ldots$ represent tensor components with respect to a complex null tetrad.) If $T = T^{\nu}_{\mu}{}^{\cdots}_{\cdots} dx^\mu \otimes \partial_\nu \otimes \cdots$ is a tensor field, then it is also true that $T = T^{b}_{a}{}^{\cdots}_{\cdots}\, \epsilon^a \otimes \mathbf{e}_b \otimes \cdots$.

The set of transformations $\mathbf{e}_a \to \mathbf{e}_a$, preserving the form (2.1) of (g_{ab}) is the set of Lorentz transformations. The proper orthochronous subgroup of these is given by

$$\begin{bmatrix} \exp(iB)\mathbf{e}_1, \\ \exp(-iB)\mathbf{e}_2, \\ \exp(A)\mathbf{e}_3, \\ \exp(-A)\mathbf{e}_4, \end{bmatrix} = |1 - \alpha\beta|^{-1} \begin{pmatrix} 1 & \bar\alpha\beta & -\bar\alpha & \beta \\ \alpha\bar\beta & 1 & -\alpha & \bar\beta \\ -\bar\beta & -\beta & 1 & -\beta\bar\beta \\ \alpha & \bar\alpha & -\alpha\bar\alpha & 1 \end{pmatrix} \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \\ \mathbf{e}_4 \end{bmatrix}, \tag{2.2}$$

where A, B, α, and β are parameters; α and β are complex; A and B are real; $\alpha\beta \neq 1$. (A bar above a symbol denotes the complex conjugate.)

The Lie bracket between any two contravariant vector fields is a vector field, $[\mathbf{X}, \mathbf{Y}] \equiv \mathbf{XY} - \mathbf{YX}$. Between vectors of the basis $\{\mathbf{e}_a\}$ the relationship

$$[\mathbf{e}_a, \mathbf{e}_b] = (\Gamma^m{}_{ba} - \Gamma^m{}_{ab})\, \mathbf{e}_m \tag{2.3}$$

holds, where the $\Gamma^m{}_{ab}$ are coefficients of the connection (see A2). If f is a scalar function, the commutation relations

$$[\mathbf{e}_b, \mathbf{e}_a] f = f_{,ab} - f_{,ba} = f_{,m}\, (\Gamma^m{}_{ab} - \Gamma^m{}_{ba}) \tag{2.4}$$

must then hold as integrability conditions on f.

In the exterior algebra a *bivector* is any 2-form. A well-known invariant classification scheme for any bivector $B_{\mu\nu} dx^\mu \wedge dx^\nu$ is given through the definition: B is *null* (or "singular") if and only if $B_{\mu\nu}B^{\mu\nu} = 0 = B^*_{\mu\nu}B^{\mu\nu}$; otherwise B is *nonnull*. In terms of the six basis bivectors $\epsilon^{\mathrm{I}}, \epsilon^{\mathrm{II}}, \ldots, \epsilon^{\mathrm{VI}}$ introduced in Ref. 1, one sees that $B = B_A \epsilon^A$ ($A = \mathrm{I}, \mathrm{II}, \ldots, \mathrm{VI}$) is null if and only if $B_A B^A = 0 = B^*_A B^A$.

It was seen in Ref. 1 that a given null bivector could be transformed by (2.2) into the canonical form

$$B = B_{\mathrm{III}}\epsilon^{\mathrm{III}} + B_{\mathrm{VI}}\epsilon^{\mathrm{VI}} = 2B_{\mathrm{III}}\epsilon^3 \wedge \epsilon^1 + 2B_{\mathrm{VI}}\epsilon^3 \wedge \epsilon^2 = 2B_{31}\epsilon^3 \wedge \epsilon^1 + 2B_{32}\epsilon^3 \wedge \epsilon^2. \tag{2.5}$$

The transformation freedom left preserving (2.5) is the subgroup of (2.2) with $\alpha \equiv 0$, the so-called *null rotations about* $\mathbf{e}_4$.

3. THE NULL KILLING BIVECTOR IN A VACUUM SPACE-TIME

Let $\mathcal{E}$ be a vacuum space-time ($R_{ab} = 0$) and $\mathbf{K} = K^a \mathbf{e}_a$, a Killing vector field. Then (see Eisenhart[2])

$$K_{a;b} + K_{b;a} = 0 \ (\Longleftrightarrow K_{a;b} = K_{[a;b]}) \qquad (3.1)$$

are Killing's equations and are satisfied locally over $\mathcal{E}$. Suppose also that the *Killing bivector* (KBV) $B \equiv K_{a;b}\epsilon^a \wedge \epsilon^b$ is null. Then from (2.5)

$$B = 2K_{\text{III}}\,\epsilon^3 \wedge \epsilon^1 + 2K_{\text{VI}}\,\epsilon^3 \wedge \epsilon^2; \qquad (3.2)$$

i.e., $K_{\text{III}} = K_{3;1}$ and $K_{\text{VI}} = K_{3;2}$ are the only non-zero covariant derivatives of $\mathbf{K}$. Hence we keep the KBV (and consequently Killing's equations) in the canonical form (3.2) by any null rotation about $\mathbf{e}_4$.

If R_{abcd} are the components of the Riemannian curvature tensor, then the first set of integrability conditions for (3.1) is given by (see Eisenhart[2]).

$$K_{a;bc} = R_{abcm}K^m. \qquad (3.3)$$

Theorem 2 in Ref. 1 [using (3.3), (3.2), and the Goldberg–Sachs Theorem[3]] gives us that *$\mathcal{E}$ must necessarily be algebraically special* and that $\mathbf{e}_4$ is geodesic and shear-free.

[It can be mentioned at this point that invariants built up from $K_{a;b}$ and R_{abcd} could be examined as was done in Ref. 1. However, $C^{(5)} = C^{(4)} = 0$ and B null are enough to make all invariants studied there equal to zero except $\mathscr{I}$ and $\mathscr{J}$, and the latter are zero if $C^{(3)} = 0$. (The $C^{(i)}$ are the conformal scalars. See Appendix A or Ref. 1). Hence, to use the invariant approach would only be redundant here to the Petrov classification itself.]

4. KILLING'S EQUATIONS AND INTEGRABILITY CONDITIONS IN CANONICAL FORM

Using the relations $K_a = g_{ab}K^b$ and $\Gamma_{411} = \Gamma_{422} = \Gamma_{414} = \Gamma_{424} = 0$ ($\mathbf{e}_4$ is geodesic and shear-free), one can write (3.1) as follows:

$$\begin{aligned}
K_{1,1} &= -K_1\Gamma_{121} + 0 + 0 + K_4\Gamma_{311},\\
K_{1,2} &= -K_1\Gamma_{122} + 0 + K_3\Gamma_{412} + K_4\Gamma_{312},\\
K_{\text{III}} &= -K_1\Gamma_{123} + 0 + K_3\Gamma_{413} + K_4\Gamma_{313} - K_{1,3},\\
K_{1,4} &= -K_1\Gamma_{124} + 0 + 0 + K_4\Gamma_{314};
\end{aligned} \qquad (4.1)$$

$$\begin{aligned}
K_{2,2} &= 0 + K_2\Gamma_{122} + 0 + K_4\Gamma_{322},\\
K_{2,1} &= 0 + K_2\Gamma_{121} + K_3\Gamma_{421} + K_4\Gamma_{321},\\
\overline{K_{\text{III}}} &= 0 + K_2\Gamma_{123} + K_3\Gamma_{423} + K_4\Gamma_{323} - K_{2,3},\\
K_{2,4} &= 0 + K_2\Gamma_{124} + 0 + K_4\Gamma_{324};
\end{aligned} \qquad (4.2)$$

$$\begin{aligned}
K_{\text{III}} &= K_1\Gamma_{321} + K_2\Gamma_{311} + K_3\Gamma_{341} + 0 + K_{3,1},\\
\overline{K_{\text{III}}} &= K_1\Gamma_{322} + K_2\Gamma_{312} + K_3\Gamma_{342} + 0 + K_{3,2},\\
-K_{3,3} &= K_1\Gamma_{323} + K_2\Gamma_{313} + K_3\Gamma_{343} + 0,\\
-K_{3,4} &= K_1\Gamma_{324} + K_2\Gamma_{314} + K_3\Gamma_{344} + 0;
\end{aligned} \qquad (4.3)$$

$$\begin{aligned}
-K_{4,1} &= K_1\Gamma_{421} + K_2\Gamma_{411} + 0 - K_4\Gamma_{341},\\
-K_{4,2} &= K_1\Gamma_{422} + K_2\Gamma_{412} + 0 - K_4\Gamma_{342},\\
-K_{4,3} &= K_1\Gamma_{423} + K_2\Gamma_{413} + 0 - K_4\Gamma_{343},\\
-K_{4,4} &= K_1\Gamma_{424} + K_2\Gamma_{414} + 0 - K_4\Gamma_{344}.
\end{aligned} \qquad (4.4)$$

Equations (3.3) take the form

$$R_{\text{I}cm}K^m = 0, \qquad (4.5)$$

$$R_{\text{II}cm}K^m = K_{\text{III}}\Gamma_{1c}, \qquad (4.6)$$

$$R_{\text{III}cm}K^m = K_{\text{III},c} + 2K_{\text{III}}\Gamma_{\text{II}c}. \qquad (4.7)$$

Since $C^{(5)} = C^{(4)} = 0$, Eqs. (4.5) are identically satisfied. The fact that $\Gamma_{424} = \Gamma_{422} = 0$ (the geodesic and shear-free conditions on $\mathbf{e}_4$) implies that Eqs. (4.6) become

$$C^{(3)}K_2 = C^{(3)}K_4 = 0, \qquad (4.6'\text{a})$$

$$C^{(3)}K_1 + 0 + 0 - C^{(2)}K_4 = 2K_{\text{III}}\Gamma_{421}, \qquad (4.6'\text{b})$$

$$0 + C^{(2)}K_2 + C^{(3)}K_3 + 0 = 2K_{\text{III}}\Gamma_{423}. \qquad (4.6'\text{c})$$

Recall that Γ_{421} is the *complex expansion* and Γ_{423} is the *rotation* of the lightlike geodesic congruence $\mathbf{e}_4$ (see, for example, the optical scalars defined by Sachs[4] or Newman and Penrose[5]). Two cases can now be considered: (A) $C^{(3)} \neq 0$ and (B) $C^{(3)} = 0$. This means that study of A is concerned only with Petrov type-II and type-D spaces, whereas B is concerned only with Petrov types III and N. We exclude flat space ($C^{(i)} = 0$) for the rest of this discussion.

5. CASE A: TYPE II AND D SPACES ADMITTING A NULL KBV

Let $C^{(3)} \neq 0$. Then (4.6′a) implies that $K_4 (\equiv K^3) = 0$ and $K_1 = K_2 = 0$. In this case we are also assuming $K_{\text{III}} \neq 0$. If $K_{\text{III}} = 0$, then $C^{(3)} \neq 0 \Rightarrow K_3 = 0 \Rightarrow \mathbf{K} = 0$. Hence

$$\mathbf{K} = K^4\,\mathbf{e}_4; \qquad (5.1)$$

it is evidently lightlike. Equation (4.6′b) now must have

$$\Gamma_{421} = 0 \qquad (5.2)$$

so that case A is in the class of spaces studied by Kundt.[6]

Using a null rotation about $\mathbf{e}_4$, one can transform K_{III} into a real function, a. Furthermore $K_3 (\equiv K^4)$ may be transformed to 1 so that $\mathbf{K} = \mathbf{e}_4$. The subgroup of (2.2) left after this transformation is now that for which $A = B = 0$. Killing's equations become

$$\begin{aligned}
a &= \Gamma_{413} = \Gamma_{423},\\
0 &= \Gamma_{343} = \Gamma_{344},\\
a &= \Gamma_{341} = \Gamma_{342}.
\end{aligned}$$

Hence (4.6′c) gives

$$C^{(3)} = 2a^2 = \overline{C^{(3)}}. \tag{5.3}$$

Equations (4.7) now take the form

$$a_{,1} + a^2 + a\Gamma_{121} = 0, \tag{5.4a}$$

$$a_{,2} + a^2 + a\Gamma_{122} = -\tfrac{1}{2}C^{(3)}, \tag{5.4b}$$

$$a_{,3} + a\Gamma_{123} = \tfrac{1}{2}C^{(2)}, \tag{5.4c}$$

$$a_{,4} + a\Gamma_{124} = 0, \tag{5.4d}$$

plus their complex conjugates. It is a simple matter to show that these together give

$$\begin{aligned} &a_{,1} = a_{,2} = -\tfrac{3}{2}a^2, \quad a_{,4} = 0, \quad a_{,3} = \tfrac{1}{2}\mathrm{Re}(C^{(2)}),\\ &\Gamma_{121} = \Gamma_{212} = \tfrac{1}{2}a, \quad \Gamma_{124} = 0,\\ &\Gamma_{123} = (2a)^{-1} i\, \mathrm{Im}(C^{(2)}). \end{aligned} \tag{5.5}$$

Through the relationship $-\Gamma_{abc} = e_{a\mu;\nu}e_b^{\mu}e_c^{\nu}$ it can be shown that a Lorentz transformation (2.2) with $A = B = 0$ and parameter β has the effect

$$\Gamma_{1'2'3'} = \Gamma_{123} + \tfrac{3}{2}a(\beta - \bar{\beta}).$$

Since $\overline{\Gamma_{123}} = \Gamma_{213} = -\Gamma_{123}$ it follows that Γ_{123} is pure imaginary. Setting $\beta - \bar{\beta} = -(2/3a)\Gamma_{123}$ transforms Γ_{123} to zero. Hence

$$C^{(2)} = \overline{C^{(2)}} \text{ and } a_{,3} = \tfrac{1}{2}C^{(2)} \tag{5.6}$$

modifies the relationships in (5.5).

The first of the structure equations, (A3a), takes the form

$$d\Gamma_{42} + \Gamma_{42}\wedge(\Gamma_{12} + \Gamma_{34}) = \tfrac{1}{2}C^{(3)}\epsilon^3\wedge\epsilon^1$$

and is satisfied identically. We note here that

$$d\Gamma_{42} = -\tfrac{1}{2}a^2(\epsilon^3\wedge\epsilon^1 + \epsilon^3\wedge\epsilon^2). \tag{5.7}$$

The second of the set, (A3b), is

$$\begin{aligned} &d(\Gamma_{12} + \Gamma_{34}) + 2\Gamma_{42}\wedge\Gamma_{31}\\ &\quad = C^{(3)}(\epsilon^1\wedge\epsilon^2 + \epsilon^3\wedge\epsilon^4) + C^{(2)}\epsilon^3\wedge\epsilon^1 \end{aligned} \tag{5.8}$$

and yields the following results on the connection coefficients:

$$\Gamma_{312} = \Gamma_{322}, \quad \Gamma_{311} = \Gamma_{321}, \quad \Gamma_{314} = \Gamma_{324}. \tag{5.9}$$

The third structure equation (A3c) is

$$\begin{aligned} &d\Gamma_{31} + 2(\Gamma_{12} + \Gamma_{34})\wedge\Gamma_{31}\\ &\quad = \tfrac{1}{2}[C^{(3)}\epsilon^4\wedge\epsilon^2 + C^{(2)}(\epsilon^1\wedge\epsilon^2 + \epsilon^3\wedge\epsilon^4)\\ &\qquad + C^{(1)}\epsilon^3\wedge\epsilon^1], \end{aligned} \tag{5.10}$$

which is not computed in detail at this point.

Consider the Bianchi identities (A4a)–(A4c). Equation (A4a) is identically satisfied and (A4b) gives

$$\begin{aligned} &C^{(2)}_{,2} + \tfrac{9}{2}aC^{(2)} - 4a^2\Gamma_{312} = 0,\\ &C^{(2)}_{,4} + 2a^3 - 2a^2\Gamma_{314} = 0. \end{aligned} \tag{5.11}$$

The commutation relations (2.4) together with (5.11) result in

$$\begin{aligned} &\Gamma_{312} = \Gamma_{322} = \Gamma_{311} = \Gamma_{321}, \quad a = \Gamma_{314} = \Gamma_{324},\\ &C^{(2)} = 4a\Gamma_{312}, \quad C^{(2)}_{,2} = -14a^2\Gamma_{312},\\ &C^{(2)}_{,4} = 0 = \Gamma_{312,4}. \end{aligned} \tag{5.12}$$

The identity (A4c) then gives

$$\begin{aligned} &C^{(2)} = 0 = \Gamma_{311},\\ &C^{(1)}_{,4} = 0 = \Gamma_{313,4},\\ &C^{(1)}_{,2} + 2aC^{(1)} = 6a^2\Gamma_{313}. \end{aligned} \tag{5.13}$$

Since the group (2.2) still can be used to transform Γ_{313} to a pure imaginary function, consider (5.10) with Γ_{313} pure imaginary. Together with the results from the Bianchi identities above, this yields

$$\begin{aligned} &C^{(1)} = -6a\Gamma_{313},\\ &C^{(1)}_{,1} = C^{(1)}_{,2} = 18a^2\Gamma_{313},\\ &\Gamma_{313,1} = -\tfrac{3}{2}a\Gamma_{313} = \Gamma_{313,2}. \end{aligned} \tag{5.14}$$

Notice that $\Gamma_{313} = 0$ implies that the space is Petrov type *D*. This is no surprise since $\Gamma_{313} = 0 = \Gamma_{322}$ is equivalent to stating that the congruence $\mathbf{e}_3$ is also geodesic and shear-free. All conditions and equations would then be satisfied.

Assuming that $\Gamma_{313} \neq 0$ (and hence Petrov type II), one finds the general solution to (5.14) to be

$$\Gamma_{313} = \sigma a, \quad \bar{\sigma} = -\sigma, \tag{5.15}$$

with $\sigma_{,1} = \sigma_{,2} = \sigma_{,4} = 0$. Therefore

$$C^{(1)} = -6\sigma a^2, \tag{5.16}$$

and all equations are satisfied.

The Lie brackets for the basis tetrad are given by

$$\begin{aligned} &[\mathbf{e}_1, \mathbf{e}_2] = -(a/2)(\mathbf{e}_1 - \mathbf{e}_2),\\ &[\mathbf{e}_1, \mathbf{e}_3] = -a(2\mathbf{e}_3 + \sigma\mathbf{e}_4),\\ &[\mathbf{e}_2, \mathbf{e}_3] = -a(2\mathbf{e}_3 - \sigma\mathbf{e}_4),\\ &[\mathbf{e}_i, \mathbf{e}_4] = 0 \quad \text{for } i = 1, 2, 3. \end{aligned}$$

6. CASE B: TYPE III AND N SPACES ADMITTING A NULL KBV.

Let $C^{(3)} = 0$ and suppose $K_{\rm III} \neq 0$. ($K_{\rm III} = 0$ is a *pp* wave and is discussed briefly in Appendix B.) If $K^3 \neq 0$, then both K^1 and K^2 may be transformed to zero by letting $\beta = -(K^2/K^3)$ in (2.2). Then Eq. (4.6′c) gives $\Gamma_{423} = 0$. Using A and B of (2.2) to transform $K_{\rm III}$ to real function and $K^3 = 1$ simplifies Killing's equations. From (4.4) one finds $\Gamma_{341} = \Gamma_{342} = 0$. But then (4.3) implies $K_{\rm III} =$

$K^4\Gamma_{342} = 0$. Hence, there is a contradiction, which shows that K^3 must be zero.

Suppose next that $K^3 = 0$ and $K_{\rm III} \neq 0$. Then

$$\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2 + K^4\mathbf{e}_4. \tag{6.1}$$

Equation (4.6′b) gives $\Gamma_{421} = 0$, so that each of the spaces under consideration again fall into the class studied by Kundt.[6] A transformation (2.2) can make $K_{\rm III}$ a real function a.

First assume $K^1 = 0$ ($\Rightarrow K^2 = 0$). Then $\mathbf{K} = K^4\mathbf{e}_4$ can be transformed to $\mathbf{K} = \mathbf{e}_4$. Hence K^4 ($= K_3$) $= 1$. Equation (4.6′c) then necessitates $a\Gamma_{423} = 0$. Killing's equations (4.2) also give $a = \Gamma_{423}$. Therefore, we obtain $a = 0 = K_{\rm III}$, a contradiction. In summary, there is no way for $K_{\rm III} \neq 0$ to be compatible with $\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2 + K^3\mathbf{e}_3 + K^4\mathbf{e}_4$ whenever $K^3 \neq 0$ or whenever $K^1 = K^2 = K^3 = 0$. Hence, the only case left to explore (for $K_{\rm III} \neq 0$) is $K^3 = 0$ with $K^1 \neq 0$.

Next consider (6.1) and assume $K^1 \neq 0$. A transformation (2.2) can now take K^4 to zero in addition to taking $K_{\rm III}$ to 1. The Killing vector then has the form

$$\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2, \tag{6.2}$$

and is spacelike. The Bianchi identities (A4b) become

$$\begin{aligned} -\Gamma_{423}C^{(2}\cdot\epsilon^3\wedge\epsilon^1\wedge\epsilon^2 &= (C^{(2)}_{,2} - 2C^{(2)}\Gamma_{312})\epsilon^3\wedge\epsilon^1\wedge\epsilon^2 + 2C^{(2)} \\ &\times \Gamma_{423}\epsilon^4\wedge\epsilon^2\wedge\epsilon^3 \\ &+ (-C^{(2)}_{,4} + 2C^{(2)}\Gamma_{341})\epsilon^3\wedge\epsilon^4\wedge\epsilon^1. \end{aligned} \tag{6.3}$$

In particular it is seen that (6.3) implies

$$C^{(2)}\Gamma_{423} = 0. \tag{6.4}$$

Equation (4.6′c) gives

$$C^{(2)}K^1 = 2\Gamma_{423}. \tag{6.5}$$

Hence $\Gamma_{423} = 0$ if and only if $C^{(2)} = 0$ and Eq. (6.4) gives

$$C^{(2)} = 0 = \Gamma_{423}. \tag{6.6}$$

Consequently the space is Petrov type N. Since Γ_{423} (the "rotation" of $\mathbf{e}_4$) is zero, this space is also a *pp wave* by Kundt's characterization (Ref. 6, p. 79). In this case $\mathbf{e}_4$ is also a Killing vector field, is a principal null vector for the KBV associated with (6.2), and is tangent to a ray congruence which is parallel.

