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Energy Spectrum According to Classical Mechanics

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The phase integral approximation for the Green's function is investigated so as to yield an approximate expression for the density of states per unit interval of energy. This quantity is shown for negative energies (bound states) to depend only on the periodic orbits, i.e., the smoothly closed trajectories, unlike the approximate wavefunctions which depend on all possible trajectories. A particle in a periodic box of one, two, and three dimensions is discussed first to demonstrate how the approximate density of states contains a continuous background besides the δ-function spikes of the discrete spectrum. Then we examine the situation in a spherically symmetric potential where special problems arise because the quasiclassical propagator has to be evaluated at a focal point of the classical trajectory. With the help of the Helmholtz–Kirchhoff formula of diffraction theory, the amplitude is shown to remain finite at the focus. The orbits which remain entirely in a region of Coulombic potential yield a spectrum of Balmer terms with appropriately reduced degeneracy. However, the orbits which penetrate the screening charge give discrete levels obeying the Bohr–Sommerfeld conditions with the correct degeneracy. The continuous background in the approximate density of states can be discussed on the basis of the formulas derived in this paper. This is necessary as an introduction to the problem of a particle in a potential where the motion is not multiply periodic.

INTRODUCTION

Most textbooks on quantum mechanics include a chapter where classical mechanics is shown to be the limit of quantum mechanics when Planck's quantum goes to zero. Examples are given to demonstrate the approximate validity of the quantization rules of Bohr and Sommerfeld. This fulfills the need to make quantum mechanics philosophically more acceptable, to recall its historical development, and to give an intuitive understanding for some of its most elementary results. Yet, the close relation between classical and quantum mechanics is hardly ever used to find approximate solutions of Schrödinger's equation except for the above purposes or in the very simplest situations.

It seemed, therefore, worthwhile to expand the scope of the phase-integral or WKB method and make it available as a method of approximation, particularly for finding the spectrum of a single particle bound in some electrostatic potential. After treating the hydrogen atom in a novel fashion,[1] it became clear that classical mechanics could indeed yield results which had been obtained previously only by solving Schrödinger's equation. On the other hand, it was shown in II that there were some unexpected features as soon as the spherically symmetric potential was not purely Coulombic. The spectrum seemed to contain not only the sharp spikes corresponding to bound states of well-defined energy, but also a relatively smooth background as if there was a continuum of states besides the discrete spectrum.

The purpose of this paper is to establish the existence of such a background in the most straightforward manner. That is not a very interesting goal in itself because this background represents something unphysical in the case of a spherically symmetric potential. It should simply be discarded as an artifact of the approximation which is of no consequence in view of the sharp spikes. There is, however, the possibility that the approximate spectrum of a particle in an anisotropic potential contains no sharp spikes because the classical motion is not multiply periodic. Yet, the spectrum might give information about the approximate energy eigenvalues exactly like any other resonance phenomenon which is broadened by some relaxation processes. It seemed very hard to investigate this idea before the much simpler case of a spherically symmetric potential was fully understood.

The problem is stated more explicitly in Sec. 1. Contrary to the previous papers, I and II, we give a formulation which gives us the approximate energy spectrum without the corresponding approximate eigenfunctions of the Hamiltonian. The method is illustrated first in Sec. 2 with two examples where the approximation happens to give the exact answers. A third example is discussed in Sec. 3, where most calculations can be performed fairly easily and the sharp spikes correspond to the exact results, but there is definitely a background, i.e., the approximate density of states does not consist only of δ functions.

The last four sections are devoted to the spherically symmetric case. It turns out that there are a number of technical difficulties to overcome which are due to the spherical symmetry. It is necessary to evaluate the approximate Green's function at a focus of the classical trajectories where the amplitude appears to be infinite at first glance. However, this problem is solved in Sec. 4 by a method which was used by

Debye for the corresponding task in optics. The approximate Green's function is integrated over all space in Sec. 5, where it is shown that only periodic orbits make a contribution to the spectrum. This result applies not only to a spherically symmetric potential, and may yield the first real generalization of the Bohr–Sommerfeld conditions.

Since a nucleus screened by a fairly well-localized charge cloud is the most interesting example, we have to discuss the effect of Kepler orbits which occur only in a limited range of energy and angular momentum. As shown in Sec. 6, this situation leads to a partial Balmer spectrum where each energy is less than n^2-fold degenerate. Finally, the sharp spikes are obtained in Sec. 7 for orbits which go through the screening charge and their strength is shown to correspond to the correct $(2l+1)$-fold degeneracy. Thus, the stage is set for a detailed calculation of the background in the density of states. It will be investigated in the following paper which is now in preparation.

1. NOTATIONS AND BASIC FORMULAS

The present paper is concerned with the approximate Green's function $\tilde{G}(q''q'E)$ of a single electron in three dimensions. The Green's function $G(q''q'E)$ is simply the probability amplitude for the particle to end up at the position q'' if it is known to have started at the position q' and was propagating with the energy E. The Hamiltonian has the ordinary form

$$H(pq) = (p^2/2m) + V(q) \tag{1}$$

with a spherically symmetric potential whose singularity at the origin $q = 0$ has the Coulomb form

$$V(q) \cong -Z_0e^2/r, \tag{2}$$

where $r = |q|$. We are interested in bound states and shall assume $E < 0$ henceforth.

In the classical limit, $G(q''q'E)$ is approximated by

$$\tilde{G}(q''q'E) = -\frac{1}{2\pi\hbar^2} \sum_{\substack{\text{classical}\\ \text{trajectories}}} |D_s|^{\frac{1}{2}} \times \exp i\left[\frac{S(q''q'E)}{\hbar}\text{-phases}\right], \tag{3}$$

where

$$S(q''q'E) = \int_{q'}^{q''} p\, dq \tag{4}$$

and D_s is the 4-by-4 determinant of second derivatives

$$D_s = \begin{vmatrix} \frac{\partial^2 S}{\partial q''\partial q'} & \frac{\partial^2 S}{\partial q''\partial E} \\ \frac{\partial^2 S}{\partial E\partial q'} & \frac{\partial^2 S}{\partial E^2} \end{vmatrix}. \tag{5}$$

The "phases" are given by $\frac{1}{2}\pi$ multiplied by the number of conjugate times along the trajectory.

In order to study the singularities of $G(q''q'E)$ along the energy axis, we start from the formula

$$G(q''q'E) = \sum_j \frac{\phi_j(q'')\phi_j^*(q')}{E - E_j}, \tag{6}$$

where $\phi_j(q)$ is the eigenfunction with label j and eigenvalue E_j of the Hamiltonian (1). After we have set $q'' = q'$ and integrated over the 3-dimensional coordinate space, we find that

$$\int d^3q G(qqE) = \sum_j (E - E_j)^{-1}. \tag{7}$$

This last formula can be written in an equivalent form if we use the well-known relation

$$(E + i\epsilon - E_j)^{-1} = P/(E - E_j) - i\pi \operatorname{sgn}\epsilon\,\delta(E - E_j), \tag{8}$$

where P is the Cauchy principal value and δ the Dirac δ function. The discontinuity $DG(q''q'E)$ of $G(q''q'E)$ across the real energy axis

$$DG(q''q'E) = \lim_{\epsilon\to 0}[G(q''q'(E + i\epsilon)) - G(q''q'(E - i\epsilon))] \tag{9}$$

has the spectrum

$$\int d^3q\, DG(qqE) = -2\pi i \sum_j \delta(E - E_j), \tag{10}$$

i.e., a δ-function singularity of strength $-2\pi i$ for each energy eigenvalue.

The question to be answered in this paper is the following: If we assume $G(q''q'E)$ to be given approximately by $\tilde{G}(q''q'E)$ as in formula (3), does the spectrum along the negative energy axis still have the simple appearance of formula (10) except that the energies E_j are to be replaced by approximate values $\tilde{E}_j$?

2. A TRIVIAL AND A SIMPLE EXAMPLE

In order to clarify the meaning of this question, two examples are discussed first where the answer is affirmative. The example of the next section is shown to yield a negative answer in spite of the simple relation to the two examples of this section. The reason for the different behavior is entirely in the dimensionality of the examples with two dimensions inherently more complicated than either one or three dimensions. Since the conditions are the same in each case, they will be described for all at the same time.

Consider a particle in a box of linear extent L, in either one, two, or three dimensions, with a constant potential (equal to zero) inside the box. Let us discuss

the situation when periodic boundary conditions are assumed, i.e., we have a torus of length L in each dimension and the standard Euclidean metric on it. The Hamiltonian is given by $H(pq) = p^2/2m$, and the action integral $S(q''q'E) = [2mE\,|q'' - q'|^2]^{\frac{1}{2}}$. The trajectories whose end point q'' coincides with the starting point q' are obtained from the condition $q_i'' = q_i' + n_iL$, where n_i are integers ranging from $-\infty$ to $+\infty$, with one such integer for each dimension.

The approximate Green's function is given by

$$\tilde{G}(q''q'E) = [m/i\hbar(2mE)^{\frac{1}{2}}] \exp\,[(i/\hbar)(2mE)^{\frac{1}{2}}\,|q'' - q'|] \quad (11)$$

for the free particle in one dimension. If this expression is summed over all closed trajectories and integrated over the box of length L, we find that

$$\begin{aligned}\int dqG(qqE) &= \frac{mL}{i\hbar(2mE)^{\frac{1}{2}}} \sum_{-\infty}^{+\infty} \exp\left[\frac{i}{\hbar}\,|n|\,L(2mE)^{\frac{1}{2}}\right] \\ &= \frac{mL}{\hbar(2mE)^{\frac{1}{2}}} \cot \frac{L(2mE)^{\frac{1}{2}}}{2\hbar} \\ &= \sum_{-\infty}^{+\infty} \frac{1}{E - (2k\pi\hbar/L)^2(2m)^{-1}}\,, \end{aligned} \quad (12)$$

which is the expected result. In this particular case, $\tilde{G}$ coincides with G. However, even if the approximate Green's function differs from the exact one, the geometric series always arises in one dimension and can be transformed into a series of the type (7) because of the partial-fraction expansion for cotangent.

In three dimensions the approximate Green's function

$$\tilde{G}(q''q'E) = -\frac{1}{2\pi\hbar^2}\frac{m}{|q'' - q'|} \times \exp\left[\frac{i}{\hbar}(2mE)^{\frac{1}{2}}\,|q'' - q'|\right] \quad (13)$$

for the free particle again coincides with the exact Green's function. The density of states $\int d^3qDG(qqE)$ for a particle in a 3-dimensional periodic box is obtained by evaluating the sum

$$-\frac{2\pi i}{(2\pi\hbar)^2} \sum_{n_1n_2n_3} \frac{2mL^2}{(n_1^2 + n_2^2 + n_3^2)^{\frac{1}{2}}} \times \sin\left(\frac{L[2mE(n_1^2 + n_2^2 + n_3^2)]^{\frac{1}{2}}}{\hbar}\right), \quad (14)$$

which includes the term $n_1 = n_2 = n_3 = 0$ correctly as $(n_1^2 + n_2^2 + n_3^2)^{\frac{1}{2}} = 0$.

This triple summation can be transformed into an expression like (7) with the help of the Fourier integral

$$\tilde{G}(q''q'E) = \frac{1}{(2\pi\hbar)^3} \int \frac{d^3p}{E - p^2/2m}\, e^{ip(q'' - q')/\hbar}. \quad (15)$$

We can insert $q_i'' = q_i' = n_iL$ and do the summation over all n_i under the integral sign. The exponential is thereby converted into a sum over products of δ functions, namely,

$$\sum \delta(\nu_1 - p_1L/2\pi\hbar)\delta(\nu_2 - p_2L/2\pi\hbar)\delta(\nu_3 - p_3L/2\pi\hbar),$$

where each ν runs from $-\infty$ to $+\infty$. The integration over p_1, p_2, and p_3 is trivial, and we find that

$$\int d^3qG(qqE) = \sum_{\nu_1\nu_2\nu_3} \left(E - \frac{(2\pi\hbar)^2}{2mL^2}(\nu_1^2 + \nu_2^2 + \nu_3^2)\right)^{-1}. \quad (16)$$

The spectrum is completely discrete, as indeed it should be when we happen to have the correct Green's function. It should be noted that, although the calculation in this case is quite simple, it cannot be generalized to arbitrary potentials as in the preceding example.

The Kepler problem is another example in three dimensions which leads to a completely discrete spectrum for the negative energies as was shown in I. The approximate Green's function $\tilde{G}$ is not equal to the exact one, however. The Coulomb potential is exceptional compared to other spherically symmetric potentials because of its discrete spectrum even in the quasiclassical approximation. This is undoubtedly due to the high degeneracy of its classical orbits.

3. A TYPICAL EXAMPLE

The approximate Green's function for a free particle in two dimensions is given by

$$\tilde{G}(q''q'E) = -\frac{e^{i\pi/4}}{(2\pi)^{\frac{1}{2}}}\frac{m}{\hbar^2} \times \left[\frac{(2mE)^{\frac{1}{2}}\,|q'' - q'|}{\hbar}\right]^{-\frac{1}{2}} \exp\left[\frac{i(2mE)^{\frac{1}{2}}\,|q'' - q'|}{\hbar}\right]; \quad (17)$$

This constitutes the asymptotic form for large distances $|q'' - q'|$ of the correct expression

$$G(q''q'E) = -(m/\pi\hbar^2)K_0([-2m(E + i\epsilon)]^{\frac{1}{2}}\,|q'' - q'|/\hbar), \quad (18)$$

where K_0 is the modified Bessel function of the second kind. It can be written as a Fourier integral exactly like (15), and we are led to a formula exactly like (16)

for the particle in a periodic box by the same argument.

It would seem futile to investigate what happens if the approximate Green's function $\tilde{G}$ is used instead of G, except to demonstrate what kind of new features are introduced into the density of states through the use of $\tilde{G}$ when it does not coincide with G. Therefore, we want to discuss the double sum

$$\int d^2q\tilde{G}(qqE) = -\frac{mL^2}{2\pi\hbar^2}\sum_{n_1n_2}{}' \frac{1}{[\eta(n_1^2+n_2^2)]^{\frac{1}{4}}} \times \exp\{2\pi i[\eta(n_1^2+n_2^2)]^{\frac{1}{2}} + \tfrac{1}{4}i\pi\}, \quad (19)$$

where $\eta = 2mL^2E/(2\pi\hbar)^2$ is the dimensionless energy. The prime in the summation sign indicates the omission of the term $n_1 = n_2 = 0$,which can be brought in only when $D\tilde{G}$ is calculated.