Case B is then a *pp wave:* the plane-fronted gravitational wave solution which is Petrov type N and has parallel rays. If one continues to examine the subcase (6.2), all equations can be satisfied so that both $\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2$ and $\mathbf{K} = K^4\mathbf{e}_4$ may coexist in the same type-N space, both having null Killing bivectors.

7. APPLICATIONS TO THE STUDY OF GEODESIC KILLING VECTORS

In this discussion, it is still assumed that $\mathcal{E}$ is a vacuum space-time ($R_{ab} = 0$) and that flat space is excluded.

Theorem 1: Let $\mathcal{E}$ be a vacuum space-time and let $\mathbf{K} = K^a\mathbf{e}_a$ be a *geodesic* Killing vector field. Then (1) $\mathbf{K}$ is lightlike, (2) $\mathbf{K}$ is geodesic and shear-free, (3) $\mathcal{E}$ is algebraically special.

Proof: That $\mathbf{K}$ is geodesic implies

$$K_{a;b}K^b = f\cdot K_a \tag{7.1}$$

for some scalar f. If $K_{a;b}$ defines a *null* bivector over $\mathcal{E}$, then $\mathcal{E}$ must be algebraically special by Theorem 2 in Ref. 1. The eigenvalue problem for a null bivector necessitates $f \equiv 0$ above. In Sec. 5 the Killing vector field $\mathbf{K}$ is necessarily lightlike, geodesic, and shear-free with $K_{\rm III} \neq 0$. In Sec. 6, one possibility for $\mathbf{K}$ is $\mathbf{K} = K^4\mathbf{e}_4$, which is lightlike, geodesic, shear-free, with $K_{\rm III} = 0 = K_{3;1}$. The other possibility here is the spacelike $\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2$, with (7.1) implying

$$K_{3;1}K_2 + K_{3;2}K_1 = 0. \tag{7.2}$$

Equation (7.2) is to be preserved under the subgroup of (2.2), with $\alpha = \beta = 0$; i.e., A and B are arbitrary real parameters. Since

$$K_{3';1'} = \exp(-A - iB)K_{3;1}$$
and
$$K_{2'} = \exp(iB)K_2,$$
then
$$e^A K_{3;1}K_2 + e^{-A}K_{3;2}K_1 = 0. \tag{7.3}$$

Letting $K_{3;1} = ae^{i\theta}$ and $K_2Ke^{i\phi}$, (7.3) is equivalent to

$$a = 0 \text{ or } K = 0 \text{ or } \sin(\theta + \phi) = \cos(\theta + \phi) = 0, \tag{7.4}$$

since $A \equiv 0$ is impossible. Clearly, none of (7.4) is possible since $K_{\rm III} \neq 0$ and $\mathbf{K} \neq 0$ are assumed. Consequently, the spacelike Killing vector field of Sec. 6 is not geodesic. Hence all geodesic Killing vector fields with a null KBV are lightlike.

If $K_{a;b}$ defines a *nonnull* bivector over $\mathcal{E}$, then it can be shown (see Ref. 1) that $\mathbf{K}$ being geodesic allows only for $\mathbf{K}$ to be lightlike and tangent to one of the principal null congruences of $K_{a;b}$. Furthermore, $K_{(a;b)} = 0 \Rightarrow \mathbf{K}$ is shear-free. Hence $\mathcal{E}$ is algebraically special by the Goldberg–Sachs theorem; $\mathbf{K}$ must then be a multiple Debever vector field. QED

Theorem 2: Let $\mathcal{E}$ be a vacuum space-time and let $\mathbf{K} = K^a\mathbf{e}_a$ be a (lightlike) geodesic Killing vector field. Then the associated Killing bivector $K_{a;b}$ is *null* and the space represents an *expansion-free radiation field*.[6] Furthermore, the only such spaces which are not *pp* waves are those encountered in Sec. 5. (That is, there are no geodesic Killing vectors in a space-time $R_{ab} = 0$ which generate a nonnull bivector.)

Proof: After the work of Theorem 1 it is necessary only to show that the nonnull KBV studied in Ref. 1 is incompatible with any geodesic Killing vector. It was shown in Ref. 1 that if $\mathbf{e}_3$ and $\mathbf{e}_4$ are tangent to principal null congruences for the nonnull KBV, then $\mathbf{K}$ being geodesic implies $\mathbf{K} = K^3\mathbf{e}_3$ or $\mathbf{K} = K^4\mathbf{e}_4$. Take first $\mathbf{K} = K^4\mathbf{e}_4$ and say that $e_{4\mu} = K_\mu$, so that $K_{\mu;\nu} = e_{4\mu;\nu}$. (The argument for $\mathbf{K} = K^3 e_3$ is completely analogous.) Then

$$\Gamma_{4ab} = -K_{\mu;\nu} e^\mu_a e^\nu_b. \tag{7.5}$$

But $K_{(\mu;\nu)} = 0$, so that $\Gamma_{4ab} = \Gamma_{4[ab]}$ and, hence,

$$\Gamma_{4(ab)} = 0. \tag{7.6}$$

So $\Gamma_{411} = \Gamma_{422} = \Gamma_{433} = 0$. Furthermore (7.6) implies $\Gamma_{4a4} = 0$; therefore $\Gamma_{414} = \Gamma_{424} = \Gamma_{434} = 0$. Since now $C^{(5)} = C^{(4)} = 0$ is implied here, the integrability conditions on Killing's equations corresponding to (3.3) necessitate $\Gamma_{423} = \Gamma_{421} = \Gamma_{412} = \Gamma_{413} = 0$. Since $K_{\mu;\nu} = K_{[\mu;\nu]}$, these relations all imply $\Gamma_{4ab} = 0$. Therefore, the independence of $\{\mathbf{e}_a\}$ gives $K_{[\mu;\nu]} = 0$ and so $K_{\mu;\nu} = 0$, contrary to $K_{a;b}$ being nonnull. Hence, a nonnull KBV (studied in Ref. 1) excludes completely any geodesic Killing vector fields. Theorem 3 of Ref. 1 can then be stated more strongly: $\mathbf{K}$ is a Killing vector and $K_{a;b}$ is a nonnull KBV $\Rightarrow$ $\mathbf{K}$ is not geodesic. QED

Corollary to Theorem 2: There are no Petrov type-III vacuum space-times admitting a geodesic Killing vector field.

Proof: Sections 5 and 6 exhaust all possibilities for geodesic Killing vectors.

If the geodesic Killing vector belongs to a space more general than a *pp* wave (type *N*), then it must belong to one of the spaces in Sec. 5. QED

The following global result can now be stated:

Theorem 3: Let $\mathcal{E}$ be a vacuum space-time and let $\mathbf{K}$ be a (lightlike) geodesic Killing vector field. Then (as a vector field over $\mathcal{E}$) $\mathbf{K}$ is complete.

Proof: This follows from results of Boyer.[7]

8. CONCLUSIONS

From the present study, it can be seen that "most" vacuum space-times with a symmetry (Killing vector field) possess a Killing bivector which is nonnull. Those space-times admitting a symmetry whose associated bivector is null fall into a very narrow category, the algebraically special spaces whose Debever vector field is also a Killing vector, and consequently is expansion-free. These were called the expansion-free radiation fields by Kundt.[6]

Further analysis of the null KBV yields the fact that both Petrov type-II and type-*D* spaces are allowed. However, types more special than this all turn out to be the plane-fronted gravitational waves with parallel rays, the *pp* waves, and are all Petrov type *N*. Hence, no type-III spaces contain a null KBV.

The earlier work of the author[1] plus work in this paper go to characterize the geodesic Killing vector in a vacuum space-time. Such a Killing vector can be found only in those (nonflat) spaces which are *expansion-free radiation fields*. The associated Killing bivector for this case is necessarily null.

Kerr and the author[8] studied vacuum space-times which (1) were algebraically special, (2) possessed an *expanding* multiple Debever vector field, and (3) admitted a Killing vector field. Since $\mathbf{e}_4$ in Secs. 5 and 6 of this work is *expansion-free*, the bivector associated with each Killing vector field in Ref. 8 must then be nonnull.

APPENDIX A: STRUCTURE EQUATIONS AND BIANCHI IDENTITIES FOR A VACUUM SPACE-TIME

In the complex null tetrad approach, the following components of the Riemann tensor are the conformal scalars for $R_{ab} = 0$:

$$\begin{aligned}
C^{(5)} &= 2R_{4242},\\
C^{(4)} &= R_{4212} + R_{4234},\\
C^{(3)} &= \tfrac{1}{2}(R_{1212} + 2R_{1234} + R_{3434}) = 2R_{4231},\\
C^{(2)} &= R_{3112} + R_{3134},\\
C^{(1)} &= 2R_{3131}.
\end{aligned} \tag{A1}$$

The space is algebraically special if and only if there exists a tetrad for which $C^{(5)} = C^{(4)} = 0$ or $C^{(1)} = C^{(2)} = 0$. Related to this, the Goldberg-Sachs theorem[3] states that the space is algebraically special if and only if there exists a geodesic and shear-free lightlike vector field; such a field is $\mathbf{e}_4$ whenever $C^{(5)} = C^{(4)} = 0$ and $\mathbf{e}_3$ whenever $C^{(1)} = C^{(2)} = 0$.

In order to introduce the connection coefficients for the space, the first structure equations are given by

$$d\epsilon^a = \Gamma^a{}_{bc}\epsilon^b \wedge \epsilon^c = \Gamma^a{}_{[b,c]}\epsilon^b \wedge \epsilon^c, \tag{A2}$$

where the $\Gamma^a{}_{bc}$ are the connection coefficients. They have the properties $\Gamma_{abc} = -\Gamma_{bac}$, where $\Gamma_{abc} \equiv g_{am}\Gamma^m{}_{bc}$, and are not necessarily skew symmetric in (bc). This also defines the connection 1-form $\Gamma_{ab} \equiv \Gamma_{abc}\epsilon^c$.

The second structure equations are equations involving 2-forms. These are

$$d\Gamma_{ab} + \Gamma_{am}\wedge\Gamma_b^m = \tfrac{1}{2}\mathcal{R}_{ab}, \quad (A3)$$

where $\mathcal{R}_{ab} \equiv R_{abcd}\epsilon^c\wedge\epsilon^d$, the curvature 2-forms. In terms of the notation of basis bivectors (see Sec. 2 and Ref. 1) these become

$$d\Gamma_{I} + 2\Gamma_{I}\wedge\Gamma_{II} = \tfrac{1}{2}\mathcal{R}_{I}, \quad (A3'a)$$

$$d\Gamma_{II} + \Gamma_{I}\wedge\Gamma_{III} = \tfrac{1}{2}\mathcal{R}_{II}, \quad (A3'b)$$

$$d\Gamma_{III} + 2\Gamma_{II}\wedge\Gamma_{III} = \tfrac{1}{2}\mathcal{R}_{III}, \quad (A3'c)$$

plus their complex conjugates.

The Bianchi identities are easily obtained by taking the exterior derivatives of (A3) above. Hence we have

$$d\mathcal{R}_{I} = 2\mathcal{R}_{I}\wedge\Gamma_{II} - 2\Gamma_{I}\wedge\mathcal{R}_{II}, \quad (A4a)$$

$$d\mathcal{R}_{II} = \mathcal{R}_{I}\wedge\Gamma_{III} - \Gamma_{I}\wedge\mathcal{R}_{III}, \quad (A4b)$$

$$d\mathcal{R}_{III} = 2\mathcal{R}_{II}\wedge\Gamma_{III} - 2\Gamma_{II}\wedge\mathcal{R}_{III}. \quad (A4c)$$

In a vacuum space-time the curvature 2-forms in Eq. (A3) become

$$\tfrac{1}{2}\mathcal{R}_{I} = \tfrac{1}{2}[C^{(5)}\epsilon^4\wedge\epsilon^2 + C^{(4)}(\epsilon^1\wedge\epsilon^2 + \epsilon^3\wedge\epsilon^4) + C^{(3)}\epsilon^3\wedge\epsilon^1], \quad (A5a)$$

$$\tfrac{1}{2}\mathcal{R}_{II} = \tfrac{1}{2}[C^{(4)}\epsilon^4\wedge\epsilon^2 + C^{(3)}(\epsilon^1\wedge\epsilon^2 + \epsilon^3\wedge\epsilon^4) + C^{(2)}\epsilon^3\wedge\epsilon^1], \quad (A5b)$$

$$\tfrac{1}{2}\mathcal{R}_{III} = \tfrac{1}{2}[C^{(3)}\epsilon^4\wedge\epsilon^2 + C^{(2)}(\epsilon^1\wedge\epsilon^2 + \epsilon^3\wedge\epsilon^4) + C^{(1)}\epsilon^3\wedge\epsilon^1]. \quad (A5c)$$

It is this latter formulation that is most useful for calculations.

APPENDIX B: THE PLANE-FRONTED WAVES

A trivial case of the Killing vector field $\mathbf{K} = K^\mu\partial_\mu$ having a null KBV is where $K_{\mu;\nu} = 0$. This means that $\mathbf{K}$ is a *parallel* vector field and, by an argument of Ehlers and Kundt,[9] is necessarily lightlike. (This case was also mentioned in passing while setting up the more general problem in Ref. 1.)

Ehlers and Kundt[9] define the *plane-fronted gravitational waves* as being those solutions to the vacuum field equations which are of Petrov type N and possess a hypersurface orthogonal, shear-free, expansion-free (lightlike) ray congruence. The *plane-fronted waves with parallel rays*, the *pp waves*, have the additional property that the ray congruence is recurrent. That is, if k^μ is tangent to the ray convergence, then $k_{\mu;\nu} = \gamma k_\mu k_\nu$, where γ is a scalar.

Six characterizations for a *pp* wave are cited in Ref. 8, with three actually proved. Furthermore, a *pp* wave has the metric

$$ds^2 = dx^2 + dy^2 + 2du dv + 2H(x,y,u)du^2,$$

where the four coordinates form a (real) harmonic system and the scalar H satisfies $H_{xx} + H_{yy} = 0$. The contravariant vector ∂_v is a covariant constant Killing vector field.

A result useful for the work in the present paper was mentioned by Kundt[6]: The expansion-free radiation fields with *vanishing rotation* have parallel rays; if the space is also Petrov type N, it is necessarily a *pp* wave.

---

1 G. C. Debney, J. Math. Phys. 12, 1088 (1971).
2 L. P. Eisenhart, *Riemannian Geometry*, (Princeton U.P., Princeton, N.J., 1960).
3 J. N. Goldberg and R. K. Sachs, Acta Phys. Polon. 22, 13 (1962).
4 R. K. Sachs, Proc. Roy. Soc. A264, 309 (1961).
5 E. T. Newman and R. Penrose, J. Math. Phys. 3, 565 (1962).
6 W. Kundt, Z. Physik 163, 77 (1961).
7 R. H. Boyer, Proc. Roy. Soc. A311, 245 (1969).
8 R. P. Kerr and G. C. Debney, J. Math. Phys. 11, 2807 (1970).
9 J. Ehlers and W. Kundt, *Gravitation* edited by L. Witten (Wiley, New York, 1962), Chap. 2.

An Explicit Basis for the Reduction $U(n+m) \downarrow U(n) \times U(m)$*

Jouko Mickelsson†
Institute of Theoretical Physics, Fack, S-402 20, Göteborg 5, Sweden
(Received 8 April 1971)

We construct lowering operators associated with the multiplicity pattern obtained in a previous paper [J. Math. Phys. 11, 2803 (1970)] for the labeling of the basis vectors in the reduction of an irreducible representation of $U(n+m)$ with respect to $U(n) \times U(m)$. Every basis vector can be written as a product of lowering operators acting on the highest-weight vector.

1. INTRODUCTION

Nagel and Moshinsky[1] have some years ago constructed a set of operators which can be used for lowering the irreducible vector spaces of $U(n-1)$ contained in an irreducible vector space of $U(n)$. With the help of these operators, one can write every basis vector as a product of lowering operators acting on the state of highest weight.

In this paper we construct a set of operators which can be used for lowering the irreducible vector spaces of $U(n) \times U(m)$ in an irreducible representation of $U(n+m)$. Here $U(m)$ is the subgroup of $U(n+m)$ which transforms the first m components of a vector in the defining representation of $U(n+m)$ and correspondingly $U(n)$ transforms the last n components. For the labeling of the various IR's of $U(n) \times U(m)$ (which have generally a multiplicity bigger than one) in an IR of $U(n+m)$, we use a pattern which we derived in a previous paper.[2] Every semimaximal state [= a basis vector of highest weight with respect to $U(n) \times U(m)$ in an IR of $U(n) \times U(m)$] can be written as a product of lowering operators acting on the highest-weight vector. An arbitrary basis vector may then be obtained by acting with the canonical lowering operators of $U(n)$ and $U(m)$ on the semimaximal states.

Work on similar lines has previously been done by Devi and Venkatarayudu in Ref. 3, where they have explicitly constructed the basis vectors using a boson operator realization for the cases $U(4) \downarrow U(2) \times U(2)$ and $U(6) \downarrow U(3) \times U(3)$.

The knowledge of the explicit form of the basis vectors is important at least in

(i) the calculation of the matrix element of the generators.
(ii) the calculation of the Wigner coefficients for $U(n)$.

When reducing the direct product of two irreducible representations of $U(n)$ to irreducible constituents, one is led to consider representations of $U(2n)$ in the chain $U(2n) \supset U(n) \times U(n)$.[4]

Finally let us mention that the knowledge of the explicit form of the IR's of $U(n+m)$ in the chain $U(n+m) \supset U(n) \times U(m)$ is useful when constructing representations of the noncompact groups $U(n,m)$. If one has a UIR (unitary irreducible representation) of $U(n+m)$ in this chain, then one may find UIR's of the group $U(n,m)$ in the chain $U(n,m) \supset U(n) \times U(m)$ [$U(n) \times U(m)$ is the maximal compact subgroup] by letting some of the labels take complex values.

2. DEFINITION OF THE LOWERING OPERATORS

We consider an irreducible representation (IR) of $U(n+m)$ characterized by the highest weight $(\lambda_1, \lambda_2, \ldots, \lambda_{n+m})$. According to Ref. 2 the Gel'fand-Zetlin (GZ) patterns of the subgroups $U(n)$ and $U(m)$ together with the pattern given below can be used for labeling of a complete set of basis vectors in the representations space:

$$\begin{bmatrix} \lambda_m & \lambda_{m+1} & \lambda_{m+2} & \cdots & \lambda_{m+n} \\ \lambda_{m-1} & k_1^{m-1} & k_2^{m-1} & \cdots & k_n^{m-1} \\ \lambda_{m-2} & k_1^{m-2} & k_2^{m-2} & \cdots & k_n^{m-2} \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \lambda_1 & k_1^1 & k_2^1 & \cdots & k_n^1 \\ & l_1 & l_2 & \cdots & l_n. \end{bmatrix} \tag{2.1}$$

There are two rules restricting the range of the labels (which are all integers):

(i) Every number in the pattern is less than or equal to the number above its left and greater than or equal to the number above it;
(ii) $S_j^i \geq S_j^{i+1}, j = 1, 2 \ldots, n$ and $i = 1, 2, \ldots, m-1$.

S_j^i is the sum of the j first numbers on the $(i+1)$ th row from the bottom minus the sum of numbers immediately below right. For example, $S_1^1 = \lambda_1 - l_1$ and $S_3^2 = \lambda_2 + k_1^2 + k_2^2 - k_1^1 - k_2^1 - k_3^1$. When reading the pattern (2.1) from left to right in an arbitrary row, the numbers never increase, and when reading from top to bottom in any column the numbers never decrease. $(l_1, l_2, \ldots, l_n)$ is a highest weight characterizing an IR of $U(n)$ and correspondingly $(j_1, j_2, \ldots, j_m)$ labels the IR's of the $U(m)$ subgroup, where

$$j_v = S_n^v + k_n^v, \quad k_n^m \equiv \lambda_{n+m}, \quad v = 1, 2, \ldots, m. \tag{2.2}$$

Because every basis vector can be obtained by acting with the known lowering operators [1] of the subgroups $U(n)$ and $U(m)$ on a semimaximal basis vector, we can restrict our attention from now on to these vectors. For the semimaximal states we can drop the GZ patterns associated with $U(n)$ and $U(m)$ and we can denote them solely by (2.1)

We denote the generators of $U(n+m)$ by $E_j^i, i, j = 1, 2, 3, \cdots, n+m, E_i^i = H_i$. They fulfill the commutation relations

$$[E_j^i, E_l^k] = \delta_{jk} E_l^i - \delta_{il} E_j^k. \tag{2.3}$$

The H_i's span the Cartan subalgebra. In unitary representation the hermiticity condition

$$(E^i_j)^\dagger = E^j_i \tag{2.3'}$$

is satisfied. Generators E^i_j with $i < j$ are raising generators for the weights and the E^i_j with $i > j$ are lowering generators. The generators with the indices less than or equal to m span the algebra of the subgroup $U(m)$ and the ones with indices greater than m, the algebra of $U(n)$. For any semimaximal state $|s.m.\rangle$ one has

$$\begin{aligned} &E^i_j\,|s.m.\rangle = 0, \quad \text{if } i < j \\ &\text{and } i,j = 1,2,\ldots,m \\ &\text{or } \; i,j = m+1, m+2, \ldots, m+n, \end{aligned} \tag{2.4}$$

$$\begin{aligned} &H_i\,|s.m.\rangle = j_i\,|s.m.\rangle, \quad \text{if } i = 1,2,\ldots,m, \\ &H_i\,|s.m.\rangle = l_{i-m}\,|s.m.\rangle, \\ &\text{if } i = m+1, m+2, \ldots, m+n. \end{aligned} \tag{2.4'}$$

For the highest-weight vector $|M\rangle$ one has

$$E^i_j|M\rangle = 0, \quad \text{if } i < j, i, j = 1,2,\ldots,m+n, \tag{2.5}$$

$$H_i|M\rangle = \lambda_i|M\rangle, \quad i = 1,2,\ldots,m+n. \tag{2.5'}$$

Comparing (2.1), (2.4′), and (2.5′) one concludes

$$|M\rangle = \begin{bmatrix} \lambda_m & \lambda_{m+1} & \lambda_{m+2} & \cdots & \lambda_{m+n} \\ \lambda_{m-1} & \lambda_{m+1} & \lambda_{m+2} & \cdots & \lambda_{m+n} \\ \vdots & \vdots & \vdots & & \vdots \\ \lambda_1 & \lambda_{m+1} & \lambda_{m+2} & \cdots & \lambda_{m+n} \\ & \lambda_{m+1} & \lambda_{m+2} & \cdots & \lambda_{m+n} \end{bmatrix}. \tag{2.6}$$

Let us now assume that we have found a set of operators $\{L^i_j, j = 1,2,\ldots,m \text{ and } i = m+1, m+2, \ldots, m+n\}$, which are polynomials in the generators and which satisfy the following equations:

$$\begin{aligned} &[E^k_l, L^i_j]\,|s.m.\rangle = 0, \quad \text{if } k < l \\ &\qquad\qquad \text{and } k,l = 1,2,\ldots,m \\ &\text{or } \; k,l = m+1, m+2, \ldots, m+n, \end{aligned} \tag{2.7}$$

$$[H_k, L^i_j] = (\delta_{ki} - \delta_{kj})L^i_j, \quad k = 1,2,\ldots,m+n. \tag{2.7'}$$

Equation (2.7) says that when acting with L^i_j on a semimaximal state the result contains only semimaximal states. Because of Eq. (2.7′) we call the L^i_j the lowering operators. Using the lowering operators one can give an operational *definition* for the general semimaximal state by writing

$$\begin{bmatrix} \lambda_m & \lambda_{m+1} & \lambda_{m+2} & \cdots & \lambda_{m+n} \\ \lambda_{m-1} & k^{m-1}_1 & k^{m-1}_2 & \cdots & k^{m-1}_n \\ \lambda_{m-2} & k^{m-2}_1 & k^{m-2}_2 & \cdots & k^{m-2}_n \\ \vdots & & & & \vdots \\ \lambda_1 & k^1_1 & k^1_2 & \cdots & k^1_n \\ & l_1 & l_2 & \cdots & l_n \end{bmatrix}$$

$$\begin{aligned} &= \prod_{i_1=m+1}^{m+n} (L^{i_1}_1)^{l_{i_1-m} - k^1_{i_1-m}} \prod_{i_2=m+1}^{m+n} (L^{i_2}_2)^{k^1_{i_2-m} - k^2_{i_2-m}} \\ &\times \cdots \times \prod_{i_{m-1}=m+1}^{m+n} (L^{i_{m-1}}_{m-1})^{k^{m-2}_{i_{m-1}-m} - k^{m-1}_{i_{m-1}-m}} \\ &\times \prod_{i_m=m+1}^{m+n} (L^{i_m}_m)^{k^m_{i_m-m} - \lambda_{i_m}} |M\rangle. \end{aligned} \tag{2.8}$$

(However, this basis is in general nonorthogonal.) In (2.8) we can choose the following convention for the order of the L^i_j with different values of the index i but with the same value of j: If one reads the formula (2.8) from the left to the right, the index i decreases. From (2.8) one can see that the effect of a single operator L^i_j is the following:

$$\begin{aligned} &L^i_j \begin{bmatrix} \lambda_j & k^j_1 & \cdots & k^j_{i-m-1} & k^j_{i-m} & k^j_{i-m+i} & \cdots & k^j_n \\ \lambda_{j-1} & k^{j-1}_1 & \cdots & k^{j-1}_{i-m-1} & k^{j-1}_{i-m} & k^j_{i-m+1} & \cdots & k^j_n \end{bmatrix} \\ &= \begin{bmatrix} \lambda_j & k^j_i & \cdots & k^j_{i-m-1} & k^j_{i-m} & k^j_{i-m+1} & \cdots & k^j_n \\ \lambda_{j-1} & k^{j-1}_1 & \cdots & k^{j-1}_{i-m-1} & k^{j-1}_{i-m}+1 & k^j_{i-m+1} & \cdots & k^j_n \end{bmatrix}, \\ &k^0_i = l_i \end{aligned} \tag{2.9}$$

The two-rowed pattern in Eq. (2.9) means the subpattern consisting of the rows beginning with λ_{j-1} and λ_j of the pattern (2.1) describing a semimaximal state for which $l_v = k^1_v = k^2_v = \cdots = k^{j-1}_v$, $v = 1,2,\ldots,n$. The operators L^i_j given by the formula (3.1) in Sec. 3 satisfy

$$\begin{aligned} &[L^i_j, L^{i'}_j]\,|s.m.\rangle = 0, \\ &\quad j = 1,2,\ldots,m,\; i,i' = m+1, m+2, \ldots, m+n. \end{aligned} \tag{2.10}$$

The proof of Eq. (2.10) for the L^i_j given by (3.1) is given in the Appendix. Using (2.10), one sees that these operators have a stronger property than (2.9), namely

$$L^i_j \begin{bmatrix} \lambda_j & k^j_1 & \cdots & k^j_{i-m-1} & k^j_{i-m} & k^j_{i-m+1} & \cdots & k^j_n \\ \lambda_{j-1} & k^{j-1}_1 & \cdots & k^{j-1}_{i-m-1} & k^{j-1}_{i-m} & k^{j-1}_{i-m+1} & \cdots & k^{j-1}_n \end{bmatrix} = \begin{bmatrix} \lambda_j & k^j_1 & \cdots & k^j_{i-m-1} & k^j_{i-m} & k^j_{i-m+1} & \cdots & k^j_n \\ \lambda_{j-1} & k^{j-1}_1 & \cdots & k^{j-1}_{i-m-1} & k^{j-1}_{i-m}+1 & k^{j-1}_{i-m+1} & \cdots & k^{j-1}_n \end{bmatrix}. \tag{2.9'}$$

3. CONSTRUCTION OF THE LOWERING OPERATORS

In a similar way as it was done in Ref. 1 for the canonical case $U(n) \supset U(n-1)$, we search for a polynomial in the generators E^i_j which satisfies (2.7) and (2.7′). If we put L^i_j equal to a sum of terms of the type $E^i_{l_1} E^{l_1}_{l_2} \cdots E^{l_{s-1}}_{l_s} E^{l_s}_j$ with some unknown coefficients containing elements from the Cartan subalgebra, then (2.7′) is automatically satisfied. We have found that if we put

$$L^i_j = \prod_{\mu=m+1}^{i-1}(\mathcal{E}_{i\mu}-1)\prod_{v=j+1}^{m}\mathcal{E}_{jv}\sum_{p=0}^{i-m-1}\;\sum_{\mu_p>\mu_{p-1}>\dots>\mu_1=m+1}^{i-1}\left(\prod_{k=1}^{p}\frac{1}{\mathcal{E}_{i\mu_k}-1}\right)\sum_{q=0}^{m-j}\;\sum_{v_q>v_{q-1}>\dots>v_1=j+1}^{m}\left(\prod_{l=1}^{q}\frac{1}{\mathcal{E}_{jv_l}}\right)$$

$$\times E^i_{\mu_p}E^{\mu_p}_{\mu_{p-1}}\cdots E^{\mu_2}_{\mu_1}E^{\mu_1}_{v_q}E^{v_q}_{v_{q-1}}\cdots E^{v_2}_{v_1}E^{v_1}_j,\quad j=1,2,\dots m,\quad i=m+1,m+2,\dots m+n, \tag{3.1}$$

where $\mathcal{E}_{kl} = H_k - H_l + l - k$,

then also (2.7) is fulfilled. Note that (3.1) is not the only solution of Eqs. (2.7) and (2.7′) but it seems to be the simplest solution. By comparing (3.1) with (2.27b′) and (2.27a″) in Ref. 1, one notices the following:

(1) The L^{m+1}_j's, $j = 1, 2, \dots m$, are the lowering operators for irreducible vector spaces of $U(m)$ in an UIR of $U(m+1)$.
(2) If the index shifts $m + k \to k$ and $m \to n + 1$, $k = 1, 2, \dots, n$, are made in the operator L^i_m, the result is a raising operator for the subgroup $U(n)$ of the group $U(n+1)$.

We now prove that (3.1) indeed satisfies (2.7). Consider first the commutators $[E^k_l, L^i_j]$ for $k, l = 1, 2, \dots, m$ and $k < l$. We take an arbitrary term in the sums over p and the μ_k in (3.1). Because E^k_l commutes with the algebra of $U(n)$, we conclude that $[E^k_l, L^i_j]|s.m.\rangle = 0$ if

$$[E^k_l, L_j(\mu_1)]|s.m.\rangle = 0,$$

where

$$L_j(\mu_1) = \prod_{v=j+1}^{m}\mathcal{E}_{jv}\sum_{q=0}^{m-j}\;\sum_{v_q>v_{q-1}>\dots>v_1=j+1}^{m}\times\left(\prod_{l=1}^{q}\frac{1}{\mathcal{E}_{jv_l}}\right)E^{\mu_1}_{v_q}E^{v_q}_{v_{q-1}}\cdots E^{v_2}_{v_1}E^{v_1}_j,\quad \mu_1 \geqq m+1. \tag{3.2}$$

We have dropped the elements from the algebra of Un. By $|s.m.\rangle$ we again denote an arbitrary semimaximal state. But $L_j(\mu_1)$ is the lowering operator for the jth weight of a UIR of $U(m)$ in a UIR of $U(m+1)$ [see Eq. (2.27b′) in Ref. 1]. Here the $(m+1)$th component of a basis vector in the defining representation is denoted by the symbol μ_1 instead of the number $m+1$. It then follows from Ref. 1 [see Eq. (2.13′)] that (3.2) is valid.

The proof of (2.7) for $k, l = m+1, m+2, \dots, m+n, k < l$, goes on similar lines. We take an arbitrary term in the sums over q and the v_k in (3.1). After dropping factors from the algebra of $U(m)$ (which commutes with E^k_l), we see that $[E^k_l, L^i_j]$, $|s.m.\rangle = 0$ if

$$[E^k_l, L^i(v_q)]|s.m.\rangle = 0, \tag{3.3}$$

where

$$L^i(v_q) = \prod_{\mu=m+1}^{i-1}(\mathcal{E}_{i\mu}-1)\sum_{p=0}^{i-m-1}\;\sum_{\mu_p>\mu_{p-1}>\dots>\mu_1=m+1}^{i-1}\left(\prod_{k=1}^{p}\frac{1}{\mathcal{E}_{i\mu_k}-1}\right)E^i_{\mu_p}E^{\mu_p}_{\mu_{p-1}}\cdots E^{\mu_2}_{\mu_1}E^{\mu_1}_{v_q},\quad v_q \le m.$$

Using the commutation relations one can write

$$L^i(v_q) = \left(\sum_{p=0}^{i-m-1}\;\sum_{\mu_p>\mu_{p-1}>\dots>\mu_1=m+1}^{i-1}E^i_{\mu_p}E^{\mu_p}_{\mu_{p-1}}\times\dots\times E^{\mu_2}_{\mu_1}E^{\mu_1}_{v_q}\prod_{k=1}^{p}\frac{1}{\mathcal{E}_{i\mu_k}}\right)\prod_{\mu=m+1}^{i-1}\mathcal{E}_{i\mu},\quad v_q \leqq m. \tag{3.4}$$

One can associate with the generators E^A_B, $A, B = m+1, m+2, \dots, m+n-1, m+n, v_q$, a group $U(n+1)$. The group $U(n)$ associated with the E^A_B with A and B different from v_q is the canonical subgroup $U(n)$. Comparing (3.4) with (2.27a″) in Ref. 1, one sees that $L^i(v_q)$ is a raising operator for this $U(n)$ subgroup. It then follows that (3.3) is fulfilled [see Eq. (2.13″) in Ref. 1]. We have now fully proven (2.7).

There exists a nice illustration for L^i_j by means of simple diagrams. First draw a straight line with $i - j + 1$ dots labeled by numbers from j to i, decreasing from left to right. Choose then k dots ($0 \le k \le i - j - 1$) between the dots i and j in every possible way and connect them to each other and to the dots i and j by curves. Associate then with every diagram a term in the operator L^i_j as follows: With each free dot v associate a factor $\mathcal{E}_{iv} - 1$ if $v \geqq m+1$ and a factor $\mathcal{E}_{jv}$ if $v \le m$. For each curve connecting two dots, say k and l, $k > l$, write a factor E^k_l in the same order from the left to the right as in the diagram. As an example, let us find L^5_2 when $m = 3$.

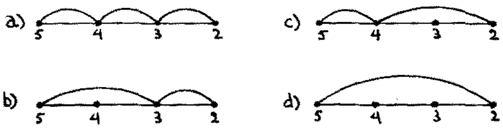

FIG 1. The operator L^5_2 when $m = 3$.

The diagram (a) in Fig. 1 does not contain any free dots and the contribution from the curves is equal to $E^5_4 E^4_3 E^3_2$. Dot 4 in diagram (b) is free and it gives a factor $H_5 - H_4 - 2$. The total contribution to L^5_2 from (b) is then $(H_5 - H_4 - 2) E^5_3 E^3_2$. After calculating in a similar way (c) and (d) one gets

$$\begin{aligned} L^5_2 = {} & E^5_4 E^4_3 E^3_2 + (H_5 - H_4 - 2) E^5_3 E^3_2 \\ & + (H_2 - H_3 + 1) E^5_4 E^4_2 \\ & + (H_5 - H_4 - 2)(H_2 - H_3 + 1) E^5_2 . \end{aligned}$$

We finally list all the lowering operators needed in the reduction $U(4) \downarrow U(2) \times U(2)$ (the simplest case possessing nontrivial multiplicity).

$$\begin{aligned} L^3_2 &= E^3_2, \\ L^3_1 &= E^3_2 E^2_1 + (H_1 - H_2 + 1) E^3_1, \\ L^4_2 &= E^4_3 E^3_2 + (H_4 - H_3 - 2) E^4_2, \\ L^4_1 &= E^4_3 E^3_2 E^2_1 + (H_1 - H_2 + 1) E^4_3 E^3_1 \\ & \quad + (H_4 - H_3 - 2) E^4_2 E^2_1 \\ & \quad + (H_4 - H_3 - 2)(H_1 - H_2 + 1) E^4_1 . \end{aligned}$$

The general semimaximal basis vector for $U(4)$ can be written as

$$\begin{bmatrix} \lambda_2 \; \lambda_3 \; \lambda_4 \\ \lambda_1 \; k^1_1 \; k^1_2 \\ l_1 \; l_2 \end{bmatrix} = (L^4_1)^{l_2 - k^1_2} (L^3_1)^{l_1 - k^1_1} \times (L^4_2)^{k^1_2 - \lambda_4} (L^3_2)^{k^1_1 - \lambda_3} |n\rangle .$$

ACKNOWLEDGMENTS

The author wishes to thank Dr. J. Nagel and Dr. U. Ottoson for many helpful discussions and Professor N. Svartholm for his hospitality at the Institute of Theoretical Physics, Göteborg.

APPENDIX: THE COMMUTATOR $[L^i_j, L^{i'}_j]$

We will prove here that

$$[L^i_j, L^{i'}_j] |s.m.\rangle = 0, \quad j = 1, 2, \ldots m, \quad i, i' = m+1, m+2, \ldots, m+n, \tag{A1}$$

where $|s.m.\rangle$ is any semimaximal state. Because of Eqs. (2.7) and (2.7′) the only matrix elements which could be different from zero are of the type

$$\langle s.m. | [L^i_j, L^{i'}_j] | s.m.\rangle' , \tag{A2}$$

where

$$\begin{aligned} H_v |s.m.\rangle &= h_v |s.m.\rangle, \\ H_v |s.m.\rangle' &= (h_v + 2\delta_{vj} - \delta_{vi} - \delta_{vi'}) |s.m.\rangle'. \end{aligned} \tag{A3}$$

We can assume that $i' < i$. Let us first calculate $\langle s.m. | L^i_j L^{i'}_j | s.m.\rangle'$. Using the explicit formula (3.1) and the fact that the lowering generators of $U(n) \times U(m)$ give zero when acting to the left, we get

$$\begin{aligned} \langle s.m. | L^i_j L^{i'}_j | s.m.\rangle' & = \prod_{\mu = m+1}^{i-1} (h_i - h_\mu + \mu - i - 1) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 1) \\ & \times \langle s.m. | E^i_j L^{i'}_j | s.m.\rangle' . \end{aligned} \tag{A4}$$

Using (3.1) once more and the fact that E^i_j commutes with the generators contained in $L^{i'}_j$, except with the elements from the Cartan subalgebra, we arrive at

$$\begin{aligned} \langle s.m. | L^i_j L^{i'}_j | s.m.\rangle' = & \prod_{\mu = m+1}^{i-1} (h_i - h_\mu + \mu - i - 1) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 1) \\ & \times \prod_{\mu = m+1}^{i'-1} (h_{i'} - h_\mu + \mu - i' - 1) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 2) \\ & \times \langle s.m. | E^i_j E^{i'}_j | s.m.\rangle' . \end{aligned} \tag{A4′}$$

For the term $\langle s.m. | L^{i'}_j L^i_j | s.m.\rangle'$ we get

$$\begin{aligned} \langle s.m. | L^{i'}_j L^i_j | s.m.\rangle' & = \prod_{\mu = m+1}^{i'-1} (h_{i'} - h_\mu + \mu - i' - 1) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 1) \\ & \times \langle s.m. | E^{i'}_j L^i_j | s.m.\rangle' . \end{aligned} \tag{A5}$$

After replacing the H_k in L^i_j by the corresponding eigenvalues according to (A3), the lowering generators of $U(n) \times U(m)$ can be commuted to the left giving zero in the matrix element $\langle s.m. | E^{i'}_j L^i_j | s.m.\rangle'$ and we eventually get

$$\begin{aligned} \langle s.m. | E^{i'}_j L^i_j | s.m.\rangle' & = \prod_{\mu = m+1}^{i-1} (h_i - h_\mu + \mu - i - 1 + \delta_{\mu i'}) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 2) \\ & \times \langle s.m. | E^{i'}_j E^i_j | s.m.\rangle' \\ & - \prod_{\mu = m+1, \, \mu \neq i'}^{i-1} (h_i - h_\mu + \mu - i - 1 + \delta_{\mu i'}) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 2) \\ & \times \langle s.m. | E^{i'}_j E^i_j | s.m.\rangle' \\ & = \prod_{\mu = m+1}^{i-1} (h_i - h_\mu + \mu - i - 1) \\ & \times \prod_{v=j+1}^{m} (h_j - h_v + v - j + 2) \\ & \times \langle s.m. | E^{i'}_j E^i_j | s.m.\rangle' . \end{aligned} \tag{A6}$$

The matrix element of $[E^{i'}_j, E^i_i, E^{i'}_j]$ between the states $|s.m.\rangle$ and $|s.m.\rangle'$ is nonzero, therefore the second term in (A6). Comparing now (A4′) with (A5) and (A6) one notices that

$$\langle s.m.|L_j^i L_j^{i'}|s.m.\rangle' = \langle s.m.|L_j^{i'} L_j^{i'}|s.m.\rangle',$$

and so (A1) is fulfilled.

* Work supported by NORDITA, Copenhagen.
† On leave of absence from the Research Institute for Theoretical Physics, Helsinki, Finland.

1 J. G. Nagel and M. Moshinsky, J. Math. Phys. 6, 682 (1965).
2 J. Mickelsson, J. Math. Phys. 11, 2803 (1970).
3 V. Syamala Devi and T. Venkatarayudu, J. Math. Phys. 9, 1057 (1968); 11, 169 (1970)
4 M. Moshinsky, J. Math. Phys. 4, 1128 (1963).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Coordinates and Democracy in the N-Body Problem*

Harold W. Galbraith†
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104
(Received 26 February 1971)

It is shown that the construction of "democratic" subgroups of O_{3N-3} in the N-body problem is greatly facilitated by the "proper" choice of relative vectors in the center of mass frame. The word "proper" is taken to mean that the set of $(N-1)$ relative vectors forms a basis for reduced representations of the corresponding democracy subgroup of S_N. The imposition of this requirement easily leads us to the reduction chains $O_6 \supset SU_3 \supset SO_3^{\text{rot}}$ and $O_9 \supset SO_3^1 \times SO_3^2 \times SO_3^3 \supset SO_3^{\text{rot}}$ in the three- and four-body problems, respectively, and to $O_{3N-3} \supset SO_{N-1} \times SO_3^{\text{rot}}$ in the $N > 4$ case.