The singularities of this last sum can be found by the following argument. The infinite sum has no upper bound if a sufficient number of terms add up in phase. These terms have to be contiguous in the double sum since otherwise the intervening terms tend to destroy any "constructive interference." For large n_1 and n_2 the phase increase of the terms $n_1 \pm 1$ and $n_2 \pm 1$ can be approximated by the partial derivatives of

$$2\pi[\eta(n_1^2+n_2^2)]^{\frac{1}{2}}$$

with respect to n_1 and n_2. Thus, we get the conditions

$$\frac{\partial}{\partial n_1}[\eta(n_1^2+n_2^2)]^{\frac{1}{2}} = \nu_1,$$
$$\frac{\partial}{\partial n_2}[\eta(n_1^2+n_2^2)]^{\frac{1}{2}} = \nu_2, \quad (20)$$

where ν_1 and ν_2 are integers between $-\infty$ and $+\infty$ which do not vanish simultaneously. The two equations can be solved only if $\eta = \nu_1^2 + \nu_2^2$ or

$$E = \frac{\hbar^2}{2m}\left[\left(\frac{2\pi\nu_1}{L}\right)^2 + \left(\frac{2\pi\nu_2}{L}\right)^2\right]. \quad (21)$$

A detailed analysis is given in Appendix A to show that the sum (19) has a simple pole with residue 1 at the energy given by (21) for each pair of integers (ν_1, ν_2) excluding (0, 0).

The neighborhood of the origin in the complex E plane can be treated very simply because the sum (19) is approximated quite well for small η by the integral

$$-\frac{mL^2}{2\pi\hbar^2}\int d\xi_1\int d\xi_2 \frac{1}{[\eta(\xi_1^2+\xi_2^2)]^{\frac{1}{4}}} \times \exp\{2\pi i[\eta(\xi_1^2+\xi_2^2)]^{\frac{1}{2}} + \tfrac{1}{4}i\pi\}, \quad (22)$$

where none of the factors changes much when n_1 or n_2 change by 1. Since this integral converges at $\xi_1 = \xi_2 = 0$, the omission of the term $n_1 = n_2 = 0$ makes no difference. If we go to polar coordinates in the (ξ_1, ξ_2) plane and give E a positive imaginary part so as to obtain good convergence at infinity, the integral (22) is found to be $\pi/2(2)^{\frac{1}{2}}E$. If the integrand had been replaced by the correct Green's function (18), the integral would have been $1/E$ as expected. The approximate Green's function (17) gives a simple pole at $E = 0$ whose residuum is, however, equal to $\pi/2(2)^{\frac{1}{2}}$ rather than 1. We can understand this "mistake" from the fact that $\tilde{G}$ is not a good approximation of G for small energies; in fact, $\tilde{G}$ is too large for small E and can thus be expected to yield too large a residuum at $E = 0$.

The important question to answer is concerned with the behavior of (19) along the real E axis between the poles (21). If we want to apply brute force and evaluate the sum on a computer, we have to make it better convergent and preferably real. The latter is achieved by considering $\int d^2qD\tilde{G}(qqE)$ and the former by integrating over E from 0 to some open upper limit. The resulting expression represents the number N of eigenstates between 0 and this upper limit. After dividing out $-2\pi i$ and integrating by parts each term, we find the expression

$$N(\eta) = -\eta f(\eta) + \tfrac{1}{4}\int_0^\eta d\eta f(\eta), \quad (23)$$

$$f(\eta) = \frac{1}{\pi}\sum_{n_1n_2}{}' \frac{1}{[\eta(n_1^2+n_2^2)]^{\frac{3}{4}}} \times \cos\{2\pi[\eta(n_1^2+n_2^2)]^{\frac{1}{2}} + \tfrac{1}{4}\pi\}. \quad (24)$$

The conditionally convergent sum for (24) can be evaluated quite easily if we let the partial sums cover all the integer points in the (n_1, n_2) plane inside a square $|n_1| \leq l$, $|n_2| \leq l$. This way of summing constitutes a partial reordering of the terms as compared to partial sums where $(n_1^2+n_2^2)^{\frac{1}{2}} \leq l$, but the two methods are equivalent in this case.

It is shown in Appendix B that $f(\eta)$ has a power-series expansion whose leading term is $\eta^{-\frac{3}{4}}$, and the further terms are $\eta^{-\frac{1}{4}}$, $\eta^{+\frac{1}{4}}$, $\eta^{+\frac{3}{4}}$, $\cdots$, all with non-vanishing coefficients. Whereas the leading term does not contribute to $N(\eta)$, all the subsequent terms do so and constitute a convergent power series for $N(\eta)$ which is valid for $\eta < 1$. There is no doubt that the number of states $N(\eta)$ does not vanish between 0 and 1, although it goes to zero for small η, i.e., like $\eta^{\frac{3}{4}}$ with a negative coefficient. The density of states is given by the analogous power series

$$\frac{dN}{d\eta} = \frac{1}{2\pi\eta^{\frac{1}{4}}}\sum_0^\infty \frac{\Gamma(n+\frac{3}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{1}{2})\Gamma(n+1)}\delta_{n+\frac{3}{4}}\eta^n - \frac{1}{2\pi}\eta^{\frac{1}{4}}\sum_0^\infty \frac{\Gamma(n+\frac{5}{4})\Gamma(n+\frac{5}{4})}{\Gamma(n+\frac{3}{2})\Gamma(n+1)}\delta_{n+\frac{5}{4}}\eta^n. \quad (25)$$

The δ's are positive except $\delta_{\frac{1}{4}}$ (cf. Appendix B). The leading negative coefficient in (25) can be understood as a compensation for the too strong δ function of $dN/d\eta$ at $\eta = 0$.

The term $n_1 = n_2 = 0$ was omitted from (19) because the approximate Green's function (17) is obviously incorrect at $q'' = q'$ since it has a stronger singularity than the correct Green's function (18). The correct contribution for the exceptional "closed orbit of zero length" follows from

$$\lim_{q''\to q'} DG(q''q'E) = -i\frac{m}{\hbar^2}. \tag{26}$$

After dividing by $-2\pi i$ and integrating over the 2-dimensional box as well as over the energy from 0 to E, one gets the contribution $\pi\eta$ to $N(\eta)$ or simply π to $dN/d\eta$. Therefore, we have to add π to the expansion (25) in order to obtain the complete density of states in the interval $0 < \eta < 1$.

The expansion (25) is useful only for small values of η, whereas η should cover the interval from 0 out to ∞. It is quite hard to find further information about the analytical behavior of $dN/d\eta$. We have, therefore, resorted to evaluating the expression which follows directly from (19),

$$\begin{aligned}\frac{dN}{d\eta} &= \frac{i}{2\pi}\frac{(2\pi\hbar)^2}{2mL^2}\int d^2q\, D\tilde{G}(qqE)\\ &= \pi + \sum_{n_1,n_2}{}' \frac{1}{[\eta(n_1^2+n_2^2)]^{\frac{1}{2}}}\\ &\quad\times \sin\{2\pi[\eta(n_1^2+n_2^2)]^{\frac{1}{2}} + \tfrac{1}{4}\pi\},\end{aligned} \tag{27}$$

on a computer. The series can be made convergent with the help of Cesaro sums, i.e., averaging over the successive partial sums. The result as shown in Fig. 1 is remarkably smooth and small (compared to 1) outside the neighborhood of the critical values $\eta = (\nu_1^2 + \nu_2^2)^{\frac{1}{2}}$.

The discontinuous behavior near $\eta = (\nu_1^2 + \nu_2^2)^{\frac{1}{2}}$ can be understood if we subtract from (27) all the δ functions. This can be done in the present simple case because we know the exact Green's function of the problem. In particular, we have from $DG(q''q'E) = -i(m/\hbar^2)J_0[(2mE)^{\frac{1}{2}}|q'' - q'|/\hbar]$ the Poisson formula

$$\sum_{\nu_1\nu_2}\delta[\eta - (\nu_1^2+\nu_2^2)^{\frac{1}{2}}] = \pi\sum_{n_1n_2} J_0\{2\pi[\eta(n_1^2+n_2^2)]^{\frac{1}{2}}\}. \tag{28}$$

If (28) is subtracted from (27), we can apply the asymptotic formula for J_0 on the right-hand side to find

$$\frac{dN}{d\eta} - \sum_{\nu_1\nu_2}\delta[\eta - (\nu_1^2+\nu_2^2)^{\frac{1}{2}}] = \tfrac{1}{16}f(\eta) + \cdots. \tag{29}$$

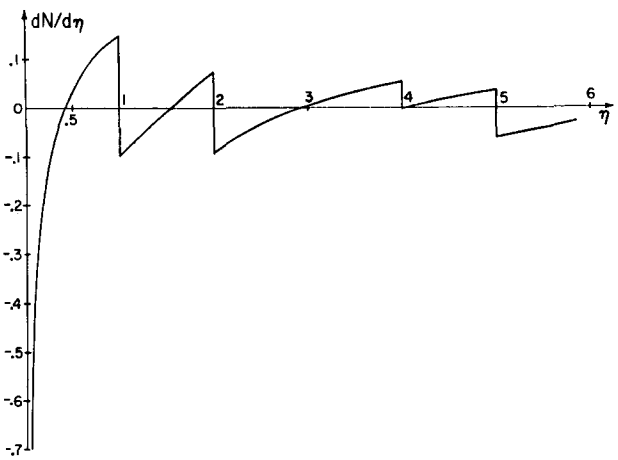

FIG. 1. The density of states (27) for a particle in a 2-dimensional periodic box according to classical mechanics after subtracting the δ-function spikes at $\eta = 1, 2, 4$, and 5 which correspond to the exact quantum states. The integral over these δ functions equals 4 for $\eta = 1, 2, 4$, and 8 for $\eta = 5$. The normalized energy η is given by $2mL^2E/(2\pi\hbar)^2$.

The omitted terms are sums like (24) and (27) with the $\frac{5}{4}$ power of $\eta(n_1^2 + n_2^2)$ and higher in the denominator. These omitted terms are, therefore, continuous at $\eta = (\nu_1^2 + \nu_2^2)^{\frac{1}{2}}$, whereas $f(\eta)$ decreases discontinuously by $4/\eta$ or $8/\eta$ according to the number of pairs (ν_1, ν_2) with $\eta = (\nu_1^2 + \nu_2^2)^{\frac{1}{2}}$. (Cf. Appendix B.)

Although it is not practical to evaluate the right-hand side of (29), one can make the following strong statement about the part of $dN/d\eta$ which is not contained in the δ-function singularities. Its integral from 0 to ∞ vanishes. Indeed, if we take the difference between the right-hand sides of (27) and (28), we can integrate term by term. The integral over the difference between terms with the same n_1 and n_2 is given by

$$\int_0^\infty d\eta\left(\frac{\sin[2\pi\mu(\eta)^{\frac{1}{2}} + \pi/4]}{[\mu(\eta)^{\frac{1}{2}}]^{\frac{1}{2}}} - \pi J_0[2\pi\mu(\eta)^{\frac{1}{2}}]\right) = 0, \tag{30}$$

where we have abbreviated $\mu = (n_1^2 + n_2^2)^{\frac{1}{2}}$. Although the approximate density of states $dN/d\eta$ does not vanish between the δ-function singularities, its integral vanishes. The approximate Green's function does not introduce any "new states" with a continuous distribution in addition to the discrete states.

4. THE VALUE OF $\tilde{G}$ WHEN $q'' = q'$

A number of technical difficulties have to be overcome which arise from the rotational symmetry of the problem in general and from the Coulomb potential in particular. We shall assume first that $V(q)$ is not purely Coulombic in any region of measure greater than zero. But this assumption will be dropped later on because we want to include the physically significant

case where $V(q)$ arises from the partial screening of the nucleus by an electronic charge cloud.

The first term in (3) is given by the Thomas–Fermi approximation (cf. I)

$$\tilde{G}(q''q'E) \cong -\frac{m}{2\pi\hbar^2 |q''-q'|} \times \exp\{i|q''-q'|[2m(E-V(q))]^{\frac{1}{2}}/\hbar\}, \quad (31)$$

where $q = \frac{1}{2}(q''+q')$. This expression is singular at $q''=q'$, but the singularity is not a consequence of the phase-integral approximation $\tilde{G}$. The exact Green's function G has the same behavior as q'' approaches q' because G solves the inhomogeneous Schrödinger equation with $\delta(q''-q')$ on the right-hand side.

The discontinuity of both (31) and G across the real energy axis remains finite. By taking the difference between (31) and its complex conjugate, we find that

$$D\tilde{G}(q''q'E) \cong -i\frac{m}{\pi\hbar^2|q''-q'|} \times \sin\{|q''-q'|[2m(E-V(q))]^{\frac{1}{2}}/\hbar\}. \quad (32)$$

This expression is valid only when $V(q) < E$. If q'' approaches q', the result is $-2\pi i m[2m(E-V(q))]^{\frac{1}{2}}/2\pi^2\hbar^3$, for $V(q) < E$ and zero elsewhere. Therefore, we find

$$\int d^3q\, D\tilde{G}(qqE) \cong -2\pi i \int d^3q \frac{m}{2\pi^2\hbar^3}[2m(E-V(q))]^{\frac{1}{2}} \quad (33)$$

for the contribution of the first term in (3) to the spectrum as defined in (10).

The remaining terms in (3) arise from a trajectory which carries the electron from q' to q'' and which does not shrink to zero as q'' approaches q'. The amplitude factor is given by the expression

$$D_s = \frac{M}{r'r''\sin\phi}\frac{m}{[2mr'^2(E-V(r'))-M^2]^{\frac{1}{2}}} \times \frac{m}{[2mr''^2(E-V(r''))-M^2]^{\frac{1}{2}}}\left(\frac{\partial\phi}{\partial M}\right)^{-1}, \quad (34)$$

where M is the angular momentum of the trajectory from q' to q'' and ϕ is the polar angle swept out in the orbital plane. As q'' approaches q', the angle ϕ goes to a multiple of 2π and we can write

$$\phi = 2\lambda\pi - \int_{r''}^{r'} \frac{dr}{r}\frac{M}{[2m(E-V(r))-M^2]^{\frac{1}{2}}}, \quad (35)$$

where r'' is assumed to approach r' from below. For the other possible circumstances, (35) has to be modified correspondingly. The derivative $\partial\phi/\partial M$ in (34) is to be taken at constant r' and r''.

If (34) is inserted into (3), it is quite obvious that one cannot go to the limit $q'' \to q'$ because of the factor $(\sin\phi)^{-\frac{1}{2}}$. This singularity does not disappear in DG as did the previous one, because the phase factor in (3) is just about arbitrary, i.e., depending on the whole trajectory from q' to q''. The origin of the singularity is the convergence of all the trajectories which left q' in different planes with the same angular momentum M. The end point $q''=q'$ is a focus for the trajectories of given energy E through q' because of the rotational symmetry. The lowest order of approximation for G in powers of $\hbar$ breaks down and has to be replaced locally by going to a higher order.