1. INTRODUCTION

The democracy concept was first introduced by Dragt[1] in his work on the three-body problem so that in solving the problem, he would obtain a set of basis states which treats all of the particles on an equal footing. Mathematically, the idea takes the form of a condition to be satisfied by certain so-called "democratic" subalgebras of the SO_6 Lie algebra. In this way, Dragt obtained the chain of subgroups[2] $O_6 \supset SU_3 \supset SO_3^{\text{rot}}$. (We use the superscript notation "rot" to distinguish the physical rotation group from other SO_3's.) The idea was later extended by Lévy-Leblond[3] who has shown that in the four-body problem, the chain giving the most highly symmetric basis functions is $O_9 \supset SO_3^1 \times SO_3^2 \times SO_3^3 \supset SO_3^{\text{rot}}$, while for $N > 4$, one has the $O_{3N-3} \supset SO_{N-1} \times SO_3^{\text{rot}} \supset SO_3^{\text{rot}}$ structure. In both of these works, primary emphasis is given to the structure of the democratic Lie algebras involved, while the role of the particular realization of the generators of these algebras in terms of the laboratory position vectors remains unclear.

The purpose of this paper is to show that the explicit choice of relative vectors should be dictated by the specific kind of "democracy" which is being considered, and is not a question to be answered by ansatz. Indeed, we show that reltative vectors carrying reduced representations of an invariant subgroup $G_N \subset S_N$ (i.e., G_N is the democracy subgroup of the permutation group S_N) are the "natural" variables for G_N democracy.

2. RELATIVE COORDINATES AND DEMOCRACY

Let the vectors $\{\mathbf{r}^\alpha : \alpha = 1, 2, \ldots, N\}$ designate the laboratory position vectors of a system of N identical particles. Taken together, the vectors constitute a basis for a real representation of the permutation group of particle indices, S_N. This representation is known[3] to be reducible into the irreducible components $\{N\} \oplus \{N\text{-}1, 1\}$ by an orthogonal transformation to the center-of-mass frame

$$\mathbf{q}^\alpha = \sum_{\beta=1}^{N} a_{\alpha\beta}\mathbf{r}^\beta, \qquad \alpha = 1, 2, \ldots, N, \tag{1}$$

where the $\{a_{\alpha\beta}\}$ are elements of an orthogonal matrix A, with

$$a_{N\beta} = N^{-1/2}, \qquad \beta = 1, 2, \ldots, N. \tag{2}$$

Equation (2) guarantees that the center-of-mass position vector is properly decoupled. The remaining $(N\text{-}1)$ independent relative vectors $\{\mathbf{q}^\alpha : \alpha = 1, 2, \ldots, N\text{-}1\}$ are a basis for the $\{N\text{-}1, 1\}$ representation of S_N. The skew symmetric Hermitian operators

$$\Lambda_{jk}^{\alpha\beta} = -i\left(q_j^\alpha \frac{\partial}{\partial q_k^\beta} - q_k^\beta \frac{\partial}{\partial q_j^\alpha}\right),$$
$$\alpha, \beta = 1, 2, \ldots, N-1, \qquad j, k = 1, 2, 3 \tag{3}$$

form a realization of the SO_{3N-3} generator algebra. (Latin indices denote the usual 3-space components of the relative vectors.)

The problem of constructing a complete set of commuting observables for the free N-body problem is equivalent to that of the construction of an appropriate chain of nested democratic subgroups of O_{3N-3}, with corresponding Casimir operators. Let $G_N = \{g_\tau : \tau = 1, 2, \ldots, h\}$ be an invariant subgroup of $S_N = \{s_\rho : \rho = 1, 2, \ldots, N!\}$. Then the set of infinitesimal operators $\{\mathcal{C}_{ij}^{(\rho)}\}$ are generators of a "G_N-democratic" subgroup of O_{3N-3}, states $|s.m.\rangle$ and $|s.m.\rangle'$ is nonzero, therefore the second term in (A6). Comparing now (A4′) with (A5) and (A6) one notices that

$$\langle s.m.|L_j^i L_j^{i'}|s.m.\rangle' = \langle s.m.|L_j^{i'} L_j^{i'}|s.m.\rangle',$$

and so (A1) is fulfilled.

* Work supported by NORDITA, Copenhagen.
† On leave of absence from the Research Institute for Theoretical Physics, Helsinki, Finland.

1 J. G. Nagel and M. Moshinsky, J. Math. Phys. 6, 682 (1965).
2 J. Mickelsson, J. Math. Phys. 11, 2803 (1970).
3 V. Syamala Devi and T. Venkatarayudu, J. Math. Phys. 9, 1057 (1968); 11, 169 (1970)
4 M. Moshinsky, J. Math. Phys. 4, 1128 (1963).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Coordinates and Democracy in the N-Body Problem*

Harold W. Galbraith†
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104
(Received 26 February 1971)

It is shown that the construction of "democratic" subgroups of O_{3N-3} in the N-body problem is greatly facilitated by the "proper" choice of relative vectors in the center of mass frame. The word "proper" is taken to mean that the set of $(N-1)$ relative vectors forms a basis for reduced representations of the corresponding democracy subgroup of S_N. The imposition of this requirement easily leads us to the reduction chains $O_6 \supset SU_3 \supset SO_3^{\text{rot}}$ and $O_9 \supset SO_3^1 \times SO_3^2 \times SO_3^3 \supset SO_3^{\text{rot}}$ in the three- and four-body problems, respectively, and to $O_{3N-3} \supset SO_{N-1} \times SO_3^{\text{rot}}$ in the $N > 4$ case.

1. INTRODUCTION

The democracy concept was first introduced by Dragt[1] in his work on the three-body problem so that in solving the problem, he would obtain a set of basis states which treats all of the particles on an equal footing. Mathematically, the idea takes the form of a condition to be satisfied by certain so-called "democratic" subalgebras of the SO_6 Lie algebra. In this way, Dragt obtained the chain of subgroups[2] $O_6 \supset SU_3 \supset SO_3^{\text{rot}}$. (We use the superscript notation "rot" to distinguish the physical rotation group from other SO_3's.) The idea was later extended by Lévy-Leblond[3] who has shown that in the four-body problem, the chain giving the most highly symmetric basis functions is $O_9 \supset SO_3^1 \times SO_3^2 \times SO_3^3 \supset SO_3^{\text{rot}}$, while for $N > 4$, one has the $O_{3N-3} \supset SO_{N-1} \times SO_3^{\text{rot}} \supset SO_3^{\text{rot}}$ structure. In both of these works, primary emphasis is given to the structure of the democratic Lie algebras involved, while the role of the particular realization of the generators of these algebras in terms of the laboratory position vectors remains unclear.

The purpose of this paper is to show that the explicit choice of relative vectors should be dictated by the specific kind of "democracy" which is being considered, and is not a question to be answered by ansatz. Indeed, we show that reltative vectors carrying reduced representations of an invariant subgroup $G_N \subset S_N$ (i.e., G_N is the democracy subgroup of the permutation group S_N) are the "natural" variables for G_N democracy.

2. RELATIVE COORDINATES AND DEMOCRACY

Let the vectors $\{\mathbf{r}^\alpha : \alpha = 1, 2, \ldots, N\}$ designate the laboratory position vectors of a system of N identical particles. Taken together, the vectors constitute a basis for a real representation of the permutation group of particle indices, S_N. This representation is known[3] to be reducible into the irreducible components $\{N\} \oplus \{N\text{-}1, 1\}$ by an orthogonal transformation to the center-of-mass frame

$$\mathbf{q}^\alpha = \sum_{\beta=1}^{N} a_{\alpha\beta}\mathbf{r}^\beta, \quad \alpha = 1, 2, \ldots, N, \tag{1}$$

where the $\{a_{\alpha\beta}\}$ are elements of an orthogonal matrix A, with

$$a_{N\beta} = N^{-1/2}, \quad \beta = 1, 2, \ldots, N. \tag{2}$$

Equation (2) guarantees that the center-of-mass position vector is properly decoupled. The remaining $(N\text{-}1)$ independent relative vectors $\{\mathbf{q}^\alpha : \alpha = 1, 2, \ldots, N\text{-}1\}$ are a basis for the $\{N\text{-}1, 1\}$ representation of S_N. The skew symmetric Hermitian operators

$$\Lambda_{jk}^{\alpha\beta} = -i\left(q_j^\alpha \frac{\partial}{\partial q_k^\beta} - q_k^\beta \frac{\partial}{\partial q_j^\alpha}\right),$$
$$\alpha, \beta = 1, 2, \ldots, N-1, \quad j, k = 1, 2, 3 \tag{3}$$

form a realization of the SO_{3N-3} generator algebra. (Latin indices denote the usual 3-space components of the relative vectors.)

The problem of constructing a complete set of commuting observables for the free N-body problem is equivalent to that of the construction of an appropriate chain of nested democratic subgroups of O_{3N-3}, with corresponding Casimir operators. Let $G_N = \{g_\tau : \tau = 1, 2, \ldots, h\}$ be an invariant subgroup of $S_N = \{s_\rho : \rho = 1, 2, \ldots, N!\}$. Then the set of infinitesimal operators $\{\mathcal{C}_{ij}^{(\rho)}\}$ are generators of a "G_N-democratic" subgroup of O_{3N-3}, denoted $\sum_{G_N}$, provided that the following four equations hold:

$$s_\rho \mathcal{C}_{ij}^{(\sigma)} s_\rho^{-1} \in \{\mathcal{C}_{ij}^{(\sigma)}\}, \quad \rho = 1, 2, \ldots, N!, \tag{4}$$

$$g_\tau \mathcal{C}_{ij}^{(\sigma)} g_\tau^{-1} = \mathcal{C}_{ij}^{(\sigma)}, \quad \tau = 1, 2, \ldots, h, \tag{5}$$

$$\mathcal{C}_{ij}^{(\sigma)} = \sum_{\alpha,\beta} \lambda_{\beta\alpha}^{(\sigma)} \Lambda_{ij}^{\alpha\beta}, \tag{6}$$

$$[\mathcal{C}_{ij}^{(\sigma)}, \mathcal{C}_{i'j'}^{(\sigma')}] = \sum_{\sigma'' i'' j''} \eta_{ij i'j', i''j''}^{\sigma\sigma'\sigma''} \mathcal{C}_{i''j''}^{(\sigma'')}. \tag{7}$$

Equation (4) states that the new generator algebra must be an invariant subspace with respect to S_N; Eq. (5) requires that each element of the G_N-democratic algebra must itself be a basis for the identity representation of G_N; Eq. (6) is the subgroup condition specifying the imbedding of the new algebra in the parent SO_{3N-3} Lie algebra. The coefficients $\eta\vdots\vdots$ are the structure constants of the subgroup $\sum_{G_N}$. The utility of democracy stems from Eq. (5). The observables of the N-particle kinematic states will be Casimir operators formed from the $\mathcal{C}_{ij}^{(\sigma)}$. Obviously then, Eq. (5) guarantees that each such Casimir operator will commute with the entire group G_N, implying that basis functions diagonalizing such observables will be highly symmetric.

We must now consider a fixed $G_N \subset S_N$ and determine: the appropriate c.m. transformation matrix $A(G_N)$, the matrix $\lambda(G_N)$ giving the embedding in SO_{3N-3}, and the structure constants $\eta\vdots\vdots$ of the $\sum_{G_N}$ group. Clearly the best choice of relative vectors $\{\mathbf{q}^\alpha\}$ will render the matrix λ simplest.

Let $\Gamma_\tau^{\{N-1,1\}}$ be the $(N-1) \times (N-1)$ orthogonal matrix representative of operator $g_\tau \in G_N$ in the $\{N-1, 1\}$ IR of S_N carried by a set of relative vectors $\{\mathbf{q}^\alpha: \alpha = 1, 2, \ldots, N-1\}$. Then Eqs. (5) and (6) and definition (3) give the matrix relation

$$\Gamma_\tau^{\{N-1,1\}} \lambda = \lambda\, \Gamma_\tau^{\{N-1,1\}}, \tau = 1, 2, \ldots, h, \tag{8}$$

as a necessary condition for G_N democracy. It now follows directly from Schur's Lemma that whenever the representation $(g_\tau \to \Gamma_\tau^{\{N-1,1\}})$ of G_N is in reduced form, the matrix λ will be diagonal. Hence we arrive at the definition: *"Proper" N-body relative coordinates for G_N democracy are those carrying reduced representations of G_N.*

It is now obvious that for S_N, which is irreducible on the $\{\mathbf{q}^\alpha: \alpha = 1, 2, \ldots, N-1\}$, one has

$$\mathcal{C}_{ij} = \sum_{\alpha=1}^{N-1} \Lambda_{ij}^{\alpha\alpha}, i < j = 1, 2, 3, \tag{9}$$

which are the generators of SO_3^{rot}. For $N > 3$ it is also the case that A_N, the alternating group, is irreducible[4] and therefore

$$\sum_{S_N} = \sum_{A_N} = SO_3^{\mathrm{rot}}. \tag{10}$$

Hence S_N democracy in general, and A_N democracy for $N > 3$, supply no conditions restricting the matrix A and give only $\sum = SO_3^{\mathrm{rot}}$.

The representation $(g_\tau \to \Gamma_\tau^{\{N-1,1\}})$ of G_N may be reducible (and reduced) in the $\{\mathbf{q}^\alpha\}$ basis. In this case, λ will have the form

$$\lambda = \begin{bmatrix} \lambda^{(i)} I_1 & & 0 \\ & \ddots & \\ 0 & & \lambda^{(j)} I_j \end{bmatrix}, \tag{11}$$

where the matrices I_k are unit matrices of dimension equal to the dimension of the corresponding G_N IR, and the $\lambda^{(\sigma)}$ are numbers determined by the remaining democracy conditions (4) and (7). We now see that the sum on α and β of Eq. (6) is to be taken only over the indices appearing in the σth submatrix of Eq. (11). The number of irreducible components of G_N carried by the relative vectors is just the number of independent operators $\{\mathcal{C}_{i'j'}^{(\sigma)}: \sigma = 1, 2, \ldots, j\}$ of like lower indices i' and j'. Hence we have the result that if j is the number of IRs of G_N in the representation$(g_\tau \to \Gamma_\tau^{\{N-1,1\}})$, then $9j$ is the maximum number of operators forming the $\sum_{G_N}$ generator algebra.

It can happen that the orthogonal transformation A cannot reduce both S_N and G_N. This is the case when an IR of G_N contained in the representation $(g_\tau \to \Gamma_\tau^{\{N-1,1\}})$ consists of complex representation matrices. The representation may however always be reduced in terms of a basis of complex vectors $\{\mathbf{z}^\alpha: \alpha = 1, 2, \ldots, N-1\}$, defined by the matrix equation

$$\begin{bmatrix} \mathbf{z}^1 \\ \mathbf{z}^2 \\ \vdots \\ \mathbf{z}^{N-1} \end{bmatrix}_{(N-1)\times 1} = U \begin{bmatrix} \mathbf{q}^1 \\ \mathbf{q}^2 \\ \vdots \\ \mathbf{q}^{N-1} \end{bmatrix}_{(N-1)\times 1}, \tag{12}$$

where U is the $(N-1) \times (N-1)$ unitary matrix reducing the matrices $\Gamma_\tau^{\{N-1,1\}}$

$$U \Gamma_\tau^{\{N-1,1\}} U^{-1} = \begin{bmatrix} \Gamma_\tau^{(1)} & & 0 \\ & \ddots & \\ 0 & & \Gamma_\tau^{(j)} \end{bmatrix}, \quad \tau = 1, 2, \ldots, h. \tag{13}$$

It now follows that in the $\{\mathbf{z}^\alpha\}$ system

$$\lambda' = U \lambda U^{-1} = \begin{bmatrix} \lambda^{(1)\prime} I_1 & & 0 \\ & \ddots & \\ 0 & & \lambda^{(j)\prime} I_j \end{bmatrix}. \tag{14}$$

Hence, it is always possible to introduce coordinates (real or complex) appropriate for G_N democracy.

3. THE CASES OF 3, 4 AND N > 4 PARTICLES

A. Three-Body Problem

S_3 has the sequence of invariant subgroups $S_3 \supset A_3 \supset$ I. Any of the six elements of S_3 may be written as products of the permutations

$$(12) = \begin{pmatrix} 123 \\ 132 \end{pmatrix}, \quad (123) = \begin{pmatrix} 123 \\ 231 \end{pmatrix}.$$

The permutation (123) is even and generates the cyclic group of order 3, A_3:

$$A_3 = \{(123), (123)^2, (123)^3 = 1\}.$$

It is one of our results that $\sum_{S_3} = SO_3^{\rm rot}$, so we turn immediately to A_3. The irreducible representations of A_3 are all one dimensional and are realized as third roots of unity. The A_3-democratic substructure of O_6 is therefore best revealed in terms of a set of coordinates $\{\mathbf{q}^1, \mathbf{q}^2\}$ obeying

$$(123)\mathbf{q}^\alpha = e^{2\pi n i/3}\ \mathbf{q}^\alpha,\ \alpha = 1, 2. \tag{15}$$

It follows that $n = 0$ gives $\mathbf{q}^\alpha\ \alpha\ \mathbf{R}_{cm}$, implying that the $\{\mathbf{q}^\alpha\}$ are necessarily complex. It is also not hard to see that we must search for only one complex 3-vector $\mathbf{z}$ such that

$$(123)\mathbf{z} = e^{2\pi i/3}\mathbf{z}, \tag{16}$$

then for the other independent vector we have $\mathbf{z}^*$, satisfying

$$(123)\mathbf{z}^* = e^{-2\pi i/3}\mathbf{z}^*. \tag{17}$$

The set $\{\mathbf{z}, \mathbf{z}^*, \mathbf{R}_{cm}\}$ are related to the lab vectors by

$$\begin{bmatrix} \mathbf{z} \\ \mathbf{z}^* \\ \frac{3}{\sqrt{3}}\mathbf{R}_{cm} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} ie^{-i\theta} & -e^{-i\theta} & 0 \\ -ie^{i\theta} & -e^{i\theta} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\cos\alpha}{\sqrt{6}} + \frac{\sin\alpha}{\sqrt{2}} & \frac{\cos\alpha}{\sqrt{6}} - \frac{\sin\alpha}{\sqrt{2}} & -\left(\frac{2}{3}\right)^{1/2}\cos\alpha \\ \frac{\sin\alpha}{\sqrt{6}} - \frac{\cos\alpha}{\sqrt{2}} & \frac{\sin\alpha}{\sqrt{6}} + \frac{\cos\alpha}{\sqrt{2}} & -\left(\frac{2}{3}\right)^{1/2}\sin\alpha \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix} \begin{bmatrix} \mathbf{r}' \\ \mathbf{r}^2 \\ \mathbf{r}^3 \end{bmatrix}, \tag{18}$$

where we have made explicit use of the fact that the last row of A determines two of the three parameters of a 3×3 orthogonal matrix. The remaining degree of freedom is expressed as an angle α. The unitary matrix of Eq. (18)

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} ie^{-i\theta} & -e^{-i\theta} \\ -ie^{i\theta} & -e^{i\theta} \end{bmatrix} \tag{19}$$

is the most general, such transformation giving $\mathbf{z}^*$ as the second independent complex vector.

Combining Eq. (18) with the condition of A_3 irreducibility, we have from Eq. (16),

$$\alpha = \tfrac{1}{2}\pi, \qquad \theta = \text{arbitrary}. \tag{20}$$

This value for α is just the one required to make A coincide with the transformation to the so-called "Jacobi" coordinate system. The factor $e^{-i\theta}$ appears as an over-all phase for $\mathbf{z}$ having no physical significance. Jacobi coordinates are given by

$$\mathbf{q}^1 = \frac{1}{\sqrt{2}}(\mathbf{r}^1 - \mathbf{r}^2), \tag{21}$$

$$\mathbf{q}^2 = \left(\tfrac{2}{3}\right)^{1/2}[\tfrac{1}{2}\mathbf{r}^1 + \tfrac{1}{2}\mathbf{r}^2 - \mathbf{r}^3]. \tag{22}$$

By setting $\theta = \frac{1}{2}\pi$, we get

$$\mathbf{z} = \frac{1}{\sqrt{2}}(\mathbf{q}^1 + i\mathbf{q}^2) \tag{23}$$

and

$$\mathbf{z}^* = \frac{1}{\sqrt{2}}(\mathbf{q}^1 - i\mathbf{q}^2). \tag{24}$$

The free three-particle Hamiltonian is proportional to the 6-Laplacian

$$\Delta_6 = \nabla_{\mathbf{z}} \cdot \nabla_{\mathbf{z}^*}. \tag{25}$$

Obviously the full symmetry group of this operator is U_3. The coordinates of Eqs. (23) and (24) were first used by Simonov[5] and give SU_3 representations automatically.

We now demonstrate explicitly how the infinitesimal generators of the Dragt-U_3 may be obtained. Equation (6), which is the defining relation of λ, is, in matrix form,

$$\mathcal{C}_{ij}^{(\sigma)} = \text{trace}\ (\lambda^{(\sigma)} \cdot \Lambda_{ij}), \tag{26}$$

where Eq. (26) is expressed in the coordinate system of the $\mathbf{q}^\alpha$. However, the trace is invariant under similarity transformations, and we have correspondingly in the $\mathbf{z}^\alpha$ system

$$\mathcal{C}_{ij}^{(\sigma)} = \text{tr}(\lambda^{(\sigma)\prime} \cdot \Lambda'_{ij}), \tag{27}$$

where in Eq. (27) λ' is diagonal and $[\Lambda'_{ij}]$ satisfies the relation

$$\Lambda'_{ij} = U\Lambda_{ij}U^{-1}. \tag{28}$$

We first construct $\mathcal{C}_{ij}^{(\sigma)}$ in terms of the $\Lambda_{ij}^{\alpha\beta}$ to recover the Dragt-U_3 explicitly, and then use Eq. (27) to express $\mathcal{C}_{ij}^{(\sigma)}$ in terms of the $\mathbf{z}$ of Eq. (23).

Using Eq. (14) with the U of Eq. (19), we have

$$\lambda = \tfrac{1}{2} \begin{bmatrix} (\lambda^{(1)} + \lambda^{(2)}) & i(\lambda^{(1)} - \lambda^{(2)}) \\ -i(\lambda^{(1)} - \lambda^{(2)}) & \lambda^{(1)} + \lambda^{(2)} \end{bmatrix}, \tag{29}$$

where we have set

$$\lambda' = \begin{bmatrix} \lambda^{(1)} & 0 \\ 0 & \lambda^{(2)} \end{bmatrix}. \tag{30}$$

Equation (26) then gives

$$\mathcal{C}_{ij} = \tfrac{1}{2}\,[\lambda^{(1)} + \lambda^{(2)})(\Lambda_{ij}^{11} + \Lambda_{ij}^{22}) - i(\lambda^{(1)} - \lambda^{(2)})(\Lambda_{ij}^{12} - \Lambda_{ij}^{21})]. \tag{31}$$

Defining the operators

$$\mathcal{L}_{ij} \equiv \Lambda_{ij}^{11} + \Lambda_{ij}^{22}, \quad i < j = 1, 2, 3 \tag{32}$$

$$N_{ij} \equiv \Lambda_{ij}^{12} - \Lambda_{ij}^{21}, \quad i, j = 1, 2, 3 \tag{33}$$

we get

$$[\mathcal{L}_{ij},\ \mathcal{L}_{i'j'}] = i(\delta_{ii'}\mathcal{L}_{jj'} + \delta_{jj'}\mathcal{L}_{ii'} - \delta_{ji'}\mathcal{L}_{ij'} - \delta_{ij'}\mathcal{L}_{i'j}), \tag{34}$$

$$[\mathcal{L}_{ij},\ N_{i'j'}] = i(\delta_{ii'}N_{jj'} - \delta_{ji'}N_{ij'} - \delta_{jj'}N_{ii'} + \delta_{ij'}N_{ji'}), \tag{35}$$

$$[N_{ij},\ N_{i'j'}] = i(\delta_{ii'}\mathcal{L}_{jj'} + \delta_{jj'}\mathcal{L}_{ii'} + \delta_{ij'}\mathcal{L}_{ji'} + \delta_{ji'}\mathcal{L}_{ij'}), \tag{36}$$

for all indices i, j of Eqs.(32) and (33). Of course the $\mathcal{L}_{ij}$ are the generators for the rotation group $SO_3^{\rm rot}$. The algebraic requirement Eq. (7) gives

$$\lambda^{(1)} = i, \ \lambda^{(2)} = 0, \tag{37}$$

and

$$\mathcal{C}_{ij} = \tfrac{1}{2}[i\mathcal{L}_{ij} + N_{ij}], \quad i, j = 1, 2, 3, \tag{38}$$

the Dragt result.

To obtain the generators in terms of **z** we use Eqs.(27),(30), and (19) along with the requirement (28). One easily finds

$$\mathcal{C}_{ij} = z_i \frac{\partial}{\partial z_j} - z_j^* \frac{\partial}{\partial z_i^*} \tag{39}$$

as the Weyl generators of U_3.

B. Four-Body Problem

Here we are dealing with the chain of invariant subgroups $S_4 \supset A_4 \supset V_4 \supset$ I. As previously noted, $\sum_{S_4} = \sum_{A_4} = SO_3^{\rm rot}$. The first possibility in the four-body case is then V_4. It is an Abelian subgroup of A_4 generated by the operations

$$(12)\,(34) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{pmatrix},$$

$$(13)\,(24) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 1 & 2 \end{pmatrix}.$$

We also have

$$[(12)\,(34)]^2 = [(13)\,(24)]^2 = 1.$$

Therefore the representation of A_3 carried by the $\{\mathbf{q}^1, \mathbf{q}^2, \mathbf{q}^3\}$ will be reduced provided that

$$(12)\,(34)\,\mathbf{q}^\alpha = \pm\,\mathbf{q}^\alpha \tag{40}$$

and

$$(13)\,(24)\,\mathbf{q}^\alpha = \pm\,\mathbf{q}^\alpha, \quad \alpha = 1, 2, 3, \tag{41}$$

are satisfied. It is easy to see that the two plus signs for any single $\mathbf{q}^\alpha$ give just $\mathbf{R}_{cm}$. Hence, we consider here the 3 IR's of V_4, corresponding to the choices (±), (∓), (=) in Eqs. (40) and (41). Furthermore any given choice fixes all but one element in row α of the A matrix, the remaining element being determined by the orthogonality of that matrix. Therefore independence of the $\{\mathbf{q}^\alpha\}$ requires that each vector transform according to a different IR. We choose

$$\mathbf{q}^1 \to (\pm), \tag{c1}$$

$$\mathbf{q}^2 \to (\mp), \tag{c2}$$

$$\mathbf{q}^3 \to (=), \tag{c3}$$

and easily get

$$\mathbf{q}^1 = \pm\tfrac{1}{2}[(\mathbf{r}^1 + \mathbf{r}^2) - (\mathbf{r}^3 + \mathbf{r}^4)], \tag{42}$$

$$\mathbf{q}^2 = \pm\tfrac{1}{2}[(\mathbf{r}^1 + \mathbf{r}^3) - (\mathbf{r}^2 + \mathbf{r}^4)], \tag{43}$$

$$\mathbf{q}^3 = \pm\tfrac{1}{2}[(\mathbf{r}^1 + \mathbf{r}^4) - (\mathbf{r}^2 + \mathbf{r}^3)]. \tag{44}$$

All other choices of (c1), (c2), and (c3) give permutations among Eqs. (42), (43), and (44). Now the λ-matrix of Eq. (11) has the form

$$\lambda = \begin{bmatrix} \lambda^{(1)} & 0 & 0 \\ 0 & \lambda^{(2)} & 0 \\ 0 & 0 & \lambda^{(3)} \end{bmatrix} \tag{45}$$

and from Eq. (26) we have

$$\mathcal{C}_{ij}^{(\alpha)} = \lambda^{(\alpha)}\,\Lambda_{ij}^{\alpha\alpha}, \quad \alpha = 1, 2, 3, \quad i < j = 1, 2, 3. \tag{46}$$

Equation (4) requires that

$$\lambda^{(1)} = \lambda^{(2)} = \lambda^{(3)} \tag{47}$$

and that the V_4-democratic algebra be the direct sum $\{\mathcal{C}_{ij}^{(1)} \oplus \mathcal{C}_{ij}^{(2)} \oplus \mathcal{C}_{ij}^{(3)}\}$. These operators are the generators of the $SO_3^1 \times SO_3^2 \times SO_3^3$ group of Lévy-Leblond.

C. $(N > 4)$-Body Problem

In this case, where we have only $S_N \supset A_N \supset I$ available, we must consider only democracy with respect to the identity operator for the construction of subgroups missing from $O_{3N-3} \supset \ldots \supset SO_3^{\rm rot}$. This is a serious failure for democracy since Eq.

(5) becomes an empty statement. Combining conditions (4), (6), and (7), we arrive at only the SO_{3N-3} and $SO_3^{\rm rot}$ generator algebras, indicating that the expansion of Eq. (6) should now also involve a restriction on the component indices i and j. We then obtain the I-democratic algebra of generators

$$L^{\alpha\beta} = \sum_{i=1}^{3} \Lambda_{ii}^{\alpha\beta}, \qquad \alpha < \beta = 1, 2, \ldots, N-1. \tag{48}$$

The set $\{L^{\alpha\beta}\}$ generates a group SO_{N-1}. The elements of this group are then proper[2] rotations in a Cartesian space whose axes are labeled by the indices $\{\alpha\}$ of the relative vectors $\{\mathbf{q}^\alpha : \alpha = 1, 2, \ldots, N-1\}$.

Since we have

$$[L^{\alpha\beta}, \mathcal{L}_{ij}] = 0, \tag{49}$$

where $\mathcal{L}_{ij} = \sum_{\alpha=1}^{N-1} \Lambda_{ij}^{\alpha\alpha}$ are generators of $SO_3^{\rm rot}$, it follows that the maximal I-democratic subalgebra of O_{3N-3} is the direct sum $\{L^{\alpha\beta} \oplus \mathcal{L}_{ij}\}$, generating the direct product group $SO_{N-1} \times SO_3^{\rm rot}$. Hence we have for $N > 4$ the chain $O_{3N-3} \supset SO_{N-1} \times SO_3^{\rm rot} \supset SO_3^{\rm rot}$.[6]

4. CONCLUSION

We have given a simple criterion for the construction of "natural" relative vectors for the N-body problem. In terms of such coordinates, the democracy substructure of O_{3N-3} is most clearly revealed.

We find that democracy with respect to the full permutation group S_N requires only that one properly decouple the position vector of the center of mass, and gives the familiar rotation group $SO_3^{\rm rot}$.

In the three-body case, the alternating group A_3 leads us to complex coordinates and the A_3-democratic SU_3 of Dragt.

In the case of 4-particles, we are led to the so-called "symmetric" coordinates by the democracy group V_4. The corresponding subgroup of O_{3N-3} being the familiar $SO_3^1 \times SO_3^2 \times SO_3^3$ of Lévy-Leblond.

Unfortunately for $N > 3$, the alternating group A_N gives only $SO_3^{\rm rot}$ and no new restrictions on the relative vectors. This means an essential failure for democracy in the $N > 4$ -body problem and we obtain only the I-democratic group structure $O_{3N-3} \supset SO_{N-1} \times SO_3^{\rm rot}$.

ACKNOWLEDGMENT

I would like to thank Professor R. D. Amado of the University of Pennsylvania for his advice and encouragement during the course of this research.

---

* This work supported in part by the National Science Foundation.

† National Science Foundation Predoctoral Fellow.

1 A. J. Dragt, J. Math. Phys. 6, 533 (1965).

2 We are noting the distinction between the Lie algebra of an orthogonal group and the group itself. The Lie algebra generates only proper rotations, i.e., SO_n in general. The permutation group S_N is, however, realized in terms of orthogonal matrices having determinants equal to both ±1. Hence, S_N is a subgroup of O_{3N-3} but not of SO_{3N-3}. As far as representations of SO_{3N-3} in the N-body problem are concerned, the distinction is superfluous since those representations are realized on the $(3N-4)$-sphere. However, in the chain $O_{3N-3} \supset SO_{N-1} \times SO_3^{\rm rot}$, where the SO_{N-1} is of a more general nature, operators of S_N (having det-1) will mix inequivalent SO_{N-1} irreducible basis vectors within the same representation space of O_{3N-3}.

3 J. M. Lévy-Leblond, J. Math. Phys. 7, 2217 (1966).

4 F. D. Murnaghan, *Theory of Group Representations* (Johns Hopkins Press, Baltimore, 1938).

5 Yu. A. Simonov, Yad. Fiz. 3, 630 (1966) [Sov. J. Nucl. Phys. 3, 461 (1966)].

6 The development given here for $N > 4$ is identical with that of Lévy-Leblond in Ref. 3.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

The Lorentz Group Symmetry of the Hydrogen Atom and the Coulomb T Matrix

A. K. Rajagopal and C. S. Shastry*
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803
(Received 17 May 1971; Revised Manuscript Received 25 June 1971)

The existence of solutions for the Lippmann–Schwinger (LS) equation for the Coulomb problem is studied by investigating whether its kernel belongs to the Hilbert–Schmidt (HS) class. The kernel for each partial wave is shown to belong to the HS class for complex energies whereas for real energies it becomes unbounded. Unlike the case of short range potentials, e.g., the Yukawa potential, even the suitably symmetrized kernel does not belong to the HS class for real, positive energies. These formal properties strongly indicate that a unique limit for the partial wave off-shell Coulomb T matrix as it approaches the unitarity axis may not exist. It is found that exploiting the $O(4)$ symmetry of the Coulomb Hamiltonian (H) in the subspace of the negative spectrum of H and the $O(3, 1)$ symmetry in the subspace of the positive spectrum of H, one can construct the off-shell Coulomb T matrix in terms of the eigensolutions (Sturmians) of the kernel of the Lippmann–Schwinger equation. These follow from the work of Perelemov and Popov, and Schwinger on the Coulomb Green's function. On the basis of the generating functions for the Sturmians, various integral, contour integral, and discrete sum representations for the complete off-shell Coulomb T matrix are derived. In this way, we explicitly demonstrate that indeed the T matrix has a nonunique limit as one approaches the unitarity axis. It is also shown that when the asymptotic Coulomb distortion is taken into account, the physical Coulomb amplitude can be deduced from this Coulomb T matrix. These results incidentally rectify some errors in the earlier works. Since for both negative and positive energies the Coulomb T matrix is obtained as the explicit solution of the LS equation, the validity of the generalized unitarity—the Low equation—in a certain sense is guaranteed. This is proved in a general way, by showing that a generalized Low equation follows when the energy is complex only from the LS equations and some defining relations; in the Coulomb case, the generalized unitarity relationship for real energies must be interpreted as the limit when the imaginary part becomes zero.

1. INTRODUCTION

A detailed knowledge of the complete off-shell two-body T matrix for each pair of interacting particles is of crucial importance in the Faddeev formulation of the three-particle scattering.[1,2] The two-body T operator obeys the well-known Lippmann–Schwinger (LS) equation. If the kernel K of the LS equation is compact, then the T matrix exists and can be shown to be unique. A kernel is compact if it belongs to the Hilbert–Schmidt (L^2) class (but a compact operator need not belong to HS class). For complex energies it can be shown that K belongs to L^2 class if the interaction H' does.[3,4] Furthermore, an existence theorem specifying the class of spherically symmetric potentials for which the kernel $(K)_l$ of the lth partial wave LS equation is compact when energy is held complex is proved recently by the present authors.[4] It was shown that in the case of Coulomb potential, $(K)_l$ belongs to the L^2 class if the energy is held complex even though $\mathrm{Tr}(K^\dagger K)$ is infinite. However, it was found that for each partial wave, $\mathrm{Tr}(K^\dagger K)_l$ diverges when the energy was made real and positive. This raises some questions about the validity of the full LS equation for the two-particle Coulomb T matrix, and the existence of the off-shell partial wave Coulomb T matrix for *real* positive energies. Such doubts were expressed by West[5] and Gerjuoy[6] based on the familiar problems of asymptotic distortion of the Coulomb solutions.

For negative energies, Schwinger[7] constructed the complete Coulomb Green's function in the momentum space by explicitly solving the LS equation after expressing it in a suitable four-dimensional space (to be explained later). Nutt[8] constructed the corresponding two-particle off-shell Coulomb T matrix and attempted to continue it analytically to positive energies. He tried to verify the off-shell unitarity relation for his T matrix and obtained zero for the discontinuity across the unitarity cut along the positive real axis in the complex energy plane. McDowell and Richards[9] and Nuttal and Stagat[10] have found errors in Nutt's calculations. They found the physically anticipated discontinuity, but with an energy dependent factor. In this paper we will describe the correct analytic continuation for the Coulomb T matrix for positive energies and resolve all the troubles faced hitherto concerning the Coulomb T matrix.

The special nature of the Coulomb problem has two facets to it: the HS nature of the LS kernel and its symmetrized form, on the one hand, and the hidden symmetry of the Coulomb Hamilton, on the other. These two apparently independent features show that the Coulomb potential stands as a unique case by itself.

The hidden symmetry of the Coulomb Hamiltonian was first exemplified by Fock.[11] The Coulomb Hamiltonian, besides being invariant under the three-dimensional spatial rotations, is also invariant under four-dimensional rotation in the Euclidean space in the subspace of negative energies and in the Minkowski space in the subspace of positive energies. Schwinger's[7] derivation uses the $O(4)$ symmetry explicitly. Hostler's work[12] on the Coulomb Green's function in the configuration space also stresses the importance of the hidden symmetry of the Coulomb Hamiltonian. The full dynamical symmetry group of the Coulomb problem is the homogeneous Lorentz group. An excellent exposition of the properties of the representations of the Lorentz groups may be found in a review article by Bander and Itzykson[13] (BI). These have been exploited by Perelomov and Popov[14] (PP) who construct the Green's function for the Coulomb problem, thus extending the work of Schwinger. By combining the works of BI and PP we have derived here the corresponding T matrix. We express the T

matrix in two more forms: one, in terms of the continuous spectrum eigensolutions of the LS kernel and, two, in terms of a one-parameter definite integral in an infinite domain. The latter follows directly from the work of PP. The last mentioned integral can be further evaluated by the method of contour integration and the results of these correspond to the work of Norcliffe *et al.*[15,16] and Roberts,[17,18] who arrived at it from an elegant analysis of the problem using classical path integral technique. Finally, a contour integral representation of the T matrix is obtained by us and this succintly displays the troubles with the analytic continuation procedure of Nutt. From the infinite integral representation, we show that, on evaluating the T matrix on the mass shell, the familiar Coulomb amplitude can be deduced.

Another aspect is the unitarity of the Coulomb T matrix. In two different ways, we demonstrate that the generalized unitarity for complex energies—the celebrated Low equation—is automatically satisfied by any T operator obeying the LS equation. However, in order to obtain the well-known on-shell unitarity relation, a proof for the existence of a unique on-shell limit of the off-shell T matrix when energy is made real positive is needed.[19] We discuss this question here with special reference to the Coulomb problem. Ford[20] analyzed in detail the cutoff Coulomb problem and found that the final result depended critically on the way one considered the mathematical limiting procedure. Faddeev[21] considers the Coulomb potential as a limit of the Yukawa potential, but with a difference, that one should renormalize the wavefunction associated with the Yukawa potential before taking the appropriate limit. It is known that a cutoff always destroys the original analytic properties of the solutions[3] and, for some recent remarks concerning such effects, one may refer to the work of Nelson *et al.*[22] In view of our results in the present paper, such an ambivalent approach to the Coulomb problem is found unnecessary. The real reason is, of course, the symmetry of the problem which is altered when the Coulomb potential is screened or cut off and the interesting aspects of the problem are lost. Moreover, the LS kernel for the cutoff or Yukawa potential belongs to the HS class while in the limit of the Coulomb potential it does not.

The plan of the paper is as follows. In Sec. 2 we investigate if the kernel of the LS equation for the Coulomb problem belongs to the HS class in order to determine the existence and uniqueness of its solutions. In Sec. 3, the symmetry of the Coulomb Hamiltonian is first briefly reviewed, and various expressions for the complete off-shell Coulomb T matrix valid in different regions of the four-dimensional hyperspace are obtained. Section 4 deals with the question of unitarity. The last section summarizes the results. In a separate paper, the implication of these results for the Faddeev approach to three-particle Coulomb problems will be discussed.

2. THE TWO PARTICLE T MATRIX—FORMAL RESULTS

In the time-independent scattering theory, the resolvent operator $G^{\pm}$ is given by

$$G^{\pm} = (E - H \pm i\delta)^{-1} \tag{2.1}$$

and satisfies the Lippmann-Schwinger (LS) equation

$$G^{\pm} = G_0^{\pm} + G_0^{\pm}H'G^{\pm} = G_0^{\pm} + G_0^{\pm}TG_0^{\pm}. \tag{2.2}$$

Here H is the Hamiltonian operator given by the sum of "kinetic energy" operator H_0 and the potential energy operator H'; E is the center of mass energy and

$$G_0^{\pm} = (E - H_0 \pm i\delta)^{-1}. \tag{2.3}$$

The T operator defined by $G_0^{\pm}T = G^{\pm}H'$ obeys the LS equation

$$T = H' + H'G_0^{+}T = H' + H'G^{+}H'. \tag{2.4}$$

For two-body scattering, the transition amplitude is given by

$$T_{\beta\alpha} = \langle\Psi_0(E,\beta)|T|\Psi_0(E,\alpha)\rangle, \tag{2.5}$$

where $\Psi_0(E,\beta)$ and $\Psi_0(E,\alpha)$ are the eigenstates of H_0 obeying the final and initial state scattering boundary conditions.

Now we will briefly discuss the existence of solutions for the LS equation (2.4) by examining if the kernel of the LS equation belongs to the HS class. It should be stressed that this is only a necessary condition for the existence of the solution. The kernel K is given by

$$K = H'G_0^{+} \tag{2.6}$$

and it belongs to the HS class if the trace over the operator product $K^{\dagger}K$ is convergent. For spherically symmetric potentials, we may write

$$\mathrm{Tr}(K^{\dagger}K) = \sum_{l=0}^{\infty}(2l+1)\mathrm{tr}(K^{\dagger}K)_l. \tag{2.7}$$

We have the result[4] for the Coulomb potential $z_1z_2e^2/r$:

$$\mathrm{tr}(K^{\dagger}K)_l = \frac{z_1^2z_2^2e^4m}{(2l+1)|\delta|}\left[1 + \frac{2}{\pi}\tan^{-1}\left(\frac{E}{|\delta|}\right)\right]. \tag{2.8}$$

This evaluation shows that as long as $\delta \neq 0$, however small, $Tr(K^{\dagger}K)_l$ exists even for $E > 0$ but the sum (2.7) diverges. However, in order to prove the uniqueness and existence of the solution of the LS equation, it is sufficient if one shows that some finite power of the kernel, say K^m, belongs to the HS class. This can be studied in detail for Coulomb-like potentials $V_\alpha(r) = g/r^\alpha$ and one finds that the mth iterate of the kernel K

belongs to L^2 class if $\alpha > 1 + 1/(2m)$ and $1 < \alpha < \frac{3}{2}$.