The point q' is enclosed by a volume W of rotational symmetry around the straight line from the origin to q'. The surface Σ of this volume is assumed to be many wavelengths $2\pi\hbar[2mr^2(E-V)]^{-\frac{1}{2}}$ away from q', yet the diameter of this surface is assumed to be small with respect to the distance r' from the origin. The expression (3) for the particular trajectory of interest is, therefore, a good approximation on Σ, but not inside. Thus, we can apply Green's formula (generally called the integral formula of Helmholtz and Kirchhoff in diffraction theory[2])

$$u(q'') = \frac{1}{4\pi}\oint d\Sigma\left(u(q)\frac{\partial v}{\partial n} - v(q)\frac{\partial u}{\partial n}\right) \quad (36)$$

in the following manner. Here u represents the two terms in (3) which are close to a particular trajectory with $q''=q'$. In one term, the trajectory has not crossed the line from 0 to q' (incoming wave); in the other, it has crossed that line and has lost an extra phase $\pi/2$ (outgoing wave). The values of u on Σ can easily be computed because the trajectories inside W differ very little from straight lines. The function v propagates the incoming and outgoing waves from the points q on Σ to q'' in the neighborhood of q'. Thus, $v(q''q')$ is given to a sufficient approximation by the Thomas–Fermi expression (31).

The evaluation of (36) presents no further difficulties. The integration over Σ is done by the stationary phase method. The details are worked out in Appendix C. For each trajectory with $q''=q'=q$, we get the contribution

$$-\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\frac{M}{\hbar}\frac{m}{r[2mr^2(E-V)-M^2]^{\frac{1}{2}}}\left|\frac{\partial\phi}{\partial M}\right|^{-\frac{1}{2}} \times \exp i\left(\frac{S(qqE)}{\hbar} - \frac{\pi}{4}\text{-phases}\right) \quad (37)$$

to $\tilde{G}(qqE)$, where the "phases" come from the conjugate points before the end point. If we had worked out the same formula in two dimensions only, the

factor $M/\hbar$ would be missing from (37). The rotational symmetry in three dimensions introduces the degeneracy given by $M/\hbar$.

5. THE SUMMATION OVER CLOSED ORBITS

With the help of the expression (37), we can now evaluate the integrals (7) or (10) for the approximate Green's function $\tilde{G}(q''q'E)$. We shall consider each term in the summation (3) over the classical trajectories separately, leaving out the first term which has been discussed already. In order to perform the integration over r, we have to introduce a more detailed discussion about the limits of integration for a given energy E and angular momentum M.

If the screening electron cloud is fairly well concentrated in a thin shell around the nucleus, the function

$$R(r) = [2mr^2(E - V(r))]^{\frac{1}{2}}$$

has a local minimum $\bar{r}$ inside the screening region. The corresponding angular momentum $\bar{M} = R(\bar{r})$ is called the critical angular momentum because for $M > \bar{M}$ the classical trajectories remain either entirely inside $\bar{r}$ or entirely outside. The equation $2mr^2(E - V(r)) = \bar{M}^2$ has two further solutions $\bar{r}_1 < \bar{r} < \bar{r}_2$. Thus for $M < \bar{M}$ there is only one pair of solutions $r_1 < \bar{r}_1 < \bar{r}_2 < r_2$ for the equation $2mr^2(E - V(r)) = M^2$, whereas for $M > \bar{M}$ the same equation has two such pairs, an "inner" pair with $\bar{r}_1 < r_1 < r_2 < \bar{r}$ and an "outer" pair with $\bar{r} < r_1 < r_2 < \bar{r}_2$. Finally, we call r_0 the radius for which $V(r) = E$.

The trajectories have been further classified in II so as to determine the number of conjugate points between q' and q''. This classification is not needed here because of the following crucial observation, which eliminates about half of the possible trajectories from our present investigation. Since $q'' = q'$, the absolute values of the momenta at the beginning and at the end are equal, i.e., $|p'| = |p''| = [2m(E - V)]^{\frac{1}{2}}$. Since the angular momentum M is constant along the trajectory, the components of p' and p'' perpendicular to $q'' = q'$ are equal. Therefore the components of p' and p'' parallel to $q'' = q'$ are either equal or the negative of each other.

Now consider the integral over (37) for a particular trajectory which starts at $q' = q$ and ends at $q'' = q$. As q moves through the volume of integration, the action integral $S(qqE)$ changes, and its rate of change with respect to q is given by

$$\frac{\partial S(qqE)}{\partial q} = \frac{\partial S(q''qE)}{\partial q''}\bigg|_{q''=q} + \frac{\partial S(qq'E)}{\partial q'}\bigg|_{q'=q} = p'' - p'. \tag{38}$$

The phase in (37) is constant provided $p'' = p'$; otherwise it changes at a rate given by twice the radial component of the momentum. In the former case the trajectory is a closed (periodic) orbit; in the latter case the trajectory is closed but not smooth since its direction changes abruptly at q.

If the expression (37) is integrated for a trajectory which does not close itself smoothly, the phase factor varies rapidly with the end point q. In the limit of small $\hbar$, the contribution from such a trajectory is negligible compared to the contribution from a closed (periodic) orbit whose phase factor remains constant throughout. The spectrum is, therefore, determined by the periodic orbits only, although the wavefunctions are made up of both types of trajectories, as was shown in II. This rule should be quite generally valid because the arguments that went into its proof used only formula (38) and the conservation of energy. If we recall the interpretation of the trajectories as geodesics in a Riemannian manifold, particularly in momentum space (cf. II), the importance of the closed geodesics for the spectrum becomes a very attractive feature.

Since only periodic orbits are of interest, we need to know only the integral

$$\gamma(E, M) = \int_{r_1}^{r_2} \frac{dr}{r} \frac{M}{[2mr^2(E - V) - M^2]^{\frac{1}{2}}}, \tag{39}$$

which gives the polar angle swept by the particle between its minimum and maximum distance from the origin. According to (35), the condition for periodicity is

$$2\nu\gamma = 2\lambda\pi, \tag{40}$$

where λ and ν are positive integers. In other words, the angular momentum M has to be chosen such as to make $\gamma(E, M)$ a rational part of π. For $M < \bar{M}$ there is only one value for γ, whereas for $M > \bar{M}$ there are two values, an inner and an outer one. All of these values for γ become infinite near $\bar{M}$, but we shall leave the discussion of the details to a later section. Each closed orbit arising from condition (40) has to be counted twice, because the radial component $p'' = p' = p$ at $q'' = q' = q$ can be negative or positive, although the shape of the orbit is exactly the same.

The number of conjugate points has been discussed in II, and we refer the reader to that paper for the relevant arguments. For the trajectories of interest in this work, the rule is simple. If $(\partial\gamma/\partial M)_E > 0$, there are $2\nu + 2\lambda - 1$ conjugate points, whereas if

$$(\partial\gamma/\partial M)_E < 0,$$

there are only $2\nu + 2\lambda - 2$. If we introduce again the

radial action integral

$$\omega(E, M) = \int_{r_1}^{r_2} \frac{dr}{r} [2mr^2(E - V) - M^2]^{\frac{1}{2}} \quad (41)$$

and the total action integral

$$\theta(E, M) = \omega(E, M) + M\gamma(E, M), \quad (42)$$

we can write the contribution from each periodic orbit to the approximate Green's function $\tilde{G}(qqE)$ as

$$-(2\pi\hbar^3)^{-\frac{1}{2}} \frac{2M}{\hbar} \frac{m}{r[2mr^2(E - V) - M^2]^{\frac{1}{2}}} \left| 2\nu \frac{\partial\gamma}{\partial M} \right|^{-\frac{1}{2}} \times \exp i(2\nu\theta/\hbar - \nu\pi - \lambda\pi - \operatorname{sgn} \dot{\gamma} \cdot \pi/4), \quad (43)$$

where $\dot{\gamma}$ is an abbreviation for $(\partial\gamma/\partial M)_E$.

It is now easy to integrate over all space, i.e., all the space which is covered by the particular orbit of energy E and angular momentum M. After multiplying (43) with $4\pi r^2\, dr$ and integrating from r_1 to r_2, we find that the factor $m/r[2mr^2(E - V) - M^2]^{\frac{1}{2}}$ is replaced by $4\pi(\partial\omega/\partial E)_M$. If we leave out the first term (31) in the summation (3) over the classical trajectories, we can now write

$$\int d^3q \tilde{G}(qqE) = -\frac{4\pi i}{(2\pi\hbar^3)^{\frac{1}{2}}} \sum_{\lambda,\nu>0} \frac{2M}{\hbar} \left(\frac{\partial\omega}{\partial E}\right)_M \left| 2\nu \left(\frac{\partial\gamma}{\partial M}\right)_E \right|^{-\frac{1}{2}} \times \exp i(2\nu\theta/\hbar - \nu\pi - \lambda\pi - \operatorname{sgn} \dot{\gamma} \cdot \pi/4). \quad (44)$$

The factor $(\partial\omega/\partial E)_M$ has a simple physical interpretation. Since $[2m(E - V) - M^2/r^2]^{\frac{1}{2}}$ is the radial component of the momentum, $(\partial\omega/\partial E)_M$ is the integral over dr divided by the radial component of the velocity. Therefore, $2\nu(\partial\omega/\partial E)_M$ is the period of the periodic orbit. We have to insert the factor ν because, if λ and ν in (40) have no common divisor, it takes ν radial periods to make the polar angle a multiple of 2π.

6. THE CONTRIBUTION OF THE KEPLER ORBITS

The assumptions about the spherically symmetric potential $V(q)$ will be relaxed henceforth so as to include a purely Coulombic region as follows:

$$V(r) = -\frac{e^2}{r} - e^2 \int_r^b \frac{Z(r) - 1}{r^2}\, dr, \quad \text{for} \quad r < b,$$
$$= -\frac{e^2}{r}, \quad \text{for} \quad r > b. \quad (45)$$

The screening charge $Z(r) - 1$ contained in a sphere of radius r is assumed to be strictly decreasing so as to avoid any other purely Coulombic region except $r > b$.

The distance r_1 of closest approach is given by solving the equation $2mr^2(E - V(r)) = M^2$. If there are two pairs of solutions, we shall concern ourselves only with the outer pair in this section. Therefore, M^2 has to be larger than $M_b^2 = 2mb^2(E + e^2/b)$ for the trajectory to remain entirely in the Coulombic region $r > b$. For $M < M_b$ there is precession, i.e., $\gamma(E, M) > \pi$, and it is important to know how γ depends on M for $M_b - M \ll M_b$. The following will be shown in the Appendix D. If the screening charge can be expanded in powers of $b - r$ for $r < b$, and the initial term in such an expansion is given by

$$Z(r) - 1 \cong c(b - r)^\alpha, \quad \text{for} \quad r < b, \quad (46)$$

then the precession for $M_b - M \ll M_b$ behaves as

$$\gamma(E, M) \cong \pi + a(1 - M/M_b)^{\alpha+\frac{1}{2}}, \quad \text{for} \quad M < M_b. \quad (47)$$

Notice that (46) includes the case $\alpha = 0$, where the screening charge decreases discontinuously at $r = b$ so that we need a charged thin shell to do the screening. We shall assume that $\alpha \geq 1$ henceforth. Even the case $\alpha = 1$ corresponds to the screening charge inside the radius b starting with a nonvanishing density, whereas one would rather expect the screening charge density to vanish at $r = b$ in a continuous manner.

The behavior of the trajectories near a point q with $|q| = r > b$ can be visualized with the help of Fig. 2. As in Sec. 4 we consider a neighborhood of q which is small enough to neglect the curvature of the trajectories. In a plane through the origin and q, we introduce the local coordinates $q_\parallel$ in the radial direction and $q_\perp$ perpendicular to $q_\parallel$. A trajectory of angular momentum M is represented by a straight line whose angle θ with the $q_\parallel$ axis is given by $M = R \sin\theta$, where $R^2 = 2mr^2(E - V(r))$. This straight line intersects the $q_\perp$ axis at $q_\perp = 2\lambda r(\gamma - \pi)$, where λ is the number of "turns" the particle has completed before reaching the neighborhood of q. For $M > M_b$, i.e., $\sin\theta > \sin\beta = R/M_b$ or $\beta < \theta < \pi - \beta$, all the trajectories go through q as in a perfect focus. For $M < M_b$, i.e., $0 < \theta < \beta$ and $\pi - \beta < \theta < \pi$, the trajectories are tangent to a focal line.

The integral formula (36) is applied to a volume W with surface Σ which completely surrounds the focus at $q_\parallel = q_\perp = 0$. The propagation function v in (36) is again approximated by the Thomas–Fermi expression (31), and u is given by the semiclassical formula (3) on the surface Σ. We investigate the particular terms of (3) which correspond to λ complete "turns." For $M > M_b$ the particle will have accumulated an action

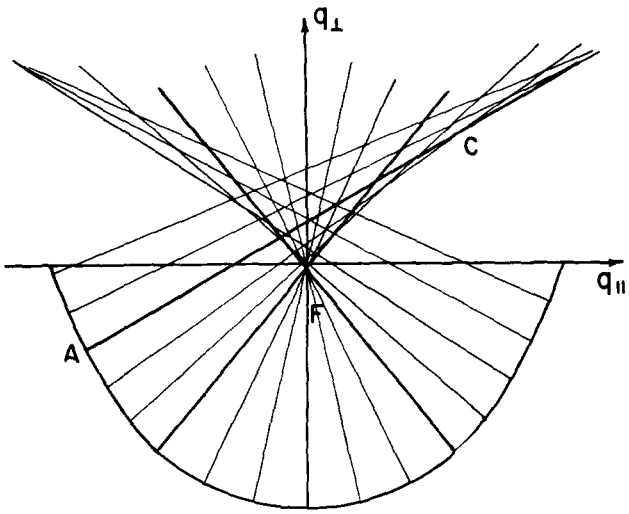

FIG. 2. Schematic picture of the classical trajectories converging onto their point of departure if the latter lies outside the screening charge. For large angular momentum, the trajectories are periodic and go through a focus. For small angular momentum, the trajectories dip into the screening charge and have some precession which leads to a focal line.

integral equal to $2\lambda\pi(me^4/2\,|E|)^{\frac{1}{2}}$ upon reaching the focus. Since it follows from (39), (41), and (42) that

$$\theta(E, M) = \int_M^{\bar{R}_2} \gamma(E, M')\, dM' + M\gamma(E, M), \quad (48)$$

we find for a particle with $M < M_b$ that

$$\theta(E, M) = 2\lambda\pi\left(\frac{me^4}{2\,|E|}\right)^{\frac{1}{2}} + 2\lambda a\left(1 - \frac{M}{M_b}\right)^{\alpha+\frac{1}{2}} M \quad (49)$$

using (47). The upper limit of integration $\bar{R}_2$ in (48) is the value of $R(r)$ at the outer maximum $\bar{r}_2$ of $R(r)$. Before reaching the neighborhood W, all the trajectories have lost a total of $(2\lambda - 1)\pi$ in phases at various conjugate times. The trajectories with $M > M_b$ lose an additional π upon traversing the focus. The trajectories with $M < M_b$ lose $\pi/2$ when crossing the $q_\parallel$ axis and another $\pi/2$ when passing the focal line. Since (49) gives the action integral when the trajectory reaches the $q_\perp$ axis, we have to add (or subtract) ps for any other point where $p = [2m(E - V(r))]^{\frac{1}{2}}$ and s is the distance along the trajectory from the point where the $q_\perp$ axis is reached.