In the analysis described above, we had restricted to $\delta > 0$ whenever E was positive. However, this does not shed light on the existence of solutions for real positive energies with $\delta = 0$, which is the case of physical interest. This point was investigated in general elsewhere by us,[19] and we summarize the results.

Unique solutions exist for the following two integral equations:

$$T(E + i\delta) = H' + H'G_0^{\dagger}T(E + i\delta) \tag{2.9}$$

and

$$\tilde{T}(E + i\delta) = H'^{1/2} + H'^{1/2}[H'^{1/2}G_0^{\dagger}H'^{1/2}]\tilde{T}(E + i\delta) \tag{2.10}$$

with

$$T(E + i\delta) = H'^{1/2}\tilde{T}(E + i\delta), \tag{2.11}$$

if the respective kernels of (2.9), (2.10) belong to the HS class. Furthermore, $\tilde{T}(E + i\delta)$ has a unique limit as $\delta \to 0$ and this provides the analytic continuation for $T(E + i\delta)$ on to the real line with $\delta = 0$. The kernel

$$\tilde{K} = H'^{1/2}G_0^{\dagger}H'^{1/2} \tag{2.12}$$

was studied in detail for spherically symmetric potentials, and it is found that $\operatorname{tr}(\tilde{K}^{\dagger}\tilde{K})_l$ is finite for a certain class of spherically symmetric potentials. It was found that $\tilde{K}^m$ belongs to L^2 for $V_\alpha(r)$ but with $1 < \alpha < 2$, if

$$\alpha > 1 + 1/m. \tag{2.13}$$

Thus the analyses of K and $\tilde{K}$ show that for the Coulomb potential, both K^m and $\tilde{K}^m$ belong to L^2 class only if $m \to \infty$ implying infinite number of iterations. In view of the presence of every power of $(z_1 z_2 e^2)$ in the asymptotic Coulomb distorted state, this result is not surprising. Therefore, the on-shell limit of the Coulomb amplitude has to be defined necessarily with respect to the Coulomb distorted asymptotic states. Interestingly enough, Green and Lanford[23] have established the existence of Møller operators and hence the S matrix for the same class of potentials defined above, showing that the time-independent and time-dependent formations of scattering theory are equivalent only for such a class of potentials.

3. SYMMETRY OF THE COULOMB PROBLEM AND THE CONSTRUCTION OF THE T MATRIX

Fock[11] showed that the Hamiltonian of the hydrogen atom, besides being invariant under the three-dimensional rotation group $O(3)$, also possesses a hidden symmetry of a larger group. For the subspace where $E < 0$, this is the four-dimensional rotation group $O(4)$. For the subspace $E > 0$, it has the symmetry of the homogeneous Lorentz group $O(1,3)$. The "complete" dynamical symmetry group of the hydrogen atom is the homogeneous Lorentz group. The irreducible representation of the symmetry groups of the hydrogen atoms are obtained from the eigensolutions of the corresponding LS kernel, the so-called Sturmian solutions used in atomic physics.

These Sturmian solutions can be constructed by solving the eigenvalue problem

$$\Psi(\mathbf{p}) = \frac{z_1 z_2 e^2}{2\pi^2}\int d^3p' \frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\,\frac{1}{E - E_{p'} + i\delta}\,\Psi(\mathbf{p}'). \tag{3.1}$$

Following PP, we find that for $E < 0$, the three-dimensional momentum space can be visualized as the stereographic projection of the four-dimensional hypersphere ($E < 0$) and hyperboloid of two sheets ($E > 0$) defined by the coordinates

$$\xi_i = 2p_0 p_i/(p^2 \pm p_0^2), \quad i = 1,2,3, \tag{3.2}$$

$$\xi_0 = (p_0^2 \mp p^2)/(p^2 \pm p_0^2) \tag{3.3}$$

with

$$\xi_0^2 \pm |\xi|^2 = 1, \quad p_0 = (2m|E|)^{1/2}. \tag{3.4}$$

$\pm$ here corresponds to $E \lessgtr 0$, respectively.

In terms of the ξ variables, Eq. (3.1) becomes

$$\Psi(\xi) \pm \frac{\eta}{2\pi^2}\int_{S_\pm} \frac{d^3\xi'}{\xi_0'}\,\frac{\Psi(\xi')}{|\xi - \xi'|^2} = 0 \tag{3.5}$$

with

$$d^3p = \left|\frac{p^2 \pm p_0^2}{2p_0}\right|^3 \frac{d^3\xi}{\xi_0}, \tag{3.6}$$

$$(\xi - \xi')^2 = 2[1 - (\xi\xi')] = \frac{\pm 4p_0^2|\mathbf{p}-\mathbf{p}'|^2}{(p^2 \pm p_0^2)(p'^2 \pm p_0^2)}, \tag{3.7}$$

$$\Psi(\xi') = \text{const}\,(p^2 \pm p_0^2)\Psi(\mathbf{p}). \tag{3.8}$$

The Coulomb parameter is given by $\eta = z_1 z_2 e^2 m/p_0$. S_+ denotes the three-dimensional surface of unit hypersphere for $E < 0$ and S_- denotes the two-sheeted surface of the unit hyperboloid with upper sheet given by $1 \leq \xi_0 < +\infty$ and the lower sheet by $-1 \geq \xi_0 > -\infty$, for $E > 0$. The $\pm$ signs correspond to $E < 0$ and $E > 0$, respectively. The negative energy solutions are given by the four-dimensional spherical harmonics $Y_{nlm}(\xi)$:

$$Y_{nlm}(\xi) = Y_{nlm}(\alpha,\theta,\varphi) = \Pi_{nl}(\alpha)Y_{lm}(\theta,\phi),$$

$$\Pi_{nl}(\alpha) = [\tfrac{1}{2}\pi n^2(n^2-1)\cdots(n^2-l^2)]^{-1/2} \times (\sin\alpha)^l\left(\frac{d}{d\cos\alpha}\right)^l \cos n\alpha, \tag{3.9}$$

with

$$\xi_0 = \cos\alpha, \quad \xi_1 = \sin\alpha\,\sin\theta\,\cos\phi, \quad \xi_2 = \sin\alpha\,\sin\theta\,\sin\phi, \quad \xi_3 = \sin\alpha\,\cos\theta.$$

$Y_{lm}(\theta,\varphi)$ is the spherical harmonic. The solutions corresponding to $E > 0$ can be obtained by making the replacement

$$\alpha \to i\alpha, \quad n \to \tfrac{1}{2}i\rho, \quad 0 \leq \rho < \infty$$

with $\cos\alpha \to \pm\cosh\alpha$, $\sin\alpha \to \sinh\alpha$. The ± sign here refers, respectively, to the upper and lower half of the hyperbola. The three-dimensional spherical harmonics form a complete orthonormal set:

$$\int \frac{d^3\xi}{\xi_0} Y_{nlm}(\xi) Y_{n'l'm'}(\xi) = \delta_{nn'}\delta_{ll'}\delta_{mm'},$$

$$\sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l} Y_{nlm}(\xi)Y^*_{nlm}(\xi') = \delta^{(3)}_{S_+}(\xi-\xi'),$$

The corresponding orthogonality conditions for the continuum eigensolutions are obtained by replacing S_+ by S_-, n by ρ, and the Kronecker symbol is changed by an appropriate delta function. The completeness condition is now similarly changed.

The set of functions $Y_{\rho lm}(\alpha, \theta, \varphi)$ with fixed ρ forms a canonical basis for the infinite-dimensional unitary irreducible representation $D(0, \rho)$ of the homogeneous Lorentz group. Thus with a given E, the Sturmian functions form a basis for irreducible representations of the homogeneous Lorentz group.

The case with $E = 0$ is discussed in detail in Refs. 13, 14. It suffices for our purposes to note that in this case the hidden symmetry of the Hamiltonian is the nonrelativistic Galilean group. For the attractive case, one has square integrable solutions while for the repulsive case, there are only unbounded solutions.

The equation for the Green's function written in momentum space is

$$\left(E - \frac{p^2}{2m} \pm i\delta\right) G^{\pm}(\mathbf{p},\mathbf{p}',E) - \frac{z_1 z_2 e^2}{2\pi^2}\int \frac{G^{\pm}(\mathbf{p}'',\mathbf{p}',E)}{|\mathbf{p}-\mathbf{p}''|^2} d^3p'' = \delta^{(3)}(\mathbf{p}-\mathbf{p}'). \quad (3.10)$$

$\pm i\delta$ here specifies the boundary condition in the usual way. By using $G^+ = G_0^+ + G_0^+ T G_0^+$, it is found that the corresponding T matrix is

$$T(\mathbf{p},\mathbf{p}',E) = [E + i\delta - \mathbf{p}^2/(2m)][G^+(\mathbf{p},\mathbf{p}',E) - G_0^+(\mathbf{p},\mathbf{p}',E)][E + i\delta - p'^2/(2m)] \quad (3.11)$$

The complete expression for $G^{\pm}(p, p', E)$ has been derived by PP[14] as an explicit solution of (3.10) using the wavefunctions just summarized. From this, the expressions for T can be derived using (3.11). We thus obtain the following results.

(i) Eigenfunction expansion:

$E < 0$:

$$T(\mathbf{p},\mathbf{p}',E) = \eta \sum_{n=1}^{\infty}\sum_{lm}\frac{1}{n+\eta}\left\{\left(\frac{4p_0^3}{m}\right)^{1/2}\frac{Y_{nlm}(\xi)}{(p_0^2+p^2)}\right\} \times \left\{\left(\frac{4p_0^3}{m}\right)^{1/2}\frac{Y^*_{nlm}(\xi')}{(p_0^2+p'^2)}\right\} \quad (3.12)$$

For the repulsive case, $\{Y_{nlm}(\xi)\}$ are not solutions of the corresponding eigenvalue problem and hence an expansion of the form (3.12) is not meaningful in the same sense as in the attractive case (See Note added in proof in Ref. 24).

$E > 0$:

$$T(\mathbf{p},\mathbf{p}',E) = -\eta\int_0^{\infty} d\rho[F_1^{\pm}(\rho) + 2\eta F_2^{\pm}(\rho)] \times \sum_{lm}\left\{\left(\frac{4p_0^3}{m}\right)^{1/2}\frac{Y_{\rho lm}(\xi)}{(p^2-p_0^2)}\right\}\left\{\left(\frac{4p_0^3}{m}\right)^{1/2}\frac{Y^*_{\rho lm}(\xi)}{(p'^2-p_0^2)}\right\} \quad (3.13)$$

$$= \frac{-\eta p_0^3}{4\pi^2 m(p_0^2-p^2)(p_0^2-p'^2)\sinh\chi_-}\int_{-\infty}^{\infty} d\rho\rho\sin(\rho\chi/2) \times [F_1^{\pm}(\rho) + 2\eta F_2^{\pm}(\rho)] \quad (3.14)$$

with

$$F_1^{\pm}(\rho) = \begin{cases} -2/\rho\coth(\pi\rho/2) \\ +2/\rho[\sinh(\pi\rho/2)]^{-1}, \end{cases} \quad (3.15)$$

$$F_2^{\pm}(\rho) = \begin{cases} \rho^{-1}\left[\dfrac{\sigma\rho/2 - \eta\coth(\pi\rho/2)}{\rho^2/4-\eta^2\pm i\delta}\right] \\ \dfrac{\eta}{\rho}\dfrac{1}{\sinh(\pi\rho/2)[\rho^2/4-\eta^2\pm i\delta]} \end{cases}, \quad (3.16)$$

and

$$\sigma = +1 \quad \text{if } \xi_0 > 0, \xi_0' > 0,$$
$$\sigma = -1 \quad \text{if } \xi_0 < 0, \xi_0' < 0. \quad (3.17)$$

From the definitions (3.6)–(3.9), the functions specified in $\{\cdots\}$ in the above are seen to be the Sturmian functions.

(ii) Infinite integral representations:

$E < 0$:

$$T(\mathbf{p},\mathbf{p}',E) = \frac{\eta p_0}{2m\pi^2|\mathbf{p}-\mathbf{p}'|^2} \times \left(1 - \frac{4\eta^2}{\epsilon_< \sin\chi_+}\int_0^{\infty}\frac{\sinh[(\pi-\chi_+)k]dk}{\sinh\pi k(k^2+\eta^2)}\right) \quad (3.18)$$

with

$\cos\chi_+ = (\xi\xi')$,

$$\epsilon_< = (p^2+p_0^2)(p'^2+p_0^2)/[p_0^2|\mathbf{p}-\mathbf{p}'|^2].$$

$E > 0$:

$$T(\mathbf{p},\mathbf{p}',E) = \frac{\eta p_0}{2m\pi^2}\frac{1}{|\mathbf{p}-\mathbf{p}'|^2} \times \left(1 - \frac{4\eta}{\epsilon_> \sinh\chi_-}\int_0^{\infty}\frac{(\sigma k - \eta\coth\pi k)\sin k\chi_-}{(k^2-\eta^2\pm i\delta)}\right) \quad (3.19)$$

with

$\cosh\chi_- = (\xi\xi')$, $\quad \xi_0\xi_0' > 0$,

$$\epsilon_> = \frac{(p^2-p_0^2)(p'^2-p_0^2)}{p_0^2|\mathbf{p}-\mathbf{p}'|^2},$$

$$T(\mathbf{p},\mathbf{p}',E)=\frac{\eta p_0}{2m\pi^2|\mathbf{p}-\mathbf{p}'|^2}\times\left(1-\frac{4\eta^2}{\epsilon_>\sinh\chi_-}\int_0^\infty dk\frac{\sinh k\chi_-}{\sinh\pi k(k^2-\eta^2\pm i\delta)}\right) \tag{3.20}$$

with $\cosh\chi_-=-(\xi\xi')$, $\xi_0\xi_0'<0$.

In all the above, $(\xi\xi')$ means the scalar product defined in conformity with the metric stated earlier for the cases $E \gtrless 0$. Alternatively, for later purposes, one could rewrite the integrals here in more convenient forms:

$$\int_0^\infty \frac{\sinh(\pi-\chi_+)k}{\sinh\pi k}\frac{dk}{k^2+\eta^2}=-\frac{1}{2i\eta}\int_{-\infty}^\infty\frac{\sinh(\pi-\chi_+)}{\sinh\pi k}\frac{dk}{k+i\eta}, \tag{3.21}$$

$$\int_0^\infty\frac{F(k)\sinh k\chi_-}{k^2-\eta^2\pm i\delta}dk=\frac{1}{2i}\int_{-\infty}^\infty F(k)\frac{e^{ik\chi_-}}{k^2-\eta^2\pm i\delta}dk, \tag{3.22}$$

where $F(k)$ can be identified from comparison with the integrals in (3.19) and (3.20) and is odd in k. The signs are here chosen so that when these integrals are evaluated by contour integration, the closing of the countour is in the upper half k plane. The above results follow directly from the work of PP.[14]

(iii) Contour integral representations: From the generating functions given by BI,[13] we can derive new contour integral representations for the T matrix. We will here give a derivation of the generating functions for positive energy regions given by BI from that valid for negative energies given by Schwinger[7] and PP by a Watson–Sommerfeld transformation. It may be shown (PP and Schwinger) that

$$\sum_{l=0}^{n-1}\sum_{m=-l}^{l}Y_{nlm}(\xi)Y^*_{nlm}(\xi')=\frac{n}{2\pi^2}\frac{\sin n\chi_+}{\sin\chi_+}. \tag{3.23}$$

χ_+ is as defined in (3.18). Similarly (see PP),

$$\sum_{lm}Y_{\rho lm}(\xi)Y^*_{\rho lm}(\xi')=\frac{\rho}{8\pi^2}\frac{\sin(\rho\chi_-/2)}{\sinh\chi_-}. \tag{3.24}$$

χ_- is as defined in (3.19) and (3.20). It was shown by Schwinger[7] that

$$\frac{1}{1-2t\cos\chi_++t^2}=\frac{1}{t}\sum_{n=0}^\infty t^n\frac{\sin n\chi_+}{\sin\chi_+}, \tag{3.25}$$

$$|t|<1,\qquad \chi_+,\ \text{real}.$$

Let us now convert the sum on the right-hand side into an integral by using the Watson–Sommerfeld transformation. To do this, we first set $\chi_+=\pi+\chi_-$ and t real and less than 1. Then the sum on the right-hand side can be written as a Watson–Sommerfeld contour integral in the usual way:

$$\frac{1}{1+2t\cos\chi_-+t^2}=\frac{-1}{2it}\int_{c_0}t^z\frac{\sin(\chi_-z)}{\sin\chi_-}\frac{dz}{\sin\pi z}. \tag{3.26}$$

c_0 here is a loop surrounding the positive and real z axis. In order to open this contour and convert it into a line integral along the imaginary z axis, the contributions from the large quadrants of circles in the right half-plane must vanish. This happens if χ_- is pure imaginary, $i\chi_-$. Then we obtain

$$\frac{1}{1+2t\cosh\chi_-+t^2}=\frac{1}{2t}\int_{-\infty}^\infty e^{i\lambda\ln t}\frac{\sin(\lambda\chi_-)}{\sinh\chi_-}\frac{d\lambda}{\sinh\pi\lambda}=\frac{1}{t}\int_0^\infty\cos(\lambda\ln t)\frac{\sin(\lambda\chi_-)}{\sinh\chi_-}\frac{d\lambda}{\sinh\pi\lambda}. \tag{3.27}$$

The t here is chosen so that one now has a cut from 0 to $-\infty$ in the complex t plane. These definitions of χ_- then correspond to (3.20). We must point out that BI have a slight difference in their definition of the angle χ_-, and with that this coincides with the result derived by them. We may also note that one may set $t=1$ in this formula in which case, we arrive at an expression for $1/(\xi-\xi')^2$ derived by PP corresponding to the case $\xi_0\xi_0'<0$. This serves as a check on this formula. (PP do not derive the generating functions in the positive energy cases).

There is another choice of χ_+ and t which gives a formula of the above structure and this corresponds to the case when $\xi_0\xi_0'>0$ and (3.19). Here we set $\chi_+=i\chi_-$ and $t\to -t$. Then

$$\frac{1}{1+2t\cosh\chi_-+t^2}=\frac{-1}{t}\sum_{n=1}^\infty t^n(-1)^n\frac{\sinh n\chi_-}{\sinh\chi_-}, \tag{3.28}$$

and the above procedure leads to the form

$$\frac{1}{1+2t\cosh\chi_-+t^2}=\frac{1}{t}\int_0^\infty\frac{\cos(\lambda\ln t)}{\sinh\pi\lambda}\frac{\sin(\lambda\chi_-)}{\sinh\chi_-}d\lambda \tag{3.29}$$

with $\cosh\chi_-$ defined as in (3.19) and the t plane now has a cut from 0 to $+\infty$. If we set $t\to e^{i\pi}$, we arrive at an expression for $1/(\xi-\xi')^2$ derived by PP for $\xi_0\xi_0'>0$, again serving as a check on our result. If we want the t plane to have the cut from 0 to $-\infty$ as in the first case even for the second situation, then one may proceed with $\cot z\pi$ instead of $1/\sin z\pi$. With the angle χ_+ now defined as $i\chi_-$, then we obtain the result

$$\frac{1}{1-2t\cosh\chi_-+t^2}=\frac{-1}{2t}\int_{-\infty}^\infty e^{i\lambda\ln t}\frac{\sin(\lambda\chi_-)}{\sinh\chi_-}\coth(\pi\lambda)d\lambda$$

$$=\frac{-1}{t}\int_0^\infty \cos(\lambda\ln t)\frac{\sin(\lambda\chi_-)}{\sinh\chi_-}\coth(\pi\lambda)d\lambda. \tag{3.30}$$

The t plane here has a cut from 0 to $-\infty$; we can thus evaluate this for $t=1$ and verify that the same answer as obtained from the last expression is obtained for $1/(\xi-\xi')^2$ when $\xi_0\xi_0'>0$.

With this alternative derivation of the generating function, the close connection between the regions in ξ space and the t plane becomes evident. This same fact is reflected in the formulas derived below. We may also state that for obtaining $\xi_0\xi_0'>0$ from the result of $\xi_0\xi_0'<0$, one merely rotates the complex t plane through an angle π in the formula for $\xi_0\xi_0'<0$.

The result for the positive energies generalizes that given by Nutt[8,25]:

$E<0$:

$$T(\mathbf{p},\mathbf{p}',E)=\frac{\eta p_0}{2m\pi^2}\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\times\left(1-4\eta\int_{R_+}\frac{t^{\eta}dt}{\epsilon_<(1-t)^2+4t}\right). \tag{3.31}$$

R_+ is a line integral going from 0 to $1(=e^{0i})$ as shown in Fig. 1. This is for the repulsive case ($\eta>0$). For the attractive case, this integral representation holds with η replaced by $-\eta$, but it should not be used to generate the "eigenfunction" expansion of the form (3.12) for the repulsive case for the reason given earlier. *For* $E>0$, the situation is somewhat more complex as is already evident. We will give only the results for the $(E+i\delta)$ case and those for $(E-i\delta)$ can be obtained by a similar procedure. In this case, we have to discuss the attractive and repulsive cases separately. We give below the results for the repulsive case and those for the attractive case are obtained by a formal complex conjugation of the corresponding results (notice these are all valid for $E+i\delta$ only). In doing this, the contours change correspondingly; for instance, L_+ becomes L_- on complex conjugation.