The detailed discussion of the Helmholtz–Kirchhoff integral is greatly simplified because we are only interested in the leading term of an expansion in inverse powers of h. The shape of Σ can be chosen such as to allow any trajectory at most two points of intersection with Σ. Thus we can clearly distinguish between incoming and outgoing waves. The focal line is made of outgoing waves and does not contribute to the amplitude at the focus any more than the rest of the outgoing waves. The incoming waves are made up of the Keplerian trajectories inside the solid angle $\beta < \theta < \pi - \beta$ and the trajectories with precession outside. The latter contribute to the amplitude at the focus in an amount proportional to $h^{-3+1/(2\alpha+1)}$, as will be shown in Appendix E. On the other hand, the Kepler orbits through q contribute

$$-\frac{m}{\pi\hbar^3}\left(2m(E - V) - \frac{M_b^2}{r^2}\right)^{\frac{1}{2}} \exp i\left(\frac{2\lambda\theta}{\hbar} + \tfrac{1}{2}i\pi\right) \quad (50)$$

to $G(qqE)$ which is, therefore, the leading term if $r > b$. Formula (44) shows that a closed orbit with precession makes a contribution proportional to $\hbar^{-\frac{1}{2}}$, whereas (50) has a factor $\hbar^{-3}$. The difference can be explained if we recall that a closed orbit with precession makes a focus with a 1-parameter family of trajectories, but there is a 2-parameter family of Kepler orbits with $M > M_b$ leading to a higher degeneracy.

The expression (50) can now be integrated over the space where $2mr^2(E - V) > M_b^2$. The result is

$$-2\pi i\,\frac{m}{\hbar^3}\left(b + \frac{e^2}{2E}\right)^2\left(\frac{me^4}{2\,|E|}\right)^{\frac{1}{2}} \exp\left[\frac{2\lambda\pi i}{\hbar}\left(\frac{me^4}{2\,|E|}\right)^{\frac{1}{2}}\right]. \quad (51)$$

Although we assume that $\lambda > 0$ and integer, it is convenient to include a term $\lambda = 0$ when we compute $\int d^3q D\tilde{G}(qqE)$. We can think of this additional term as part of (33), namely, the part coming from the Coulombic region $r > b$. Then we can write

$$\begin{aligned}\int d^3q\, D\tilde{G}(qqE) &= -2\pi i\,\frac{m}{\hbar^3}\left(b + \frac{e^2}{2E}\right)^2\left(\frac{me^4}{2\,|E|}\right)^{\frac{1}{2}} \sum_{\lambda=-\infty}^{+\infty} \\ &\quad \times \exp\left[\frac{2\lambda i\pi}{\hbar}\left(\frac{me^4}{2\,|E|}\right)^{\frac{1}{2}}\right] \\ &= -2\pi i\left(1 + \frac{2bE}{e^2}\right)^2\left(-\frac{me^4}{2E\hbar^2}\right)\sum_{n=1}^{\infty}\delta\left(E + \frac{me^4}{2n^2\hbar^2}\right)\end{aligned} \quad (52)$$

for the Coulomb part of the spectrum.

The energy eigenvalues are given by the Bohr formula, but their multiplicity is reduced from n^2 to $n^2(1 + 2bE/e^2)^2$. Since b is essentially arbitrary, provided $b < e^2/2\,|E|$, we have here an instance where the degeneracy of an approximate eigenvalue is not an integer. The orbits which do not dip into the screening charge are still quantized by the same rules as the hydrogen atom. These are the orbits with large angular momentum whose quantum defect is small. Their share among all orbits of a given energy E increases with E.

7. THE POLES ALONG THE NEGATIVE-ENERGY AXIS

The contributions from the Kepler orbits are completely accounted for by (52). Formula (44) can now be used to find the contributions from the precessing orbits separately. According to the condition (40), each periodic orbit is described by two integers, λ and ν, so that (44) is a summation over these two integers. The spherical symmetry (hidden in the factor $2M/\hbar$) is responsible for making (44) very similar to formula (19) for the 2-dimensional box. It is, therefore, not surprising that the poles of (44) can be found in much the same manner as the poles of (19) were located in (20) and Appendix A.

The integers λ and ν of (40) will be treated as independent variables which are only subject to certain inequalities such as $\lambda > \nu$ because $\gamma > \pi$. Furthermore, γ has certain upper limits which depend on the energy E. For E small enough so that

$$R(r) = [2mr^2(E - V(r))]^{\frac{1}{2}}$$

has no local minimum, the precession γ reaches a finite upper limit. However, for E large enough to allow $R(r)$ to have a local minimum $\bar{M}$ at $\bar{r}$, the precession γ becomes infinite as M approaches $\bar{M}$. For values of M close to $\bar{M}$, there are three possible orbits, all with large precession γ, one orbit with $M < \bar{M}$ and two with $M > \bar{M}$ (cf. Sec. 5). Each of these three orbits gives rise to a pair (λ, ν) whose ratio varies in the corresponding range.

If the energy E is given, the ratio λ/ν determines the angular momentum M of the periodic orbit through (40) for each of the possible types of trajectories. It is, therefore, natural to consider $\gamma = \lambda\pi/\nu$ as independent variable instead of M and to rewrite the action integrals ω and θ as functions of E and γ, rather than E and M. It follows from (39) and (41) that

$$\left(\frac{\partial\omega}{\partial M}\right)_E = -\gamma \tag{53}$$

and with the help of (42) that

$$\left(\frac{\partial\theta}{\partial E}\right)_\gamma = \left(\frac{\partial\omega}{\partial E}\right)_M. \tag{54}$$

Similarly, we find the formulas

$$\left(\frac{\partial\theta}{\partial\gamma}\right)_E = M(E, \gamma), \tag{55}$$

$$\left(\frac{\partial^2\theta}{\partial\gamma^2}\right)_E = \left(\frac{\partial M}{\partial\gamma}\right)_E = \left[\left(\frac{\partial\gamma}{\partial M}\right)_E\right]^{-1}. \tag{56}$$

The formula (44) can now be written as

$$\int d^3q\tilde{G}(qqE) = -\frac{8\pi i}{(2\pi\hbar^5)^{\frac{1}{2}}}\sum_{\lambda,\nu}\frac{\partial\theta}{\partial\gamma}\frac{\partial\theta}{\partial E}\left|\frac{1}{2\nu}\frac{\partial^2\theta}{\partial\gamma^2}\right|^{\frac{1}{2}} \times \exp i\left[\frac{2\nu\theta}{\hbar} - \nu\pi - \lambda\pi - \operatorname{sgn}\left(\frac{\partial^2\theta}{\partial\gamma^2}\right)\cdot\frac{\pi}{4}\right], \tag{57}$$

where only the total action θ as defined in (42), but now considered as function of E and γ, occurs.

The argument which led to the condition (20) can now be applied exactly as in Sec. 3. The sum (57) becomes singular when contiguous terms are in phase. The phase angle $2\nu\theta/\hbar - \nu\pi - \lambda\pi$ depends on λ and ν directly and indirectly through $\gamma = \lambda\pi/\nu$. Its increase upon changing λ to $\lambda + 1$ or ν to $\nu + 1$ is well represented by its partial derivatives with respect to λ or ν when λ and ν are large. If we set these derivatives equal to $2l\pi$ and $2n\pi$, we get with the help of (55) and (42) the quantum conditions

$$M = (l + \tfrac{1}{2})\hbar, \qquad \omega = (n + \tfrac{1}{2})2\pi\hbar, \tag{58}$$

in agreement with II.

In order to find the behavior of (57) for energies E close to the energy defined by (58), we proceed as follows. Define $\bar{\gamma}(E)$ as the value of (39) for $M = (l + \frac{1}{2})\hbar$. Moreover, define $\bar{\lambda}$ for arbitrary ν according to (40) by $\bar{\lambda} = \nu\bar{\gamma}/\pi$. The phase $2\nu\theta/\hbar - \nu\pi - \lambda\pi$ in (57) is a function of λ and ν which can be expanded in powers of $(\lambda - \bar{\lambda})$. If we indicate with $\bar{\theta}$ and $\bar{\omega}$ the values of θ and ω for $\bar{\gamma}$, the phase factor in (57) becomes

$$\exp i\left[\nu\left(\frac{2\bar{\omega}}{\hbar} - \pi\right) + \frac{\pi^2}{\nu\hbar}\frac{\partial^2\theta}{\partial\gamma^2}(\lambda - \bar{\lambda})^2 - \operatorname{sgn}\left(\frac{\partial^2\theta}{\partial\gamma^2}\right)\cdot\frac{\pi}{4}\right], \tag{59}$$

where powers higher than $(\lambda - \bar{\lambda})^2$ are neglected because they would have a correspondingly higher power of ν in the denominator. The second derivative $\partial^2\theta/\partial\gamma^2$ in the last term of (59) is assumed to have the same sign for all values of λ which contribute effectively. Similarly, the variation of the amplitude factor in (57) with λ is neglected, and the various factors are replaced by their value for $M = (l + \frac{1}{2})\hbar$. Since the singularity is determined by the terms with large ν, the summation of (59) over λ can be replaced by the corresponding integral. Thus, the expression (57) becomes

$$\int d^3q\tilde{G}(qqE) \cong -\frac{2i}{\hbar}\sum_{\nu>0}(2l + 1)\left(\frac{\partial\bar{\omega}}{\partial E}\right)_M \exp i\nu\left(\frac{2\bar{\omega}}{\hbar} - \pi\right) = (2l + 1)\frac{1}{\hbar}\frac{\partial\bar{\omega}}{\partial E}\left(i + \sum_n \frac{\hbar}{\bar{\omega} - (n + \frac{1}{2})\pi\hbar}\right). \tag{60}$$

The poles in (60) all have the residue $(2l+1)$ in accordance with the degeneracy of the angular momentum $M=(l+\frac{1}{2})\hbar$. The factor $\hbar^{-1}\partial\bar{\omega}/\partial E$ converts the pole $\hbar/[\bar{\omega}-(n+\frac{1}{2})\pi\hbar]$ into a pole $(E-E_{l,n})^{-1}$, where the energy $E_{l,n}$ is determined by (58).

APPENDIX A

Suppose that $|\nu_2|\leq|\nu_1|$ in (20). The values of n_1 and n_2 which are responsible for the singularity lie closer to the n_1 axis than to the n_2 axis. For any fixed values of n_1 and η, we can define the real (rather than integer) $\bar{n}_2=\nu_2|n_1|(\eta-\nu_2^2)^{-\frac{1}{2}}$ so that

$$\frac{\partial}{\partial\bar{n}_2}[\eta(n_1^2+\bar{n}_2^2)]^{\frac{1}{2}}=\nu_2.$$

The phase angle in (19) is expanded in powers of $n_2-\bar{n}_2$. Up to second-order terms,

$$2\pi[\eta(n_1^2+n_2^2)]^{\frac{1}{2}}=2\pi|n_1|(\eta-\nu_2^2)^{\frac{1}{2}}+\pi(\eta)^{\frac{1}{2}}\left(1-\frac{\nu_2^2}{\eta}\right)^{\frac{3}{2}}\frac{(n_2-\bar{n}_2)^2}{|n_1|}. \tag{A1}$$

Higher-order terms in $(n_2-\bar{n}_2)$ are neglected because they have correspondingly higher powers of $|n_1|$ in the denominator. Since the singularity comes from the buildup of many terms, the large values of $|n_1|$ are important. The summation over n_2 is well represented by the corresponding integral, where we replace n_2 by $\bar{n}_2$ in the amplitude factor. Thus we find that

$$\sum_{n_2}\frac{1}{[\eta(n_1^2+n_2^2)]^{\frac{1}{4}}}\exp\{2\pi i[\eta(n_1^2+n_2^2)]^{\frac{1}{2}}\}\cong\frac{1}{(\eta-\nu_2^2)^{\frac{1}{4}}}\exp[2\pi i|n_1|(\eta-\nu_2^2)^{\frac{1}{2}}+i\pi/4] \tag{A2}$$

with the help of Fresnel's integral.

The last formula is obviously incorrect for small $|n_1|$, but it is convenient to keep the expression (A2) even for small $|n_1|$ in order to get a simple expression for the singularities. Thus, we find, by adding over all n_1, the simple sequence of expressions

$$\begin{aligned}-\frac{mL^2}{2\pi\hbar^2}\sum_{n_1n_2}{}'\frac{1}{[\eta(n_1^2+n_2^2)]^{\frac{1}{4}}}\exp\{2\pi i[\eta(n_1^2+n_2^2)]^{\frac{1}{2}}+i\pi/4\}&\cong-i\frac{mL^2}{2\pi\hbar^2}\frac{1}{(\eta-\nu_2^2)^{\frac{1}{2}}}\sum_{n_1}\exp[2\pi i|n_1|(\eta-\nu_2^2)^{\frac{1}{2}}]\\&=\frac{mL^2}{2\pi\hbar^2}\frac{1}{(\eta-\nu_2^2)^{\frac{1}{2}}}\operatorname{cotg}\pi(\eta-\nu_2^2)^{\frac{1}{2}}\\&=\frac{mL^2}{2\pi^2\hbar^2}\left(\frac{1}{\eta-\nu_2^2}+2\sum_{\nu_1>0}\frac{1}{\eta-\nu_1^2-\nu_2^2}\right)\\&=\sum_{-\infty}^{+\infty}\left(E-\frac{2\pi^2\hbar^2}{mL^2}(\nu_1^2+\nu_2^2)\right)^{-1}.\end{aligned} \tag{A3}$$

In this manner the singularities for a given ν_2 are found, provided $|\nu_2|\leq|\nu_1|$. All the other singularities can be found in a similar fashion, except $\nu_1=\nu_2=0$.

APPENDIX B

In order to transform $f(\eta)$ by the analog of Poisson's formula, we need the Fourier transform

$$\begin{aligned}\int dx_1\int dx_2(x_1^2+x_2^2)^{-\frac{3}{4}}&\times\exp[-2\pi i(x_1y_1+x_2y_2)-2\pi\xi(x_1^2+x_2^2)^{\frac{1}{2}}]\\&=2\pi\int_0^\infty\rho^{-\frac{1}{2}}\,d\rho J_0(2\pi\rho\sigma)\exp(-2\pi\xi\rho)=I(\sigma,\xi),\end{aligned} \tag{B1}$$

where $\rho=(x_1^2+x_2^2)^{\frac{1}{2}}$ and $\sigma=(y_1^2+y_2^2)^{\frac{1}{2}}$. We shall always deduce from I the Fourier transform I_c which is obtained if $\exp[-2\pi\xi(x_1^2+x_2^2)^{\frac{1}{2}}]$ is replaced by $\pi^{-1}\eta^{-\frac{3}{4}}\cos\{2\pi[\eta(x_1^2+x_2^2)]^{\frac{1}{2}}+\pi/4\}$ so that

$$I_c(\sigma,\eta)=\frac{1}{2\pi\eta^{\frac{3}{4}}}\{e^{+i\pi/4}I[\sigma,-i(\eta)^{\frac{1}{2}}]+e^{-i\pi/4}I[\sigma,+i(\eta)^{\frac{1}{2}}]\}. \tag{B2}$$

Without relating I to any of the standard transcendental functions, we can find an integral representation with the help of the Mellin transforms[3]

$$\int_0^\infty J_0(2\pi\rho\sigma)\rho^{s-1}\,d\rho=2^{s-1}\Gamma(s/2)/[(2\pi\sigma)^s\Gamma(1-s/2)],\quad\text{for } 0<\operatorname{Re}s<\tfrac{3}{2},$$

$$\int_0^\infty\rho^{-\frac{1}{2}}e^{-2\pi\xi\rho}\rho^{s-1}\,d\rho=\Gamma(s-\tfrac{1}{2})/(2\pi\xi)^{s-\frac{1}{2}},\quad\text{for } \operatorname{Re}s>\tfrac{1}{2}.$$

Parseval's formula for Mellin transforms gives

$$I(\sigma,\xi)=\frac{1}{i}\int ds\,\frac{\Gamma(s-\frac{1}{2})}{(2\pi\xi)^{\frac{1}{2}-s}}\frac{2^{s-1}\Gamma(s/2)}{(2\pi\sigma)^s\Gamma(1-s/2)}, \tag{B3}$$

where the integral is to be taken along a parallel to the imaginary axis in the strip $0<\operatorname{Re}s<\frac{1}{2}$.

With the help of the duplication formula[4]

$$2^{2z-1}\Gamma(z)\Gamma(z+\tfrac{1}{2})=(\pi)^{\frac{1}{2}}\Gamma(2z),$$

the last integral becomes, after changing the variable of integration from s to $t=-s/2$,

$$I(\sigma,\xi)=\xi^{-\frac{1}{2}}\frac{1}{2\pi i}\int dt\,\frac{\Gamma(t+\frac{1}{4})\Gamma(t+\frac{3}{4})\Gamma(-t)}{\Gamma(t+1)}\left(\frac{\sigma}{\xi}\right)^{2t}, \tag{B4}$$

where $-\frac{1}{4}<\operatorname{Re}t<0$. Thus, $I(\sigma,\xi)$ is a hypergeometric function, as can be seen by pulling the contour

of integration to the right across the poles of $\Gamma(-t)$:

$$I(\sigma, \xi) = \xi^{-\frac{1}{2}} \sum_0^\infty \frac{\Gamma(n+\frac{1}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+1)\Gamma(n+1)}\left(-\frac{\sigma^2}{\xi^2}\right)^n. \quad \text{(B5)}$$

This series converges for $|\sigma^2/\xi^2| < 1$ and leads to $I_c(\sigma, \eta) = 0$ for $\sigma^2 < \eta$.

A series which converges in the range $|\sigma^2/\xi^2| > 1$ can be obtained by pulling the contour in (B4) to the left across the poles of $\Gamma(t+\frac{1}{4})$ and $\Gamma(t+\frac{3}{4})$:

$$I(\sigma, \xi) = (2\sigma)^{-\frac{1}{2}} \sum_0^\infty \frac{\Gamma(n+\frac{1}{4})\Gamma(n+\frac{1}{4})}{\Gamma(n+\frac{1}{2})\Gamma(n+1)}\left(-\frac{\xi^2}{\sigma^2}\right)^n$$
$$- (2\sigma)^{-\frac{1}{2}} \sum_0^\infty \frac{\Gamma(n+\frac{3}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{3}{2})\Gamma(n+1)}\left(-\frac{\xi^2}{\sigma^2}\right)^n \frac{\xi}{\sigma}. \quad \text{(B6)}$$

The corresponding expansion for $I_c(\sigma, \eta)$ is given by

$$I_c(\sigma, \eta) = \frac{1}{2\pi\sigma^{\frac{1}{2}}\eta^{\frac{3}{4}}} \sum_0^\infty \frac{\Gamma(n+\frac{1}{4})\Gamma(n+\frac{1}{4})}{\Gamma(n+\frac{1}{2})\Gamma(n+1)}\left(\frac{\eta}{\sigma^2}\right)^n$$
$$- \frac{1}{2\pi\sigma^{\frac{3}{2}}\eta^{\frac{1}{4}}} \sum_0^\infty \frac{\Gamma(n+\frac{3}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{3}{2})\Gamma(n+1)}\left(\frac{\eta}{\sigma^2}\right)^n, \quad \text{(B7)}$$

which converges in the range $\sigma^2 > \eta$. For a given σ the Fourier transform $I_c(\sigma, \eta)$ is discontinuous as a function of η, since it vanishes identically for $\eta > \sigma^2$.

The value of $I_c(\sigma, \eta)$ as η approaches σ^2 from below can be obtained with the help of Barnes' lemma,[5] which gives the integral

$$I(\sigma, \xi) = \frac{1}{\pi(2\xi)^{\frac{1}{2}}}$$
$$\times \frac{1}{2\pi i}\int dt\,\Gamma(t+\tfrac{1}{4})\Gamma(t+\tfrac{3}{4})\Gamma(-t)\Gamma(-t)\left(1+\frac{\sigma^2}{\xi^2}\right)^t, \quad \text{(B8)}$$

where again $-\frac{1}{4} < \operatorname{Re} t < 0$. If the contour of integration is pushed across the double pole to $\frac{1}{2} < \operatorname{Re} t < 1$, the remaining contour integral can be shown to vanish faster than $|1 + \sigma^2/\xi^2|^{\frac{1}{2}}$ as ξ^2 tends to $-\sigma^2$. The contribution from the double pole is found to be

$$-\xi^{-\frac{1}{2}}\left[\psi(\tfrac{1}{4}) + \psi(\tfrac{3}{4}) - 2\psi(1) + \log\left(1+\frac{\sigma^2}{\xi^2}\right)\right]. \quad \text{(B9)}$$

Whereas $I(\sigma, \xi)$ has a logarithmic infinity as ξ^2 tends to $-\sigma^2$, $I_c(\sigma, \eta)$ remains finite as η tends to σ^2 from below. If we insert $\xi = \pm i(\eta)^{\frac{1}{2}}$ into the above expression, we find that

$$\log(1 + \sigma^2/\xi^2) = \pm i\pi + \log(-1 + \sigma^2/\eta)$$

and $\xi^{-\frac{1}{2}} = \eta^{-\frac{1}{4}} \exp(\pm i\pi/4)$. Therefore, it follows that

$$\lim_{\eta \to \sigma^2} I_c(\sigma, \eta) = \frac{1}{\sigma^2}. \quad \text{(B10)}$$

More generally, we obtain for $\eta < \sigma^2$ the expansion

$$I_c(\sigma, \eta) = \frac{1}{\eta} \sum_0^\infty \frac{\Gamma(n+\frac{1}{4})\Gamma(n+\frac{3}{4})}{\Gamma(\frac{1}{4})\Gamma(\frac{3}{4})n!\,n!}\left(1-\frac{\sigma^2}{\eta}\right)^n. \quad \text{(B11)}$$

The expansion (B7) converges rapidly for $0 < \eta \leq \sigma^2/2$, and the expansion (B11) in the range $\sigma^2/2 \leq \eta \leq \sigma^2$.

The function $f(\eta)$ can now be evaluated in the form

$$f(\eta) = \sum_{n_1 n_2}{}' \int dy_1 \int dy_2 I_c[(y_1^2 + y_2^2)^{\frac{1}{2}}, \eta] e^{2\pi i(n_1 y_1 + n_2 y_2)}$$
$$= \sum_{\nu_1 \nu_2} I_c[(\nu_1^2 + \nu_2^2)^{\frac{1}{2}}, \eta] - \int dy_1 \int dy_2 I_c[(y_1^2 + y_2^2)^{\frac{1}{2}}, \eta]. \quad \text{(B12)}$$

Since $I_c(\sigma, \eta) = 0$, for $\sigma^2 < \eta$, the term $\nu_1 = \nu_2 = 0$ never appears, and the integral covers only the area $y_1^2 + y_2^2 > \eta$ in the (y_1, y_2) plane. An inspection of the two series in (B7) reveals that both the summation and the integration in (B12) do not converge for the terms $n = 0$, although there is no problem with the terms $n > 0$. On the other hand, it is clear that the difference between the sum and the integral remains finite provided the variables of summation and of integration go to ∞ in the same way.

For this purpose, let us do the integration over the region in the (y_1, y_2) plane which is bounded by the square $|y_1| < \omega$, $|y_2| < \omega$. The terms in (B7) with $n = 0$ converge at the origin of the (y_1, y_2) plane but not at ∞, whereas the terms with $n > 0$ converge at ∞ but not at the origin. Therefore, we calculate the integrals $Q(\nu, \omega)$ given by

$$\int_{|y_1|<\omega} dy_1 \int_{|y_2|<\omega} dy_2 \frac{1}{(y_1^2 + y_2^2)^\nu}, \quad \text{for } \nu < 1,$$
$$\int_{|y_1|>\omega} dy_1 \int_{|y_2|>\omega} dy_2 \frac{1}{(y_1^2 + y_2^2)^\nu}, \quad \text{for } \nu > 1. \quad \text{(B13)}$$

In both cases we have the simple formulas

$$\frac{\partial Q}{\partial \omega} = \pm 8 \int_0^\omega \frac{dy}{(y^2+\omega^2)^\nu} = \pm \frac{8}{\omega^{2\nu-1}} \int_0^1 \frac{dz}{(1+z^2)^\nu} \quad \text{(B14)}$$

with the upper (lower) sign for $\nu < 1$ ($\nu > 1$). We have also the "initial" condition $Q(\nu, 0) = 0$ for $\nu < 0$ and $Q(\nu, \infty) = 0$ for $\nu > 1$. Thus, we find

$$Q = \pm 4\gamma_\nu \frac{\omega^{2(1-\nu)}}{1-\nu} \quad \text{with} \quad \gamma_\nu = \int_0^1 \frac{dz}{(1+z^2)^\nu}. \quad \text{(B15)}$$

The "constant" γ_ν is obtained by expanding the integrand

$$\gamma_\nu = \sum_0^\infty \frac{\nu(\nu+1)\cdots(\nu+n-1)}{1\cdot 2\cdots n}\frac{(-1)^n}{2n+1} = F(\nu, \tfrac{1}{2}; \tfrac{3}{2}; -1), \tag{B16}$$

which converges for $\nu < 2$. There seems to be no obvious way to reduce the last expression to simpler functions.

It is now possible to evaluate the integral

$$\int_{\nu_1^2+\nu_2^2>\eta} d\nu_1 \int_{|\nu_1|<\omega, |\nu_2|<\omega} d\nu_2 \frac{1}{(\nu_1^2+\nu_2^2)^\nu} = \frac{\pi}{\nu-1}\eta^{1-\nu} + \frac{4\gamma_\nu}{1-\nu}\omega^{2(1-\nu)} \tag{B17}$$

for all $\nu > 0$ with the exception of $\nu = 1$. Therefore, after inserting (B17), the integral in (B12) consists of a term which comes from the first part of (B17) and is given by

$$\sum_0^\infty \frac{\Gamma(n-\frac{3}{4})\Gamma(n+\frac{1}{4})}{\Gamma(n+\frac{1}{2})\Gamma(n+1)} - \sum_0^\infty \frac{\Gamma(n-\frac{1}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{3}{2})\Gamma(n+1)} = 0$$

and a term from the second part of (B17) which is given by

$$+\frac{2}{\pi}\sum_0^\infty \frac{\Gamma(n-\frac{3}{4})\Gamma(n+\frac{1}{4})}{\Gamma(n+\frac{1}{2})\Gamma(n+1)}\gamma_{n+\frac{1}{4}}\left(\frac{\eta}{\omega^2}\right)^{n-\frac{3}{4}} - \frac{2}{\pi}\sum_0^\infty \frac{\Gamma(n-\frac{1}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{3}{2})\Gamma(n+1)}\gamma_{n+\frac{3}{4}}\left(\frac{\eta}{\omega^2}\right)^{n-\frac{1}{4}}. \tag{B18}$$

If ω is allowed to go to ∞, all terms except $n = 0$ vanish. The terms $n = 0$, however, diverge, and one has to proceed more cautiously.

Each term in (B18) behaves for large ω as the corresponding term in the sum over ν_1 and ν_2 of (B12) when $|\nu_1| \le \omega$ and $|\nu_2| \le \omega$. Therefore, we can write

$$f(\eta) = \frac{1}{2\pi\eta^{\frac{3}{4}}}\sum_0^\infty \frac{\Gamma(n+\frac{3}{4})\Gamma(n+\frac{1}{4})}{\Gamma(n+\frac{1}{2})\Gamma(n+1)}\delta_{n+\frac{1}{4}}\eta^n - \frac{1}{2\pi\eta^{\frac{1}{4}}}\sum_0^\infty \frac{\Gamma(n+\frac{3}{4})\Gamma(n+\frac{3}{4})}{\Gamma(n+\frac{3}{2})\Gamma(n+1)}\delta_{n+\frac{3}{4}}\eta^n, \tag{B19}$$

where the coefficients δ_ν are defined as the difference

$$\delta_\nu = \lim_{\omega\to 0}\left[\sum\left(\begin{matrix}\nu_1^2+\nu_2^2>\eta \\ |\nu_1|<\omega,\quad |\nu_2|<\omega\end{matrix}\right) \times \frac{1}{(\nu_1^2+\nu_2^2)^\nu} - \frac{4\gamma_\nu}{1-\nu}\omega^{2(1-\nu)}\right] \tag{B20}$$

and ω is assumed to have only half-integer values. If $\nu > 1$, the second term in (B2) can be omitted because the sum over ν_1 and ν_2 converges all by itself.