$E>0$ (repulsive case with $E+i\delta$):

$$T(\mathbf{p},\mathbf{p}',E)=\frac{\eta p_0}{2\pi^2m|\mathbf{p}-\mathbf{p}'|^2}\left(1-4i\eta e^{-\pi\eta}\int_{L_-}\frac{t^{i\eta}dt}{\epsilon_>(1+t)^2+4t}\right),$$

$$\xi_0>0,\ \xi_0'>0, \tag{3.32}$$

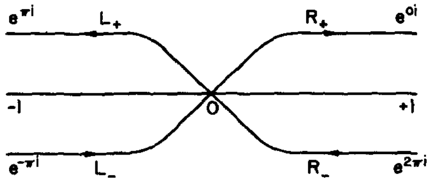

FIG. 1. Contours used in the expressions (3.36), (3.37), and (3.38).

$$=\frac{\eta p_0}{2\pi^2m|\mathbf{p}-\mathbf{p}'|^2}\left(1-4i\eta e^{\pi\eta}\int_{L_+}\frac{t^{i\eta}dt}{\epsilon_>(1+t)^2+4t}\right),$$

$$\xi_0<0,\ \xi_0'<0, \tag{3.33}$$

$$=\frac{\eta p_0}{2\pi^2m|\mathbf{p}-\mathbf{p}'|^2}\left(1+4i\eta\int_{R_+}\frac{t^{i\eta}dt}{\epsilon_>(1-t)^2-4t}\right),$$

$$\xi_0\xi_0'<0. \tag{3.34}$$

These follow if we note that

$$\int_{L_\pm}dt\,t^{i\eta-1}\cos(k\ln t)=\frac{e^{\mp\pi\eta}}{(\eta^2-k^2)i}(k\sinh\pi k\pm\eta\cosh\pi k),$$

$$\int_{R_+}dt\,t^{i\eta-1}\cos(k\ln t)=\frac{\eta}{(\eta^2-k^2)i}. \tag{3.35}$$

The $\ln t$ is here defined on a cut plane from 0 to $-\infty$ along the Ret axis. $p_0^2\to p_0^2+i\delta$ in all the above. The contours L_+, R_+ are shown in Fig. 1. If one formally expresses the contour integrals in (3.32)–(3.34) as real integrals ranging from 0 to 1, they reduce to the form (3.31).

All these representations are mutually equivalent. Several remarks can now be made. Nutt[8] tried to analytically continue (3.31) for $E>0$, and essentially he ended up examining only (3.34) and missed (3.32) and (3.33) entirely. This is the case for all the subsequent troubles he faced. It is clear that *analytic continuation with respect to* E does not bring the expression (3.12) to (3.13). It becomes quite clear if we note that the coefficient of expansion of T for negative E are the representations $D(j,j)$ with $j=(n-1)/2$, and those for positive E are the representation $D(0,\rho)$ of the Lorentz group and these are not analytic continuations of one another. This is after all the manifestation of the different topology for $E \gtrless 0$ associated with the surface $\xi^\mu\xi_\mu=1$ (Ref. 14). For $\epsilon_>=\epsilon_<=0$ with no imaginary parts in them, the T matrix vanishes identically; for $\epsilon\neq0$ however small, as will be seen from (3.36), a Taylor expansion in ϵ does not exist. This was Nutt's mistake. We must stress that these expressions were obtained by explicit solution of the LS equation following PP who explicitly obtained the Green's functions for $E>0$ by solving Eq. (3.10). In our discussion in Sec. 4, we show that these T matrices then automatically obey the generalized unitarity. It should be mentioned that an analytic continuation in E which takes cognizance of the above properties also gives (3.32)–(3.34) from (3.31).

We will now demonstrate that the correct Coulomb amplitude is obtained from an evaluation of the T matrix for positive energies near $p_0^2=p^2=p'^2$. Using (3.14), the actual evaluation of T near the mass shell can be carried out and this displays the on-shell behavior of T quite transparently. Notice that (3.14) has explicitly subsumed in it the Born term in either set of expressions (3.18)–

(3.20) or (3.32)–(3.34). Without making any approximations, the integrals (3.14) can be evaluated and the result is

$$T(\mathbf{p},\mathbf{p}',E)=\pm\frac{4p_0^3\eta}{2\pi m(p^2-p_0^2)(p'^2-p_0^2)}\times\left(\frac{\eta e^{-i\eta\chi_-}\theta(\eta)}{\sinh\chi_-(1-e^{-2\pi\eta})}+\frac{1}{\pi}\sum_{n=1}^{\infty}\frac{e^{-n\chi_-}s_n}{\sinh\chi_-}\frac{n^2}{n^2+\eta^2}\right),$$
$$E>0, \tag{3.36}$$

with

$$\theta(\eta)=e^{-2\pi\eta},\quad s_n=1,\quad \text{for } \xi_0>0,\quad \xi_0'>0,$$
$$\theta(\eta)=1,\quad s_n=1,\quad \text{for } \xi_0<0,\quad \xi_0'<0,$$
$$\theta(\eta)=e^{-\pi\eta},\quad s_n=(-1)^n,\quad \text{for } \xi_0\xi'<0, \tag{3.37}$$

$$T(\mathbf{p},\mathbf{p}',E)=\frac{p_0^3\eta}{\pi^2 m(p^2+p_0^2)(p'^2+p_0^2)}\times\left((1-\cos\chi_+)^{-1}-\eta\pi\frac{\sin(\pi-\chi_+)\eta}{\sin\chi_+}+\frac{2\eta^2}{\sin\chi_+}\sum_{m=1}^{\infty}(-1)^m\frac{\sin(\pi-\chi_+)m}{\eta^2-m^2}\right),\quad E<0. \tag{3.38}$$

$\pm$ signs go with $\xi_0\xi_0' \gtrless 0$. This expression was recently derived by Roberts using the classical path integral techniques. Very near the points $p^2=p_0^2$ and/or $p'^2=p_0^2$ (and vice versa), $(p^2-p_0^2)(p'^2-p_0^2)\sinh\chi_-$ remains finite and $e^{-\chi_-}$ becomes very small as can be seen from expression (3.17) and the definition χ_-, and so the terms in the series can all be ignored compared to the first term in (3.36):

$$T(\mathbf{p},\mathbf{p}',E)\approx\frac{2\eta^2p_0^3\theta(\eta)e^{-i\eta\chi_-}}{\pi m\,|(p^2-p_0^2)(p'^2-p_0^2)|}\,\frac{1}{(1-e^{-2\pi\eta})\sinh\chi_-}. \tag{3.39}$$

It can be noted that in the case of the off-shell Coulomb T matrix, the limit as energy becomes real exists but at the on-shell point $p_0^2=p^2=p'^2$, $e^{-i\eta\chi_-}$ for real η oscillates rapidly and does not tend to any unique limit. However, these oscillating terms can be isolated in terms of momentum space wavefunctions for asymptotic Coulomb distorted states, and the definition of the physical Coulomb amplitude is with respect to the Coulomb distorted waves. Using the explicit expression for χ_- and the Mullin–Guth wavefunctions[8] in the Sturmian form (this is equivalent to using a distorted G_0^+ as was done by Schwinger[7])

$$\langle\mathbf{p}'|\Phi_c^+(\mathbf{p},E)\rangle=-\delta^{(3)}(\mathbf{p}-\mathbf{p}')e^{-\pi\eta/2}|\Gamma(1-i\eta)|\left(\frac{p^2-p_0^2}{p_0^2}\right)^{i\eta}, \tag{3.40}$$

we obtain the usual Coulomb scattering amplitude.

In summary, we may state that the nature of the Coulomb T matrix near the mass-shell depends on the approach to the mass shell; this appears in (3.39) as the multiplicative factor $\theta(\eta)$. This is missing in the analysis of Nutt in Ref. 8. The second important point is that the Born term gets cancelled by a portion of the term VGV on the mass-shell, an observation made earlier by us[22] elsewhere only for short range potentials obeying the constraint $\int_0^\infty r|V(r)|dr<\infty$. The off-shell unitarity relationships are obeyed by these T matrices by virtue of our general demonstration given in the next section. An easy direct verification of these can be accomplished by using (3.13) and a transformation to the four-dimensional space.

In the next section, we will discuss the generalized unitarity and its implications to the Coulomb T matrix.

4. OFF-SHELL UNITARITY

The erroneous calculation of the discontinuity of the Coulomb T matrix[8] across the unitarity cut has led some authors to investigate validity of on the energy shell Low equation for this T matrix.[9,10] We now show that for complex energies, if a unique solution of the LS equation for T is obtained, the generalized Low equation is guaranteed for complex energies and further study of the unitarity for real energies reduces to one of careful limiting process.

We have from the LS equation for complex energies, Eq. (2.4), the corresponding one for $T^\dagger$. Then

$$T-T^\dagger=H'[G^+-G^-]H' \tag{4.1}$$
$$=TG_0^+[(G^-)^{-1}-(G^+)^{-1}]G_0^-T^\dagger \tag{4.2}$$
$$=-2i\delta TG_0^+G_0^-T^\dagger. \tag{4.3}$$

Equation (4.3) is the Low equation for complex energies depicting the generalized unitarity relation.

Somewhat more subtle manipulations are needed to obtain (4.3) from the LS equation for G^+. We write from the second expression in Eq. (2.2)

$$T=(E-H_0+i\delta)[G^+-G_0^+](E-H_0+i\delta). \tag{4.4}$$

Then

$$T-T^\dagger=-2i\delta\left((E-H_0)\frac{1}{(E-H_0)^2+\delta^2}(E-H_0)\right)+2i\delta\left((E-H)\frac{1}{(E-H)^2+\delta^2}(E-H_0)+(E-H_0)\frac{1}{(E-H)^2+\delta^2}(E-H)\right)+\frac{2i\delta^3}{(E-H)^2+\delta^2}-2i\delta \tag{4.5}$$

$$=-2i\delta\left(-H'\frac{1}{(E-H)^2+\delta^2}(E-H_0)\right.$$

$$-(E-H_0)\frac{1}{(E-H)^2+\delta^2}H' + (E-H_0)\frac{1}{(E-H)^2+\delta^2}(E-H_0)\Big) + \frac{2i\delta^3}{(E-H)^2+\delta^2} - 2i\delta \tag{4.6}$$

$$= -2i\delta\Big(2TG_0^+G_0^-T^\dagger + TG_0^+G^-(E-H) + (E-H)G^+G_0^-T^\dagger + 1 - \frac{\delta^2}{(E-H)^2+\delta^2}\Big) + \{2i\delta(E-H_0)G^+G^-(E-H_0)\}. \tag{4.7}$$

The last line in $\{\cdots\}$ can be further simplified to give

$$\{\cdots\} = 2i\delta\Big(1 + TG_0^+G_0^-T^\dagger - \frac{\delta^2}{(E-H)^2+\delta^2} + TG_0^+ + G_0^-T^\dagger + i\delta(H'G^+G^- - G^+G^-H')\Big). \tag{4.8}$$

Substitutions of this expression in (4.7) immediately leads to the generalized unitarity relation for complex energies. In the above manipulations, only the LS equation and the definitions of $G^\pm$, $G_0^\pm$, H, and T are used. It is important to stress that δ was not set equal to zero anywhere in the derivation. Roberts[18] writes the equation

$$T - T^\dagger = -2i\pi(E-H_0)\delta(E-H)(E-H_0) \tag{4.9}$$

to express unitarity. Our above analysis shows that this cannot be correct for the usual T operator. To obtain from (4.3) the on-shell unitarity valid for physical energies, it is important to prove the existence of the limit $\delta \to 0$ for $T(E+i\delta)$. The analysis described in Sec. 2 and the explicit expression for the Coulomb T matrix obtained in the last section show the on-shell limit is not unique for the Coulomb T matrix. One thus substitutes the Coulomb T in (4.3) and computes the limit $\delta \to 0$ with care. When the limit exists for T, however, then the usual form of the Low equation is obtained by setting $\delta = 0$ in (4.3).

5. SUMMARY

In this paper, we have shown that the partial wave off-shell two particle Coulomb T matrix obeys the usual Lippmann–Schwinger equation for complex energies. The proof was accomplished by explicitly showing that the corresponding kernel is L^2. But this is not the case for the full LS equation. However, via the Sturmian eigenfunctions and following the procedure of Schwinger and PP, the full LS equation was solved for T and various general expressions for the off-shell T matrix were obtained. The Hilbert–Schmidt analysis of the kernel of the symmetrized form of LS equation indicated that the limit $\delta \to 0$ of $T(E+i\delta)$ may not be well defined, and this is found to be true by studying the on-shell behavior of the Coulomb T matrix for real positive energies. If proper overlap between the Coulomb distorted asymptotic states of the plane wave representation of the Coulomb T matrix is taken, then the physical Coulomb amplitude is obtained. Moreover, the generalized (off-shell) unitarity—the Low equation—was shown to be valid if T is the solution of the LS equation.

In a separate communication, the implications of some of the above remarks as well as the use of the various representations of the off-shell Coulomb T matrix in the Faddeev theory of the three-particle Coulomb systems, will be presented.

ACKNOWLEDGMENTS

We thank Professor J. Callaway for providing us with the necessary impetus to examine the various puzzles concerning the Coulomb T matrix. We thank the referee of the original version of the paper for his very valuable suggestions which resulted in the present form of the paper.

---

* Present address: Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan, India.

[1] L. D. Faddeev, *Mathematical Aspects of the Three-Body Problem in the Quantum Scattering Theory*, translated by Ch. Gutfreund, Israel Program for Scientific Translations (Jerusalem, 1965).

[2] C. S. Shastry and A. K. Rajagopal, *Faddeev Theory of Three-Particle Scattering and Some Applications*, Lecture Notes in Physics Series (Springer-Verlag, Berlin) (To be published in 1971). This contains an exhaustive account of the formalism along with a fairly extensive bibliography.

[3] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[4] A. K. Rajagopal and C. S. Shastry, J. Math. Phys. 12, 1515 (1971).

[5] G. B. West, J. Math. Phys. 8, 942 (1967); see also T. Sasakawa Suppl. Progr. Theoret. Phys. (Kyoto) 27, 1 (1964).

[6] E. Gerjuoy, lecture at the *Second International Conference On Atomic Physics*, Oxford, England, July 21-24, 1970.

[7] J. Schwinger, J. Math Phys. 5, 1606 (1964).

[8] G. L. Nutt, J. Math. Phys. 9, 796 (1968).

[9] M. R. C. McDowell and D. Richards, preprint (1970).

[10] J. Nuttall and R. W. Stagat, Phys. Rev. A 3, 1355 (1971).

[11] V. A. Fock, Z. Physik 98, 145 (1935).

[12] L. Hostler, J. Math. Phys. 8, 142 (1967); also see 5, 591, 1235 (1964) for his earlier works on the Coulomb Green's function. A closed integral form for the Coulomb Green's function given in the third paper may be shown to be equivalent to Schwinger's result for $E < 0$.

[13] M. Bander and C. Itzykson, Rev. Mod. Phys. 38, 330, 346 (1966).

[14] A. M. Perelomov and V. S. Popov, Zh. Eksp. Teor. Fiz 50, 179, (1966)[Sov. Phys. JETP 23, 118 (1966)].

[15] A. Norcliffe and I. C. Percival, J. Phys. B1, 784 (1968).

[16] A. Norcliffe, I. C. Percival, and M. J. Roberts, J. Phys. B2, 578, 590 (1969).

[17] M. J. Roberts, Chem. Phys. Letters 6, 46 (1970).

[18] M. J. Roberts, J. Phys. B3, L115 (1970).

[19] C. S. Shastry and A. K. Rajagopal, J. Math. Phys. (1971)(to be published).

[20] W. F. Ford, J. Math. Phys. 7, 626 (1966).

[21] L. D. Faddeev, in *Three-Body Problem*, edited by J. S. C. McKee and P. M. Rolph (North-Holland, New York, 1970), p. 154, and preprint of Vaselova (1971).

[22] C. A. Nelson, A. K. Rajagopal, and C. S. Shastry, J. Math. Phys. 12, 737 (1971).

[23] T. A. Green and E. Lanford, J. Math. Phys. 1, 139 (1960).

[24] S. Radhakant, C. S. Shastry, and A. K. Rajagopal, Phys. Rev. A 3, 234 (1971).

[25] C. S. Shastry and A. K. Rajagopal, Phys. Rev. A 2, 781 (1970). In this paper, starting from the representation (3.31), the eigenfunction expansion (3.12) was obtained.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

Exterior-Algebraic Derivation of Einstein Field Equations Employing a Generalized Basis

Frederick J. Ernst
Illinois Institute of Technology, Chicago, Illinois, 60616
(Received 1 July 1971)

A tetrad vector formulation of Einstein's field equations is developed in which the orthogonality properties of the tetrad are permitted to vary in any prescribed smooth way from one space-time point to another. The components of the Riemann tensor with respect to such a basis are derived by means of exterior calculus. The approach facilitates a simple direct derivation of the Harrison-Ernst equations.

I. INTRODUCTION

Recently, the author developed a formulation of the stationary axially symmetric gravitational field problem in which a key role was played by a complex potential ϵ related to the metric tensor by means of certain integrability conditions.[1] In terms of this complex potential even the Kerr metric[2] could be simply described, and a whole set of perturbation theory solutions generalizing the Kerr metric was found. Subsequently, Harrison suggested an extension of the ϵ formulation to the case of stationary nonaxially symmetric fields.[3] It is the author's desire to find a further generalization of the formalism in which even time dependence is taken into account, and in which interior as well as vacuum fields may be considered.

If these desires are to be realized, it will be necessary first to comprehend thoroughly the Harrison-Ernst field equations. As a step in this direction we shall give a simple direct derivation of these equations utilizing the methods of exterior calculus. Our approach will differ from that commonly employed[4] in that we shall permit the orthogonality properties of the tetrad system to vary from one space-time point to another. However, we shall assume that the reader is familiar with the general properties of p-vectors and p-forms.

II. THE USE OF A NONORTHONORMAL BASIS

Let us denote the *natural* basis for 1-forms by dx^α and the *natural* basis for 1-vectors by $\mathbf{a}_\alpha$, $\alpha = 0, 1, 2, 3$. It is convenient to regard dx as a row matrix and $\mathbf{a}$ as a column matrix. If $\mathbf{b}$ is an arbitrary basis for the 1-vectors, then σ is the corresponding basis induced for the 1-forms by requiring that

$$\sigma \mathbf{b} = dx\mathbf{a}. \tag{1}$$

For a space with a symmetric connection we then immediately have the important formula

$$d(\sigma \mathbf{b}) = 0. \tag{2}$$

We shall also introduce a metric matrix

$$G = \mathbf{b} \cdot \mathbf{b}^{\sim}, \tag{3}$$

which reduces to the metric tensor if the natural basis is employed. If an orthonormal or quasi-orthonormal tetrad system is employed, the G matrix is a constant matrix. It does not seem to be widely realized that there is no need to consider just these extreme points of view. We shall proceed under the assumption that G may depend upon position without necessarily coinciding with the metric tensor.

A Christoffel matrix

$$K = (d\mathbf{b}) \cdot \mathbf{b}^{\sim} \tag{4}$$

and a Riemann matrix

$$\Theta = (d^2\mathbf{b}) \cdot \mathbf{b}^{\sim} \tag{5}$$

are now defined, the former consisting of 1-forms and the latter of 2-forms. Under a change of basis Θ undergoes a linear homogeneous transformation, although this is not true for K. We define an object with the symmetries of the Riemann tensor as follows:

$$\Theta_{\alpha\beta} = \tfrac{1}{2} R_{\alpha\beta\gamma\delta}\sigma^\gamma\sigma^\delta. \tag{6}$$

In fact, when the natural basis is employed $R_{\alpha\beta\gamma\delta}$ is precisely the Riemann tensor. In other cases $R_{\alpha\beta\gamma\delta}$ is related to the Riemann tensor by a linear homogeneous relationship, which may be obtained easily from the definition of Θ. The symmetric matrix

$$R_{\alpha\gamma} = G^{\beta\delta} R_{\alpha\beta\gamma\delta} \tag{7}$$

is equal to the Ricci tensor in the case of a natural basis, and it is related to the Ricci tensor by a linear homogeneous relationship otherwise. No matter what basis is employed, Einstein's vacuum field equations may be written

$$R_{\alpha\gamma} = 0. \tag{8}$$

From Eqs. (2), (3), and (4) it follows directly that

$$(d\sigma)G = \sigma K \tag{9}$$

and that

$$dG = K + K^{\sim}. \tag{10}$$

In practice these two equations are easily solved for K.[5] Once K is determined, Θ may be evaluated, for from Eqs. (3)-(5), and (10) it follows that

$$\Theta = dK + KG^{-1}K^{\sim}. \tag{11}$$

For certain problems it is convenient to write this equation in the form

$$\Theta G^{-1} = d\Gamma - \Gamma\Gamma, \tag{12}$$

where $\Gamma = KG^{-1}$.