The choice of half-integer values for ω is motivated by the following consideration. The second term in (B20) represents the integral (B13) which can be written as a sum of terms

$$\int_{\nu_1-\frac{1}{2}}^{\nu_1+\frac{1}{2}} d\nu_1 \int_{\nu_2-\frac{1}{2}}^{\nu_2+\frac{1}{2}} d\nu_2 \frac{1}{(\nu_1^2+\nu_2^2)^\nu}, \tag{B21}$$

provided ω is a half-integer. This integral can be evaluated if we expand the integrand in a Taylor series around $\nu_1 = \nu_1$ and $\nu_2 = \nu_2$. The first two terms of the resulting series are given by

$$1/(\nu_1^2+\nu_2^2)^\nu + \nu^2/12(\nu_1^2+\nu_2^2)^{\nu+1} + \cdots. \tag{B22}$$

As ω increases, the contribution from the first term in (B22) cancels the successive terms in the summation over ν_1 and ν_2 in (B20). We are left, therefore, with a sum over ν_1 and ν_2 of the second term in (B22) which converges for $\nu > 0$ as ω goes to ∞. All δ_ν are expected to be well-defined real numbers which will have to be evaluated on a computer, however. It follows from the above argument that $\delta_\nu < 0$, for $\nu < 1$, and $\delta_\nu > 0$, for $\nu > 1$.

The values for γ_ν are as follows: $\gamma_{\frac{1}{4}} = 0.93748975$, $\gamma_{\frac{3}{4}} = 0.83089621$, $\gamma_{\frac{5}{4}} = 0.744303$, and $\gamma_{\frac{7}{4}} = 0.673368$. The resulting values of δ are given by $\delta_{\frac{1}{4}} = -1.917$, $\delta_{\frac{3}{4}} = -10.077$, $\delta_{\frac{5}{4}} = 15.23807$, $\delta_{\frac{7}{4}} = 7.00987$, $\delta_{\frac{9}{4}} = 5.45641$, $\delta_{\frac{11}{4}} = 4.83917$, etc., for $\eta < 1$ in (B19).

APPENDIX C

A small volume W around q' is chosen with a shape like a football whose axis of rotation coincides with the straight line from the origin to q'. The surface Σ of W is described by two parameters, σ and ψ, if we write $q = [q_\perp(\sigma)\cos\psi, q_\perp(\sigma)\sin\psi, q' + q_\parallel(\sigma)]$, where $-1 \le \sigma \le +1$ and $0 \le \psi \le 2\pi$. The z axis has been chosen along the direction through q', and $q_\perp(\sigma) \ge 0$. The football shape of W is convenient because it allows none of the trajectories of interest to intersect Σ more than twice. That excludes the case where $M = 0$, but it will turn out that there is no contribution from such trajectories anyway.

For the present purpose we can approximate

$$\begin{aligned} S(qq'E) &= S(q'q'E) - p'(q-q'), \quad \text{incoming wave,} \\ &= S(q'q'E) + p'(q-q'), \quad \text{outgoing wave,} \end{aligned} \tag{C1}$$

where $p' = hk(\sin\theta\cos\psi, \sin\theta\sin\psi, \cos\theta)$ is the momentum of the trajectory through q' in the plane of longitude ψ around the z axis. The propagating function $v(q''q)$ inside W is approximated by

$$v(q''q) = \frac{1}{|q''-q|}e^{ik|q''-q|}, \tag{C2}$$

where $k = [2m(E - V(q'))/\hbar]^{\frac{1}{2}}$. Obviously v is the simplified expression for the Thomas–Fermi approximation (31). In both (C1) and (C2) the trajectories have been approximated by straight lines.

Apart from a factor $-(2\pi\hbar^2)^{-1}$, the function u in the Helmholtz–Kirchhoff formula (36) is defined by

$$|D_s|^{\frac{1}{2}} \exp i[S(qq'E)/\hbar\text{-phases}],$$

where D_s and $S(qq'E)$ are given by (34) and (C1). Obviously, all the factors in $|D_s|^{\frac{1}{2}}$ can be replaced by their value at q' with the exception of $(\sin\phi)^{-\frac{1}{2}}$. Since ϕ is small, we can write $r \sin\phi \cong q_\perp$. Finally,we have to discuss the effect of $\partial/\partial n$, the derivative along the inward normal on Σ upon u and v. If $\partial/\partial n$ acts on the phase factor of u or v, it introduces a factor $\sim k$; if $\partial/\partial n$ acts on the amplitude of u or v, a factor $\sim |q - q'|^{-1}$ appears. We shall assume that the latter is negligible with respect to the former, i.e., that the radius of W is many wavelengths $2\pi/k$.

After all these approximations we are left with

$$-\frac{1}{2\pi\hbar^2}\left(\frac{M}{r'^2}\frac{m^2}{2mr^2(E - V(r')) - M^2}\left|\frac{\partial\phi}{\partial M}\right|^{-1}\right)^{\frac{1}{2}} \times \exp i\left[\frac{1}{\hbar}S(q'q'E)\text{-phases}\right] \times \frac{1}{4\pi}\oint\frac{d\Sigma}{|q - q'|}\left(\frac{r}{q_\perp}\right)^{\frac{1}{2}}\left(ik\frac{(n, q - q')}{|q - q'|} \pm i\frac{(p', n)}{\hbar}\right) \times \exp[ik|q - q'| \mp ip'(q - q')/\hbar], \quad \text{(C3)}$$

where the upper sign is valid for the incoming wave and the lower sign for the outgoing wave. In the latter case we also have to add the phase-loss factor $\exp(-i\pi/2)$. If we insert $(q_\perp^2 + q_\parallel^2)^{\frac{1}{2}}$ for $|q - q'|$ and $k(q_\perp \sin\theta + q_\parallel \cos\theta)$ for $p'(q - q')/\hbar$, we recognize immediately that the phase factor becomes stationary only for the incoming wave, namely,when $(q_\perp, q_\parallel) = (q_\perp^2 + q_\parallel^2)^{\frac{1}{2}}(\sin\theta, \cos\theta)$.

The outgoing wave does not contribute to the value of the approximate Green's function G at the focus $q'' = q'$. The evaluation of the integral for the incoming wave by the stationary phase method follows the standard procedure. The phase vanishes at the stationary value σ_0, and its second derivative there with respect to σ is given by

$$\Phi = k(q_\perp^2 + q_\parallel^2)^{-\frac{3}{2}}\left(q_\perp\frac{dq_\parallel}{d\sigma} - q_\parallel\frac{dq_\perp}{d\sigma}\right)^2. \quad \text{(C4)}$$

The integration over ψ is trivial so that we are left with the integration over σ:

$$-ik\int d\sigma\frac{(rq_\perp)^{\frac{1}{2}}}{q_\perp^2 + q_\parallel^2}\left(q_\perp\frac{dq_\parallel}{d\sigma} - q_\parallel\frac{dq_\perp}{d\sigma}\right) \times \exp i[\Phi(\sigma - \sigma_0)^2/2]. \quad \text{(C5)}$$

If $q_\parallel$ increases monotonically from some negative to some positive value as σ goes from -1 to $+1$, the factor $q_\perp\, dq_\parallel/d\sigma - q_\parallel\, dq_\perp/d\sigma$ remains always positive. The integral becomes $-i(2\pi kr\sin\theta)^{\frac{1}{2}}\exp(+i\pi/4)$ after inserting $q_\perp = \sin\theta(q_\perp^2 + q_\parallel^2)^{\frac{1}{2}}$. Finally we use the fact that $M = rp\sin\theta = rhk\sin\theta$ to get the simple result $(2\pi M/\hbar)^{\frac{1}{2}}\exp(-i\pi/4)$ for (C5) and the second line of (C3). The formula (37) follows at once.

APPENDIX D

The integral in (45) can be evaluated with the help of the first term (46) of an expansion in powers of $(b - r)$. Thus, the potential in $r < b$ differs from $-e^2/r$ by

$$\int_r^b\frac{Z(r) - 1}{r^2}dr \cong\int_r^b\frac{c(b - r)^\alpha}{[b - (b - r)]^2}dr = c\left(\frac{(b - r)^{\alpha+1}}{(\alpha + 1)b^2} + 2\frac{(b - r)^{\alpha+2}}{(\alpha + 2)b^3} + \cdots\right). \quad \text{(D1)}$$

The integral (39) is worked out by choosing a variable of integration which imitates the Coulomb potential. We define $\rho = r$ for $r > b$, and

$$2mr^2(E - V(r)) = 2m\rho^2(E + e^2/\rho)$$

for $r < b$ as long as the approximation (D1) is valid. The angle of precession is then given by

$$\gamma(E, M) = \int_{\rho_1}^{\rho_2}\frac{dr}{r}\frac{M}{[2m\rho^2(E + e^2/\rho) - M^2]^{\frac{1}{2}}}, \quad \text{(D2)}$$

where ρ_1 and ρ_2 are the solutions of

$$2m\rho^2(E + e^2/\rho) = M^2.$$

It follows from (D1) that

$$r = \rho - \frac{c(b - \rho)^{\alpha+1}}{(\alpha + 1)(1 + 2Eb/e^2)} + \cdots, \quad \text{for} \quad \rho < b, \quad \text{(D3)}$$

$$\frac{dr}{r} = \left(1 + \frac{c(b - \rho)^\alpha}{1 + 2Eb/e^2} + \cdots\right)\frac{d\rho}{\rho} \quad \text{(D4)}$$

in the range $\rho_1 < \rho < b$, whereas $dr/r = d\rho/\rho$ in $b < \rho$.

The further manipulations are straightforward. With a new variable τ with

$$\rho = \frac{e^2}{2|E|}\left(1 - \epsilon\frac{1 - \tau^2}{1 + \tau^2}\right), \quad \text{(D5)}$$

and $\epsilon^2 = 1 + 2M^2E/me^4$, we find that

$$\frac{d\rho}{\rho}\frac{M}{2m\rho^2(E + e^2/\rho) - M^2} = 2\left(\frac{1 + \epsilon}{1 - \epsilon}\right)^{\frac{1}{2}}\frac{d\tau}{1 + (1 + \epsilon)\tau^2/(1 - \epsilon)}. \quad \text{(D6)}$$

The limit of integration τ_b corresponding to $\rho = b$ is given by the expression

$$\tau_b = [2E(M^2 - M_b^2)/me^4]^{\frac{1}{2}}(1 + \epsilon + 2Eb/e^2)^{-1}, \quad \text{(D7)}$$

and the quantity $b - \rho$ can be written as

$$b - \rho = \left(\frac{\epsilon e^2}{|E|}\right)\frac{\tau_b^2 - \tau^2}{(1 + \tau^2)(1 + \tau_b^2)}. \quad \text{(D8)}$$

The lower limit of integration ρ_1 becomes simply $\tau = 0$, and $\tau_b \ll 1$ as long as $M_b^2 - M^2 \ll M_b^2$. Therefore, we can neglect the denominator in (D8) in the range $\rho_1 < \rho < b$ where the second term of (D4) appears. The right-hand side of (D6) is integrated from 0 to $+\infty$ and yields π, whereas the correction due to the second term in (D4) becomes

$$2\left(\frac{1 + \epsilon}{1 - \epsilon}\right)^{\frac{1}{2}}\frac{c}{1 + 2bE/e^2}\left(\frac{\epsilon e^2}{|E|}\right)^{\alpha}\tau_b^{2\alpha+1}\int_0^{\tau_b}\frac{d\tau}{\tau_b}\left(1 - \frac{\tau^2}{\tau_b^2}\right)^{\alpha}. \quad \text{(D9)}$$

The last integral over τ is given by $\Gamma(\frac{1}{2})\Gamma(\alpha + 1)/2\Gamma(\alpha + \frac{3}{2})$. All the factors remain obviously finite and nonvanishing as $M \to M_b$ with the exception of $\tau_b^{2\alpha+1}$, which leads to (47).

APPENDIX E

It is evident from Fig. 2 and (47) that the trajectories through W with $M < M_b$ are given by the equations

$$q_{\parallel} = s\cos\theta,$$
$$q_{\perp} = 2\lambda ra\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha+\frac{1}{2}} + s\sin\theta, \quad \text{(E1)}$$

where s is the distance along the trajectory as measured from its intersection with the $q_{\perp}$ axis. The caustic is obtained by a standard calculation as

$$(q_{\parallel}, q_{\perp}) = 2\lambda ra\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha+\frac{1}{2}} \times \left[(0, 1) + \frac{(\alpha + \frac{1}{2})\cos^2\theta}{\sin\beta - \sin\theta}(\cos\theta, \sin\theta)\right]. \quad \text{(E2)}$$

Since θ is the angle of the tangent to the envelope, its radius of curvature $\tilde{R}$ is immediately obtained from the formula $d\sigma = \tilde{R}\,d\theta$, where $d\sigma$ is the distance between two corresponding points of (E2). Thus, we get

$$\tilde{R} = \frac{(2\alpha + 1)\lambda ra}{\sin\beta}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha-\frac{1}{2}} \times \left(\frac{(\alpha - \frac{1}{2})\cos^3\theta}{\sin\beta - \sin\theta} + 3\sin\theta\cos\theta\right). \quad \text{(E3)}$$

In the case of a thin shell ($\alpha = 0$), the radius of curvature goes to ∞ as $\theta \to \beta$; this remains true even for a nonvanishing screening charge density at $r = b$ when $\alpha = 1$. For $\alpha > \frac{3}{2}$, however, $\tilde{R}$ vanishes at $\theta = \beta$ because the precession is small and the trajectories remain almost focused.

Let us now consider a line of constant phase in the $(q_{\parallel}, q_{\perp})$ plane. In the region $\beta < \theta < \pi - \beta$ it will be a circle of radius ρ around the focus with the phase integral $2\lambda\pi(me^4/2|E|)^{\frac{1}{2}} - p\rho$. In the regions $\theta < \beta$ and $\pi - \beta < \theta$ we have to determine s for (E1) such that adding ps to (49) gives again $2\lambda\pi(me^4/2|E|)^{\frac{1}{2}} - p\rho$ as for $\beta < \theta < \pi - \beta$. Therefore,

$$s = -\rho - 2\lambda ar\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha+\frac{1}{2}}\sin\theta. \quad \text{(E4)}$$

The distance ρ' of the corresponding point A from the focus F is easily worked out as long as θ is close to β or $\pi - \beta$, and we have to retain only the lowest power in $(\sin\beta - \sin\theta)$:

$$\rho' = \rho + 2\frac{\lambda^2 a^2 r^2}{\rho}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{2\alpha+1}\cos^2\theta + \cdots. \quad \text{(E5)}$$

The difference between ρ' and ρ is responsible for the destructive interference of the incoming waves from outside the solid angle $\beta < \theta < \pi - \beta$.

The element of area $d\Sigma$ in the surface of constant phase can be obtained from its curvature, which is the inverse of the distance AC along the trajectory to its contact C with the caustic. This last distance equals ρ plus the length FC of the caustic from the focus F to the point of contact C. From (E2) we find for the length FC the leading term

$$\frac{(2\alpha + 1)\lambda ra}{\sin\beta}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha-\frac{1}{2}}\cos^2\theta. \quad \text{(E6)}$$

If θ is used as variable of integration in Σ, we have

$$d\Sigma = 2\pi\sin\theta\,d\theta \times \left[\rho + \frac{(2\alpha + 1)\lambda ra}{\sin\beta}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha-\frac{1}{2}}\cos^2\theta^2\right]. \quad \text{(E7)}$$

We can choose W as in Appendix C such that only the terms where $\partial/\partial n$ acts on the phase factor are important in the lim $\hbar \to 0$. Also, the directions of the normal n and of the vector toward the focus differ only an amount of order $(\beta - \theta)$.

The amplitude of the incoming wave according to (34) has $(\sin\phi\partial\phi/\partial M)^{\frac{1}{2}}$ in the denominator where

$$\sin\phi \cong \phi \cong -q_{\perp}/r \quad \text{(E8)}$$

and we have to insert (E1) with (E4). The derivative $\partial\phi/\partial M$ is to be taken at constant r' and r'', i.e., at

constant q''. If (E8) is expressed in terms of q'' and M, the derivative $\partial\phi/\partial M$ follows at once. Thus, we find

$$D_s \cong \frac{m^2}{\rho}\left[\rho + \frac{(2\alpha+1)\lambda a r}{\sin\beta}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha-\frac{1}{2}}\cos^2\theta\right]^{-1} \tag{E9}$$

for the amplitude squared of the incoming wave if we retain only the leading terms in $(\sin\beta - \sin\theta)$. In both (E7) and (E9) the second term can be neglected compared to ρ only if $\alpha > \frac{1}{2}$, i.e., if there is no infinitely thin shell carrying a nonvanishing screening charge. With that assumption both $d\Sigma$ and D_s can be reduced to their values for a pure Coulomb field.

The Helmholtz–Kirchhoff integral is thereby reduced to the simple expression

$$-\frac{m}{2\pi\hbar^2}\int \sin\theta\, d\theta\, \frac{ip}{\hbar} \times \exp i\left[\frac{2\lambda\pi}{\hbar}\left(\frac{me^4}{2|E|}\right)^{\frac{1}{2}} - (2\lambda-1)\pi\right] \tag{E10}$$

in the solid angle $\beta < \theta < \pi - \beta$, with an additional phase factor

$$\exp i\left[\frac{2p\lambda^2a^2r^2}{\hbar\rho}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{2\alpha+1}\cos^2\theta\right] \tag{E11}$$

in the solid angle $\theta < \beta$ and $\pi - \beta < \theta$. If (E10) is integrated from β to $\pi - \beta$ and

$$M_b = (2mr^2(E - V))^{\frac{1}{2}}\sin\beta$$

is inserted, the formula (50) is obtained. On the other hand, the argument of the exponential (E11) can be simplified because θ varies only in the neighborhood of β. If we expand everything in powers of $(\beta - \theta)$ and keep only the leading term, we are left with the integral

$$\int_{-\infty}^{\beta} d\theta \exp\left[i\kappa(\beta-\theta)^{2\alpha+1}\right] = \kappa^{-1/(2\alpha+1)}e^{-i\pi/2(2\alpha+1)}\frac{\Gamma(1/(2\alpha+1))}{2\alpha+1},$$

where

$$\kappa = 2p\lambda^2a^2r^2(\cos\beta)^{2\alpha+3}(\sin\beta)^{-2\alpha-1}\hbar^{-1}\rho^{-1}$$

is just what is left in the exponent of (E11) besides the factor $(\beta - \theta)^{2\alpha+1}$. The factor κ to the $-1/(2\alpha+1)$ power in (E12) introduces an $h^{+1/(2\alpha+1)}$ which makes the whole term of lower order than the contribution from the Kepler orbits.

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[5] Reference 4, p. 290.

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Further Generalization of the Generalized Master Equation

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For a system described in a phase space of generalized coordinates **w** and momenta **J**, the generalized master equation gives the time evolution of the reduced-density distribution function $\rho(t, \mathbf{J})$ for the momenta. A generalization of the generalized master equation, having a similar non-Markoffian form, is derived for the full distribution function $\rho(t, \mathbf{w}, \mathbf{J})$. This equation is an alternate form of the Liouville equation. The derivation is an extension of a previous derivation of the generalized master equation from the Liouville equation utilizing projection operators in a Hilbert space. The time-evolution equation for the reduced distribution function $\rho_r(t, \mathbf{w}_r, \mathbf{J})$, depending on the subset $\mathbf{w}_r$ of the set of coordinates **w**,is derived. The approach to a stationary state for $t \to \infty$ is discussed.

1. INTRODUCTION

In a previous paper,[1] a derivation was given of the generalized master equation. For a classical system described by generalized coordinates **w** and momenta **J** in phase space, the generalized master equation is an integro-differential equation for the time evolution of the reduced distribution function $\rho(t, \mathbf{J})$ for the momenta, first obtained for a gas by perturbation theory.[2] The derivation given in Paper I used projection-operator methods[3] applied to a Hilbert-space description of an arbitrary system with time-independent Hamiltonian. The basic projector required was the

constant q''. If (E8) is expressed in terms of q'' and M, the derivative $\partial\phi/\partial M$ follows at once. Thus, we find

$$D_s \cong \frac{m^2}{\rho}\left[\rho + \frac{(2\alpha+1)\lambda a r}{\sin\beta}\left(1 - \frac{\sin\theta}{\sin\beta}\right)^{\alpha-\frac{1}{2}}\cos^2\theta\right]^{-1} \tag{E9}$$

for the amplitude squared of the incoming wave if we retain only the leading terms in $(\sin\beta - \sin\theta)$. In both (E7) and (E9) the second term can be neglected compared to ρ only if $\alpha > \frac{1}{2}$, i.e., if there is no infinitely thin shell carrying a nonvanishing screening charge. With that assumption both $d\Sigma$ and D_s can be reduced to their values for a pure Coulomb field.

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1. INTRODUCTION

In a previous paper,[1] a derivation was given of the generalized master equation. For a classical system described by generalized coordinates **w** and momenta **J** in phase space, the generalized master equation is an integro-differential equation for the time evolution of the reduced distribution function $\rho(t, \mathbf{J})$ for the momenta, first obtained for a gas by perturbation theory.[2] The derivation given in Paper I used projection-operator methods[3] applied to a Hilbert-space description of an arbitrary system with time-independent Hamiltonian. The basic projector required was the

projector onto the "vacuum state of correlations" in the terminology of perturbation theory, the state for wave vector $\mathbf{k} = \mathbf{0}$.[4]

The generalized master equation, being a description of the reduced distribution function $\rho(t, \mathbf{J})$ from which the coordinates have been eliminated, does not readily provide information about those reduced distribution functions, such as the 1-particle or 2-particle distribution functions, which depend on some of the coordinates $\mathbf{w}$. It is shown in this paper that the methods of Paper I are readily extended to generalize further the generalized master equation and to obtain an integro-differential equation of the same form as the generalized master equation but for the entire distribution function $\rho(t, \mathbf{w}, \mathbf{J})$. Time-evolution equations of this form are also given for reduced coordinate-dependent distribution functions. The projector required for these generalizations projects onto a state of arbitrary $\mathbf{k}$. We work in the continuous spectrum of $\mathbf{k}$.

In Sec. 2, the separation of the Hamiltonian $H(\mathbf{w}, \mathbf{J})$ into a part H_1, which is the Fourier component of $H(\mathbf{w}, \mathbf{J})$ independent of $\mathbf{w}$, and the remaining part H_2, which comprises all other Fourier components, is described. This separation entails a corresponding separation of the Liouville operator

$$L(\mathbf{w}, \mathbf{J}) = i\left(\frac{\partial H}{\partial \mathbf{w}} \cdot \frac{\partial}{\partial \mathbf{J}} - \frac{\partial H}{\partial \mathbf{J}} \cdot \frac{\partial}{\partial \mathbf{w}}\right)$$

into a part L_1, which is diagonal in $\mathbf{k}$ representation, and the interaction part L_2, which is off-diagonal. It is the Liouville operator itself which separates in this way, not the exponential operator e^{-itL} as assumed by Zwanzig.[5] This separation is not necessarily the same as that used in perturbation theory. If Fourier analysis of the perturbation term in the Hamiltonian yields a Fourier coefficient which is independent of $\mathbf{w}$, this term must be included in H_1; a renormalization of generalized velocities occurs.

In Sec. 3, the description of classical dynamical (phase-space) variables as eigenvalues of Hilbert-space operators, introduced in Paper I, is extended. The Hilbert space is one spanned by the eigenkets of the coordinate operator $|\mathbf{w}\rangle$. In this space the Liouville operator, including the interaction term, is not Hermitian.

The derivation of the non-Markoffian equation for $\rho(t, \mathbf{w}, \mathbf{J})$ is given in Sec. 4. As in the generalized master equation for $\rho(t, \mathbf{J})$, a term appears which depends on an operator $\sigma_0(t, \mathbf{J})$ [denoted by $\rho_0^{\text{in}'}(t, \mathbf{J})$ in Paper I]. This operator is itself the solution of an integral equation, which is discussed in Sec. 5. As time passes from $t \to -\infty$ to $t \to +\infty$, $\sigma_0(t, \mathbf{J})$ changes asymptotically from one solution σ_0^{in} to another solution σ_0^{out} of the Liouville equation without interaction. As was shown in Paper I, the same behavior is exhibited by $\rho_0(t, \mathbf{J})$, the Hilbert-space density operator whose eigenvalues are $\rho(t, \mathbf{w}, \mathbf{J})$. For $t \to -\infty$,

$$\rho_0(t, \mathbf{J}) \to \rho_0^{\text{in}}(t, \mathbf{J}), \quad \text{where} \quad \rho_0^{\text{in}}(t, \mathbf{J}) = \sigma_0^{\text{in}}(t, \mathbf{J}).$$

For $t \to +\infty$,

$$\rho_0(t, \mathbf{J}) \to \rho_0^{\text{out}}(t, \mathbf{J}),$$

also a solution of the Liouville equation without interaction. This approach to a stationary state as $t \to \pm\infty$ is considered in Sec. 6. In Sec. 7, reduced distribution functions and their Hilbert-space density operators are discussed, and the non-Markoffian time-evolution equation for reduced distribution functions is derived. If the reduced distribution function $\rho_r(t, \mathbf{w}_r, \mathbf{J})$ depends on the set of coordinates

$$\mathbf{w}_r = \{w_1, w_2, \cdots, w_r\},$$

then the density operator $\rho_0^r(t, \mathbf{J})$ operates in a reduced Hilbert space spanned by the eigenkets of the coordinate operator $|\mathbf{w}_r\rangle$.

2. IDENTIFICATION OF THE INTERACTION TERM IN THE HAMILTONIAN

For a system with a time-independent Hamiltonian H, assume that

$$H(\mathbf{w}, \mathbf{J}) = H^0(\mathbf{J}) + \Delta H(\mathbf{w}, \mathbf{J}), \tag{2.1}$$

where $\mathbf{w}, \mathbf{J}$ is a set of canonical generalized coordinate and momentum variables. They are angle-action variables for the Hamiltonian $H^0(\mathbf{J})$ of the unperturbed system. The separation of the Hamiltonian in (2.1) into an unperturbed piece $H^0(\mathbf{J})$ and a perturbation $\Delta H(\mathbf{w}, \mathbf{J})$ is not unique. If ΔH is expanded as a Fourier integral

$$\Delta H(\mathbf{w}, \mathbf{J}) = \int d\mathbf{s} e^{2\pi i \mathbf{w}\cdot\mathbf{s}} h(\mathbf{s}, \mathbf{J}), \tag{2.2}$$

the term in $h(\mathbf{0}, \mathbf{J})$ can be separated out:

$$\begin{aligned}\Delta H(\mathbf{w}, \mathbf{J}) &= \int d\mathbf{s} e^{2\pi i \mathbf{w}\cdot\mathbf{s}} \{h(\mathbf{s}, \mathbf{J})\delta(\mathbf{s}) + h(\mathbf{s}, \mathbf{J})[1 - \delta(\mathbf{s})]\} \\ &= h(\mathbf{0}, \mathbf{J}) + \int_{[\mathbf{0}]} d\mathbf{s} e^{2\pi i \mathbf{w}\cdot\mathbf{s}} h(\mathbf{s}, \mathbf{J}).\end{aligned} \tag{2.3}$$

The symbol $\int_{[\mathbf{0}]} d\mathbf{s}$ indicates that the point $\mathbf{s} = \mathbf{0}$ is omitted in the integration.

Accordingly, instead of the separation of H assumed in (2.1), a unique separation is obtained by setting

$$H(\mathbf{w}, \mathbf{J}) = H_1(\mathbf{J}) + H_2(\mathbf{w}, \mathbf{J}), \tag{2.4}$$

where

$$H_1(\mathbf{J}) = H^0(\mathbf{J}) + h(\mathbf{0}, \mathbf{J}),$$
$$H_2(\mathbf{J}) = \Delta H(\mathbf{w}, \mathbf{J}) - h(\mathbf{0}, \mathbf{J})$$
$$= \int_{[0]} d\mathbf{s} e^{2\pi i \mathbf{s}\cdot\mathbf{w}} h(\mathbf{s}, \mathbf{J}). \tag{2.5}$$

$H_1(\mathbf{J})$ is the Fourier component of total Hamiltonian $H(\mathbf{w}, \mathbf{J})$ which is independent of $\mathbf{w}$ and all other Fourier components are included in $H_2(\mathbf{w}, \mathbf{J})$. The separation (2.4) instead of (2.1) is significant when $\partial h(\mathbf{0}, \mathbf{J})/\partial \mathbf{J}$ does not vanish. In this case, the generalized velocities $\boldsymbol{\nu}(\mathbf{J})$ of the unperturbed system,

$$\boldsymbol{\nu}(\mathbf{J}) = \frac{\partial H^0(\mathbf{J})}{\partial \mathbf{J}}, \tag{2.6}$$

are renormalized in the presence of the perturbation. They become

$$\boldsymbol{\nu}_1(\mathbf{J}) = \frac{\partial H_1(\mathbf{J})}{\partial \mathbf{J}} = \boldsymbol{\nu}(\mathbf{J}) + \frac{\partial h(\mathbf{0}, \mathbf{J})}{\partial \mathbf{J}}. \tag{2.7}$$

In this paper, the separation of the Hamiltonian is made according to (2.4). $H_1(\mathbf{J})$ is the Hamiltonian of the system without interaction and $H_2(\mathbf{w}, \mathbf{J})$ is the interaction term. It is convenient to write the Fourier expansion of $H_2(\mathbf{w}, \mathbf{J})$ as

$$H_2(\mathbf{w}, \mathbf{J}) = \int d\mathbf{s} e^{2\pi i \mathbf{w}\cdot\mathbf{s}} h(\mathbf{s}, \mathbf{J}), \tag{2.8}$$

where

$$h(\mathbf{0}, \mathbf{J}) = \int d\mathbf{w} H_2(\mathbf{w}, \mathbf{J})$$
$$= \int d\mathbf{s} \delta(\mathbf{s}) h(\mathbf{s}, \mathbf{J}) = 0, \tag{2.9}$$

so that $H_2(\mathbf{w}, \mathbf{J})$ has no Fourier component independent of $\mathbf{w}$.