We are at liberty to choose the symmetric matrix

G in any convenient way. If G were chosen to be the ordinary metric tensor, we would simply have an exterior algebraic version of the traditional method of calculation involving Christoffel symbols. On the other hand, if G were chosen to be the Minkowski metric, we would then have the formalism described in detail in Ref. 4. Rather than adopt either one of these extremes, we shall in this paper suppose that

$$G = \begin{pmatrix} -1 & 0 \\ 0 & \gamma \end{pmatrix}, \tag{13}$$

where the three-dimensional symmetric matrix γ may vary from one point of space–time to another. In this case it is fruitful to introduce complex three-dimensional matrices

$$\mathbf{K}_{\alpha\beta} = K_{\alpha\beta} + i\epsilon_{\alpha\beta\mu}\gamma^{\mu\nu}(\det\gamma)^{1/2}K_{\nu 0}, \tag{14}$$

$$\mathbf{\Theta}_{\alpha\beta} = \Theta_{\alpha\beta} + i\epsilon_{\alpha\beta\mu}\gamma^{\mu\nu}(\det\gamma)^{1/2}\Theta_{\nu 0}, \tag{15}$$

where $\epsilon_{\alpha\beta\mu}$ is the Levi–Civita symbol, for one may show that

$$\mathbf{\Theta} = d\mathbf{K} + \mathbf{K}\gamma^{-1}\mathbf{K}^{\sim}. \tag{16}$$

III. DERIVATION OF THE HARRISON–ERNST EQUATIONS

We shall suppose that the coordinate system has been chosen so that

$$\sigma^0 = f^{1/2}(dx^0 - \omega_\alpha dx^\alpha), \tag{17}$$

$$\sigma^\alpha = f^{-1/2}dx^\alpha, \qquad \alpha = 1, 2, 3, \tag{18}$$

where the ten functions $\gamma_{\alpha\beta}$, ω_α, and f are independent of x^0. A straightforward calculation yields

$$\mathbf{K}_{\alpha\beta} = [\delta\alpha, \beta]\, dx^\delta + \epsilon_{\alpha\beta\mu}\gamma^{\mu\nu}(\det\gamma)^{1/2}\mathcal{K}_\nu, \tag{19}$$

where $[\delta\alpha, \beta]$ is a Christoffel symbol of the first kind for the three-dimensional space with metric tensor $\gamma_{\alpha\beta}$, and where

$$\mathcal{K}_\alpha = \tfrac{1}{2} f^{-1/2}\{\epsilon_{\alpha\delta\mu}\gamma^{\mu\nu}(\det\gamma)^{1/2}M_\nu\sigma^\delta - iM_\alpha\sigma^0\} \tag{20}$$

$$M_\alpha = f_{,\alpha} + i(f^2 Z_\alpha). \tag{21}$$

The axial vector Z_α may be obtained from the skew symmetric tensor

$$h_{\alpha\beta} = -2\omega_{[\alpha,\beta]} = \epsilon_{\alpha\beta\mu}\gamma^{\mu\nu}(\det\gamma)^{1/2}Z_\nu. \tag{22}$$

On the other hand, substitution of Eq. (19) into Eq. (16) yields

$$\mathbf{\Theta}_{\alpha\beta} = \tfrac{1}{2}P_{\alpha\beta\gamma\delta}dx^\gamma dx^\delta + \epsilon_{\alpha\beta\mu}\gamma^{\mu\nu}(\det\gamma)^{1/2}D\mathcal{K}_\nu + \mathcal{K}_\alpha\mathcal{K}_\beta, \tag{23}$$

where the new differential operator D is defined so that

$$D\mathcal{K}_\nu = d\mathcal{K}_\nu - dx^\alpha \textstyle\sum^\delta_{\alpha\nu}\mathcal{K}_\delta. \tag{24}$$

Here $\sum^\delta_{\alpha\nu}$ and $P_{\alpha\beta\gamma\delta}$ are, respectively, the Christoffel symbol and Riemann tensor associated with the three-dimensional metric tensor $\gamma_{\alpha\beta}$.

For any stationary gravitational field such that the Ricci tensor component $R_{\alpha 0}$ vanishes, M_α can be shown to be a gradient.

$$M_\alpha = \epsilon_{,\alpha}, \tag{25}$$

where $\epsilon = f + i\varphi$. This is demonstrated by looking at the terms proportional to $\sigma^0\sigma^\delta$ in $\mathrm{Re}\mathbf{\Theta}_{\alpha\beta}$. The remaining components of the vacuum field equations are then found to be given by

$$\mathrm{Re}[(\mathrm{Re}\epsilon)\gamma^{\alpha\beta}\epsilon_{;\alpha\beta} - \gamma^{\alpha\beta}\epsilon_{,\alpha}\epsilon_{,\beta}] = 0 \tag{26}$$

$$[(\mathrm{Re}\epsilon)^2 P_{\alpha\beta} + \tfrac{1}{4}(\epsilon_{,\alpha}\epsilon^*_{,\beta} + \epsilon^*_{,\alpha}\epsilon_{,\beta})] = 0. \tag{27}$$

On the other hand, the integrability condition

$$h_{\alpha\beta,\gamma} + h_{\beta\gamma,\alpha} + h_{\gamma\alpha,\beta} = 0,$$

implies that

$$\gamma^{\alpha\beta}(f^{-2}\varphi_{,\alpha})_{;\beta} = 0$$

or

$$\mathrm{Im}\,\{(\mathrm{Re}\epsilon)\gamma^{\alpha\beta}\epsilon_{.\alpha\beta} - \gamma^{\alpha\beta}\epsilon_{,\alpha}\epsilon_{,\beta}\} = 0. \tag{28}$$

In conclusion, the field equations for a stationary vacuum metric can be written in the simple form

$$(\mathrm{Re}\epsilon)\gamma^{\alpha\beta}\epsilon_{;\alpha\beta} = \gamma^{\alpha\beta}\epsilon_{,\alpha}\epsilon_{,\beta}, \tag{29}$$

$$(\mathrm{Re}\epsilon)^2 P_{\alpha\beta} + \tfrac{1}{4}(\epsilon_{,\alpha}\epsilon^*_{,\beta} + \epsilon^*_{,\alpha}\epsilon_{,\beta}) = 0. \tag{30}$$

Alternatively, these equations may be obtained from the variational principle

$$\delta\int\Big\{P + \frac{1}{2}\,\frac{\gamma^{\alpha\beta}\epsilon_{,\alpha}\epsilon^*_{,\beta}}{(\mathrm{Re}\epsilon)^2}\Big\}(\det\gamma)^{1/2}d^3x = 0. \tag{31}$$

Although Harrison and Ernst have developed analogous equations valid in the presence of electrostatic and magnetostatic fields, it is not known at present whether or not any fruitful extension exists for fields inside of matter, or whether one can treat time-dependent fields in the same spirit.[6] It is not likely to be easy to find the desired generalization, but, if it can be found, the formalism is liable to be very useful with regard to astrophysical applications, because the stationary axially symmetric problem has already been made quite manageable in terms of this formalism.

ACKNOWLEDGMENTS

The author is grateful to Dr. I. Hauser for frequent discussions concerning the mathematics of general relativity, and to Dr. B. K. Harrison for calling his attention to the possibility of defining the complex potential ϵ for a nonaxially symmetric stationary field.

1 F. J. Ernst, Phys. Rev. **167**, 1175 (1968) and **168**, 1415 (1968). Receipt of the present article was acknowledged over three years ago by the former editor of the *Journal of Mathematical Physics*. However, no action was taken concerning its publication until this year, when the author inquired about its fate. Although the state of the art has developed during the intervening years, the author has not revised the manuscript, for his principal objective in publishing this work at this late date is to call attention to the contribution of B. Kent Harrison, to whom full credit should be given for observing that an Ernst-type complex potential can be introduced whenever one has a spacelike *or* a timelike Killing vector.

2 R. P. Kerr, Phys. Rev. Letters **11**, 237 (1963).

3 B. K. Harrison, J. Math. Phys. **9**, 1744 (1968).

4 H. Flanders, *Differential Forms with Applications to the Physical Sciences* (Academic, New York, 1963); C. W. Misner, J. Math. Phys. **4**, 924 (1963).

5 Introduce the skew symmetric matrix $\mathbf{\Omega} = \frac{1}{2}(K - K^{\sim})$, which satisfies the equation $(d\sigma)G - \frac{1}{2}\sigma dG = \sigma\Omega$. The left side is a calculable 2-form, which may be cast into the form $\frac{1}{2}f_{\alpha\beta\gamma}\sigma^{\alpha}\sigma^{\beta}$, where $f_{\alpha\beta\gamma}$ is skew symmetric in the first two indices. Similarly $\sigma\Omega\sigma^{\sim}$ may be cast into the form $\frac{1}{6}h_{\alpha\beta\gamma}\sigma^{\alpha}\sigma^{\beta}\sigma^{\gamma}$, where $h_{\alpha\beta\gamma}$ is skew symmetric in all pairs of indices. Then, it can be shown that $\Omega_{\alpha\beta} = (f_{\alpha\beta\gamma} - \frac{1}{2}h_{\alpha\beta\gamma})\sigma^{\gamma}$.

6 The author expects to submit for publication an article describing further insights into the complex potential description of fields possessing a single Killing vector. However, now, three years later, it appears unlikely that a way will be found to describe in terms of a complex potential space-times which lack symmetries.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

On the Bounds of the Average Value of a Function*

Robert H. T. Yeh

Department of Physics and Astronomy, State University of New York, Buffalo, New York 14214

(Received 30 October 1970)

We describe here how one can obtain upper and lower bounds of the average value of a function $\overline{f(E)}$ in terms of the bounds of the variable E and $\overline{E}, \overline{E^2}$.

In physics as well as other sciences, sometimes we may like to estimate the average value of a quantity, even though we have only limited informations about this quantity; e.g., we may like to estimate the higher-order moments of a certain (charge, mass, etc.) distribution in terms of some known lowest order moments. In theories of polymer solutions,[1] the average of the inverse distance between monomers $\overline{(1/r)}$ is usually difficult to compute directly, and most theories make approximate estimation of this number in terms of $\overline{r}$ or $\overline{r^2}$. In a previous article,[2] by using the concave upward property of exponential function, we obtain fairly simple bounds for its average value. The same reasoning should lead us to similar bounds for other concave upward functions. We now would like to investigate what are the simplest possible bounds that one can construct for the average value of an arbitrary function.

Consider first a real value concave upward function $f(E)$, i.e., $f''(E) \geq 0$, or $f'(E)$ is a nondecreasing function as we increase E. From Taylor's theorem, we have

$$f(E) = f(\epsilon) + (E-\epsilon)f'(\epsilon) + (E-\epsilon)^2 \int_0^1 (1-t) \times f''[\epsilon + t(E-\epsilon)]dt. \qquad (1)$$

We note that the remainder term is nonnegative for concave upward function; hence

$$f(E) \geq f(\epsilon) + (E-\epsilon)f'(\epsilon), \qquad (2)$$

for arbitrary E and ϵ. For concave downward function ($f'' \leq 0$), we have instead

$$f(\epsilon) + (E-\epsilon)f'(\epsilon) \geq f(E), \qquad (3)$$

for arbitrary E and ϵ.

The average value of a function $\overline{f(E)}$ is given by

$$\overline{f(E)} = \sum_i p_i f(E_i), \qquad (4)$$

where $p_i \geq 0$ and $\sum_i p_i = 1$. We also denote the maximum value of the set $\{E_i\}$ by E_m, and the minimum value by E_0.

From Eqs. (2) and (3), using the same arguments as in Ref. 2, we easily find that for concave upward function

$$\overline{f(E)} \geq f(\overline{E}). \qquad (5a)$$

and for concave downward function

$$\overline{f(E)} \leq f(\overline{E}). \qquad (5b)$$

Eq. (5) can easily be generalized to functions of several variables. Taylor's theorem for functions of N variables gives

$$f(\{x_i\}) = f(\{x_{i0}\}) + \Sigma_i(x_i - x_{i0})(\partial f/\partial x_i)_0 + R_2, \qquad (6)$$

where $R_2 = \frac{1}{2}d^2 f(x_{i0} + \theta(x_i - x_{i0}))$, with $0 < \theta < 1$. It is easy to see that if we have

$$\left(\frac{\partial^2 f}{\partial x_i^2}\right)\left(\frac{\partial^2 f}{\partial x_j^2}\right) \geq (N-1)^2 \left(\frac{\partial f}{\partial x_i}\right)^2 \left(\frac{\partial f}{\partial x_j}\right)^2 \qquad (7a)$$

and

$$\frac{\partial^2 f}{\partial x_i^2} \geq 0, \qquad (7b)$$

for all values of all variables, then $R_2 \geq 0$. Hence, if Eq. (7) holds, we would have

$$\overline{f(\{x_i\})} \geq f(\{\overline{x}_i\}). \qquad (8)$$

If the inequality sign is reversed in Eq. (7b), then

[1] F. J. Ernst, Phys. Rev. **167**, 1175 (1968) and **168**, 1415 (1968). Receipt of the present article was acknowledged over three years ago by the former editor of the *Journal of Mathematical Physics*. However, no action was taken concerning its publication until this year, when the author inquired about its fate. Although the state of the art has developed during the intervening years, the author has not revised the manuscript, for his principal objective in publishing this work at this late date is to call attention to the contribution of B. Kent Harrison, to whom full credit should be given for observing that an Ernst-type complex potential can be introduced whenever one has a spacelike *or* a timelike Killing vector.

[2] R. P. Kerr, Phys. Rev. Letters **11**, 237 (1963).

[3] B. K. Harrison, J. Math. Phys. **9**, 1744 (1968).

[4] H. Flanders, *Differential Forms with Applications to the Physical Sciences* (Academic, New York, 1963); C. W. Misner, J. Math. Phys. **4**, 924 (1963).

[5] Introduce the skew symmetric matrix $\Omega = \frac{1}{2}(K - K^{\sim})$, which satisfies the equation $(d\sigma)G - \frac{1}{2}\sigma dG = \sigma\Omega$. The left side is a calculable 2-form, which may be cast into the form $\frac{1}{2}f_{\alpha\beta\gamma}\sigma^\alpha\sigma^\beta$, where $f_{\alpha\beta\gamma}$ is skew symmetric in the first two indices. Similarly $\sigma\Omega\sigma^{\sim}$ may be cast into the form $\frac{1}{6}h_{\alpha\beta\gamma}\sigma^\alpha\sigma^\beta\sigma^\gamma$, where $h_{\alpha\beta\gamma}$ is skew symmetric in all pairs of indices. Then, it can be shown that $\Omega_{\alpha\beta} = (f_{\alpha\beta\gamma} - \frac{1}{2}h_{\alpha\beta\gamma})\sigma^\gamma$.

[6] The author expects to submit for publication an article describing further insights into the complex potential description of fields possessing a single Killing vector. However, now, three years later, it appears unlikely that a way will be found to describe in terms of a complex potential space-times which lack symmetries.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 11 NOVEMBER 1971

On the Bounds of the Average Value of a Function*

Robert H. T. Yeh

Department of Physics and Astronomy, State University of New York, Buffalo, New York 14214

(Received 30 October 1970)

We describe here how one can obtain upper and lower bounds of the average value of a function $\overline{f(E)}$ in terms of the bounds of the variable E and $\bar{E}, \overline{E^2}$.

In physics as well as other sciences, sometimes we may like to estimate the average value of a quantity, even though we have only limited informations about this quantity; e.g., we may like to estimate the higher-order moments of a certain (charge, mass, etc.) distribution in terms of some known lowest order moments. In theories of polymer solutions,[1] the average of the inverse distance between monomers $\overline{(1/r)}$ is usually difficult to compute directly, and most theories make approximate estimation of this number in terms of $\bar{r}$ or $\overline{r^2}$. In a previous article,[2] by using the concave upward property of exponential function, we obtain fairly simple bounds for its average value. The same reasoning should lead us to similar bounds for other concave upward functions. We now would like to investigate what are the simplest possible bounds that one can construct for the average value of an arbitrary function.

Consider first a real value concave upward function $f(E)$, i.e., $f''(E) \geq 0$, or $f'(E)$ is a nondecreasing function as we increase E. From Taylor's theorem, we have

$$f(E) = f(\epsilon) + (E-\epsilon)f'(\epsilon) + (E-\epsilon)^2\int_0^1 (1-t) \times f''[\epsilon + t(E-\epsilon)]dt. \quad (1)$$

We note that the remainder term is nonnegative for concave upward function; hence

$$f(E) \geq f(\epsilon) + (E-\epsilon)f'(\epsilon), \quad (2)$$

for arbitrary E and ϵ. For concave downward function ($f'' \leq 0$), we have instead

$$f(\epsilon) + (E-\epsilon)f'(\epsilon) \geq f(E), \quad (3)$$

for arbitrary E and ϵ.

The average value of a function $\overline{f(E)}$ is given by

$$\overline{f(E)} = \textstyle\sum_i p_i f(E_i), \quad (4)$$

where $p_i \geq 0$ and $\sum_i p_i = 1$. We also denote the maximum value of the set $\{E_i\}$ by E_m, and the minimum value by E_0.

From Eqs. (2) and (3), using the same arguments as in Ref. 2, we easily find that for concave upward function

$$\overline{f(E)} \geq f(\bar{E}). \quad (5a)$$

and for concave downward function

$$\overline{f(E)} \leq f(\bar{E}). \quad (5b)$$

Eq. (5) can easily be generalized to functions of several variables. Taylor's theorem for functions of N variables gives

$$f(\{x_i\}) = f(\{x_{i0}\}) + \Sigma_i(x_i - x_{i0})(\partial f/\partial x_i)_0 + R_2, \quad (6)$$

where $R_2 = \frac{1}{2}d^2 f(x_{i0} + \theta(x_i - x_{i0}))$, with $0 < \theta < 1$. It is easy to see that if we have

$$\left(\frac{\partial^2 f}{\partial x_i^2}\right)\left(\frac{\partial^2 f}{\partial x_j^2}\right) \geq (N-1)^2\left(\frac{\partial f}{\partial x_i}\right)^2\left(\frac{\partial f}{\partial x_j}\right)^2 \quad (7a)$$

and

$$\frac{\partial^2 f}{\partial x_i^2} \geq 0, \quad (7b)$$

for all values of all variables, then $R_2 \geq 0$. Hence, if Eq. (7) holds, we would have

$$\overline{f(\{x_i\})} \geq f(\{\bar{x}_i\}). \quad (8)$$

If the inequality sign is reversed in Eq. (7b), then

$R_2 \le 0$; hence the inequality sign in Eq. (8) must also be reversed.

Let us now consider $f_n(E) = (E - E_0)^n$, where n is an integer and $n \ge 3$. Since $f_n(E)$ is concave upward (for $E \ge E_0$), from Eq. (2), we have

$$(E - E_0)^n \ge (\epsilon - E_0)^n + (E - \epsilon) f_n'(\epsilon) \qquad (9a)$$

and

$$(E - E_0)^{n-1} \ge (\epsilon_1 - E_0)^{n-1} + (E - \epsilon_1) f_{n-1}'(\epsilon_1). \qquad (9b)$$

From Eq. (9a), with $\epsilon = \overline{E}$, we get

$$\overline{(E - E_0)^n} \ge (\overline{E} - E_0)^n. \qquad (10a)$$

Multiplying Eq. (9b) by $(E_m - E)$ and setting

$$\epsilon_1 = E_m - \overline{(E_m - E)^2}/(E_m - \overline{E}),$$

we get the following recursive upper bound for f_n:

$$(E_m - E_0)\overline{(E - E_0)^{n-1}} - (E_m - \overline{E})(\epsilon_1 - E_0)^{n-1} \ge \overline{(E - E_0)^n}. \qquad (10b)$$

Hence for any function $f(E)$ which has a Taylor expansion about E_0, or

$$f(E) = f(E_0) + \sum_{n=1}^{\infty} (n!)^{-1} (E - E_0)^n f^{(n)}(E_0),$$

we can in principle find bounds of $\overline{f(E)}$ in terms of $E_0, E_m, \overline{E}$ and $\overline{E^2}$. Or

$$\sum_{n=3}^{\infty} (n!)^{-1} B_l(n) f^{(n)}(E_0)$$

$$\le \overline{f(E)} - f(E_0) - (\overline{E} - E_0) f'(E_0) \tfrac{1}{2} f^{(2)}(E_0) \overline{(E - E_0)^2}$$

$$\le \sum_{n=3}^{\infty} (n!)^{-1} B_u(n) f^{(n)}(E_0), \qquad (11)$$

where if $f^{(n)}(E_0) > 0$, then $B_u(n)$ is the upper bound of $\overline{(E - E_0)^n}$, (Eq. 10b) and $B_l(n)$ is the lower bound of $\overline{(E - E_0)^n}$ (Eq. 10a). And, if $f^{(n)}(E_0) < 0$, then $B_u(n)$ is the lower bound of $\overline{(E - E_0)^n}$, while $B_l(n)$ is the upper bound.

If we have more input information about the function or about the distribution (e.g., $E_i \ge 0$), then we can improve our bounds; e.g., the average value of an even function $[f(E) = f(-E)]$ can be bounded in terms of $\overline{E^2}$, E_m and $\overline{E^4}$, via

$$E_m^2 \overline{E^{2n-2}} - (E_m^2 - \overline{E^2})\, \epsilon_2^{2n-2} \ge \overline{E^{2n}} \ge (\overline{E^2})^n,$$

where $\epsilon_2^2 = E_m^2 - \overline{(E_m^2 - E^2)^2}/(E_m^2 - \overline{E^2})$. Consider the case of $E_0 = 0$, $E_m = 1$ and $p(E) = (s+1)E^s$ with integer s; then we find that $\overline{E^{2n}} = (s+1)/(2n+s+1)$ and $(\overline{E^2})^n = [(s+1)/(s+3)]^n$. These bounds are poor for large n $(n > s)$, but improve with increasing s $(s > n)$.

---

* This work was supported by a Faculty Research Fellowship from the Research Foundation of State University of New York.

1 R. Yeh and A. Isihara, J. Chem. Phys. 51, 1215 (1969).

2 R. H. T. Yeh, J. Math. Phys. 11, 1521 (1970) and references therein. There are mistakes in Ref. 6 of this article: F should read $F - E_0$ and $\langle\psi|e^{-\beta H}|\psi\rangle$ should read $\langle\psi|e^{-\beta H'}|\psi\rangle$.