In accordance with (2.4), (2.8), and (2.9), the Liouville operator in phase space separates into

$$L(\mathbf{w}, \mathbf{J}) = L_1(\mathbf{w}, \mathbf{J}) + L_2(\mathbf{w}, \mathbf{J}), \tag{2.10}$$

where

$$L_1 = -i\boldsymbol{\nu}_1(\mathbf{J}) \cdot \frac{\partial}{\partial \mathbf{w}}, \tag{2.11}$$

$$L_2 = -\int d\mathbf{s} e^{2\pi i \mathbf{w}\cdot\mathbf{s}} \left[h(\mathbf{s}, \mathbf{J}) \left(2\pi \mathbf{s} \cdot \frac{\partial}{\partial \mathbf{J}} \right) + i \left(\frac{\partial h(\mathbf{s}, \mathbf{J})}{\partial \mathbf{J}} \right) \cdot \frac{\partial}{\partial \mathbf{w}} \right]. \tag{2.12}$$

3. THE HILBERT SPACE

In the Hilbert space introduced in Paper I, the dynamical variables $A(t, \mathbf{w}, \mathbf{J})$ of classical phase space are eigenvalues of Hermitian operators $A_o(t\mathbf{J})$ (subscript "o" denotes operator),

$$A_o(t, \mathbf{J}) = \int d\mathbf{w} \, |\mathbf{w}\rangle \, A(t, \mathbf{w}, \mathbf{J}) \, \langle \mathbf{w}|,$$
$$A(t, \mathbf{w}, \mathbf{J}) = \mathrm{Tr}\, [A_o(t, \mathbf{J}) \, |\mathbf{w}\rangle \langle \mathbf{w}|], \tag{3.1}$$

where the eigenvectors $|\mathbf{w}\rangle$ are assumed complete and orthonormal on the real domain of $\mathbf{w}$, so that

$$\int d\mathbf{w} \, |\mathbf{w}\rangle \langle \mathbf{w}| = \mathbf{1}, \quad \langle \mathbf{w}' \mid \mathbf{w} \rangle = \delta(\mathbf{w}' - \mathbf{w}). \tag{3.2}$$

Clearly,

$$A_o(t, \mathbf{J}) \, |\mathbf{w}\rangle = A(t, \mathbf{w}, \mathbf{J}) \, |\mathbf{w}\rangle,$$

so that

$$\mathrm{Tr}\, [A_o(t, \mathbf{J}) \, |\mathbf{w}\rangle \langle \mathbf{w}|] = \int d\mathbf{w}' \langle \mathbf{w}| \, A_o(t, \mathbf{J}) \, |\mathbf{w}'\rangle, \tag{3.3}$$

$$\mathrm{Tr}\, [A_o(t, \mathbf{J})] = \int d\mathbf{w} \int d\mathbf{w}' \langle \mathbf{w}| \, A_o(t, \mathbf{J}) \, |\mathbf{w}'\rangle. \tag{3.4}$$

These expressions for the traces are appropriate in the continuous spectrum where only the diagonal elements contribute because of the δ-function singularity[6]

$$\langle \mathbf{w}'| \, A_o(t, \mathbf{J}) \, |\mathbf{w}\rangle = A(t, \mathbf{w}, \mathbf{J}) \delta(\mathbf{w}' - \mathbf{w}). \tag{3.5}$$

The Fourier-transform kets $|\mathbf{k}\rangle$,

$$|\mathbf{k}\rangle = \int d\mathbf{w} e^{2\pi i \mathbf{w}\cdot\mathbf{k}} \, |\mathbf{w}\rangle, \quad \langle \mathbf{w} \mid \mathbf{k} \rangle = e^{2\pi i \mathbf{w}\cdot\mathbf{k}}, \tag{3.6}$$

are also complete and orthonormal on the real domain of $\mathbf{k}$. According to (3.1), (3.3), and (3.4), since $A(t, \mathbf{w}, \mathbf{J})$ is real,

$$A(t, \mathbf{w}, \mathbf{J}) = \langle \mathbf{w}| \, A_o(t, \mathbf{J}) \, |\mathbf{0}\rangle = \langle \mathbf{0}| \, A_o(t, \mathbf{J}) \, |\mathbf{w}\rangle, \tag{3.7}$$

$$\mathrm{Tr}\, [A_o(t, \mathbf{J})] = \langle \mathbf{0}| \, A_o(t, \mathbf{J}) \, |\mathbf{0}\rangle. \tag{3.8}$$

The ket $|\mathbf{0}\rangle$ is defined in this paper as

$$|\mathbf{0}\rangle \equiv |\mathbf{k} = \mathbf{0}\rangle. \tag{3.9}$$

Since, according to (3.7) and (3.6),

$$A(t, \mathbf{w}, \mathbf{J}) = \int d\mathbf{k} \langle \mathbf{w} \mid \mathbf{k} \rangle \langle \mathbf{k}| \, A_o(t, \mathbf{J}) \, |\mathbf{0}\rangle$$
$$= \int d\mathbf{k} e^{2\pi i \mathbf{k}\cdot\mathbf{w}} \langle \mathbf{k}| \, A_o(t, \mathbf{J}) \, |0\rangle, \tag{3.10}$$

the matrix element $\langle \mathbf{k}| \, A_o(t, \mathbf{J}) \, |\mathbf{0}\rangle$ is the Fourier transform of $A(t, \mathbf{w}, \mathbf{J})$.

The Hilbert-space Liouville operator corresponding to $L(\mathbf{w}, \mathbf{J})$ is

$$\mathfrak{L}(\mathbf{J}) = \mathfrak{L}_1(\mathbf{J}) + \mathfrak{L}_2(\mathbf{J}), \tag{3.11}$$

where

$$\mathfrak{L}_1(\mathbf{J}) = \int d\mathbf{w} \, |\mathbf{w}\rangle \, L_1(\mathbf{w}, \mathbf{J}) \, \langle \mathbf{w}|,$$
$$\mathfrak{L}_2(\mathbf{J}) = \int d\mathbf{w} \, |\mathbf{w}\rangle \, L_2(\mathbf{w}, \mathbf{J}) \, \langle \mathbf{w}|. \tag{3.12}$$

The Fourier-transform kets $|\mathbf{k}\rangle$ of (3.6) are eigenkets of $\mathfrak{L}_1$, since

$$\mathfrak{L}_1 |\mathbf{k}\rangle = \int d\mathbf{w}\, |\mathbf{w}\rangle \left(-i\boldsymbol{\nu}_1(\mathbf{J}) \cdot \frac{\partial}{\partial \mathbf{w}}\right) \langle \mathbf{w} \mid \mathbf{k}\rangle = 2\pi \boldsymbol{\nu}_1(\mathbf{J}) \cdot \mathbf{k}\, |\mathbf{k}\rangle. \tag{3.13}$$

$\mathfrak{L}_1(\mathbf{J})$ is Hermitian with eigenvalues

$$\lambda(\mathbf{k}, \mathbf{J}) = 2\pi \mathbf{k} \cdot \boldsymbol{\nu}_1(\mathbf{J}), \tag{3.14}$$

continuous in $\mathbf{k}$.[7] In the $\mathbf{k}$ representation, the matrix elements of $\mathfrak{L}_1$ and $\mathfrak{L}_2$ are

$$\langle \mathbf{k}|\, \mathfrak{L}_1\, |\mathbf{k}'\rangle = 2\pi \mathbf{k} \cdot \boldsymbol{\nu}_1(\mathbf{J}) \delta(\mathbf{k} - \mathbf{k}'), \tag{3.15}$$

$$\langle \mathbf{k}|\, \mathfrak{L}_2\, |\mathbf{k}'\rangle = 2\pi \left[\mathbf{k}' \cdot \left(\frac{\partial h(\mathbf{k} - \mathbf{k}', \mathbf{J})}{\partial \mathbf{J}}\right) - h(\mathbf{k} - \mathbf{k}', \mathbf{J})(\mathbf{k} - \mathbf{k}') \cdot \frac{\partial}{\partial \mathbf{J}}\right]. \tag{3.16}$$

In the $\mathbf{k}$ representation, $\mathfrak{L}_1$ is diagonal, but the diagonal elements $\langle \mathbf{k}|\, \mathfrak{L}_2\, |\mathbf{k}\rangle$ of $\mathfrak{L}_2$ all vanish according to (2.9). This result is a consequence of the separation of the Hamiltonian (2.4), according to which $h(\mathbf{0}, \mathbf{J})$ is included in $H_1(\mathbf{J})$, rather than in the interaction $H_2(\mathbf{w}, \mathbf{J})$. Note that the Liouville operator is separated into diagonal and nondiagonal parts in (3.11), but the exponential operator $e^{-i\mathfrak{L}t}$ is not. The latter separation was assumed by Zwanzig.[5] From (3.15) and (3.16),

$$\mathrm{Tr}\, [\mathfrak{L}_1 |\mathbf{k}\rangle\langle \mathbf{k}|] = \int d\mathbf{k}'\, \langle \mathbf{k}|\, \mathfrak{L}_1\, |\mathbf{k}'\rangle = 2\pi \mathbf{k} \cdot \boldsymbol{\nu}_1(\mathbf{J}), \tag{3.17}$$

$$\mathrm{Tr}\, [\mathfrak{L}_2 |\mathbf{k}\rangle\langle \mathbf{k}|] = 0, \tag{3.18}$$

$$\langle \mathbf{k}|\, \mathfrak{L}_1\, |\mathbf{k}'\rangle^* = -\langle -\mathbf{k}|\, \mathfrak{L}_1\, |-\mathbf{k}'\rangle,$$
$$\langle \mathbf{k}|\, \mathfrak{L}_2\, |\mathbf{k}'\rangle^* = -\langle -\mathbf{k}|\, \mathfrak{L}_2\, |-\mathbf{k}'\rangle. \tag{3.19}$$

According to (3.16), it is apparent that $\mathfrak{L}_2$ is not Hermitian in the Hilbert space. This is surprising, since the Liouville operator is Hermitian in phase space, where[8]

$$\int d\mathbf{J} \int d\mathbf{w} f^*(\mathbf{w}, \mathbf{J}) L(\mathbf{w}, \mathbf{J}) g(\mathbf{w}, \mathbf{J}) = \int d\mathbf{J} \int d\mathbf{w} g(\mathbf{w}, \mathbf{J}) [L(\mathbf{w}, \mathbf{J}) f(\mathbf{w}, \mathbf{J})]^* \tag{3.20}$$

for functions f and g vanishing at the boundaries. But (3.20) is equivalent to

$$\int d\mathbf{J}\, \mathrm{Tr}\, [f_0(\mathbf{J}) \mathfrak{L}(\mathbf{J}) g_0(\mathbf{J})] = \int d\, \mathrm{Tr}\, [g_0(\mathbf{J}) \mathfrak{L}(\mathbf{J}) f_0(\mathbf{J})]^*. \tag{3.21}$$

Integration on $\mathbf{J}$ is required for Hermiticity of the Liouville operator. It is not Hermitian in the reduced Hilbert space spanned by the $|\mathbf{w}\rangle$ kets alone. (A Hilbert space spanned by simultaneous eigenkets of coordinates and momenta $|\mathbf{w}, \mathbf{J}\rangle$ was introduced in Paper I.)

If we use the notation

$$\mathfrak{P}(\mathbf{k}) \equiv |\mathbf{k}\rangle\langle \mathbf{k}| \tag{3.22}$$

and

$$\mathbf{1}[\mathbf{k}] \equiv \mathbf{1} - \mathfrak{P}(\mathbf{k}) = \int_{[\mathbf{k}]} d\mathbf{k}'\, |\mathbf{k}'\rangle\langle \mathbf{k}'|, \tag{3.23}$$

omitting the point $\mathbf{k}' = \mathbf{k}$, then it follows from the preceding discussion that

$$\mathfrak{P}(\mathbf{k}) \mathfrak{L}_2 \mathfrak{P}(\mathbf{k}) = 0, \tag{3.24}$$

$$\mathfrak{P}(\mathbf{k}) \mathfrak{L} \mathfrak{P}(\mathbf{k}) = \mathfrak{P}(\mathbf{k}) \mathfrak{L}_1 \mathfrak{P}(\mathbf{k}) = |\mathbf{k}\rangle\, \mathrm{Tr}\, [\mathfrak{L}_1 \mathfrak{P}(\mathbf{k})]\, \langle \mathbf{k}| = 2\pi \mathbf{k} \cdot \boldsymbol{\nu}_1(\mathbf{J})\, |\mathbf{k}\rangle\langle \mathbf{k}|, \tag{3.25}$$

$$\mathbf{1}[\mathbf{k}] \mathfrak{L}_1 \mathfrak{P}(\mathbf{k}) = \mathfrak{P}(\mathbf{k}) \mathfrak{L}_1 \mathbf{1}[\mathbf{k}] = 0, \tag{3.26}$$

$$\mathbf{1}[\mathbf{k}] \mathfrak{L} \mathfrak{P}(\mathbf{k}) = \mathbf{1}[\mathbf{k}] \mathfrak{L}_2 \mathfrak{P}(\mathbf{k}) = \mathfrak{L}_2 \mathfrak{P}(\mathbf{k}), \tag{3.27}$$

$$\mathfrak{P}(\mathbf{k}) \mathfrak{L}_2 \mathbf{1}[\mathbf{k}] = \mathfrak{P}(\mathbf{k}) \mathfrak{L}_2. \tag{3.28}$$

4. GENERALIZATION OF THE GENERALIZED MASTER EQUATION

Corresponding to the phase-space probability density $\rho(t, \mathbf{w}, \mathbf{J})$, a Hilbert-space density operator is defined as

$$\rho_0(t, \mathbf{J}) = \int d\mathbf{w}\, |\mathbf{w}\rangle\, \rho(t, \mathbf{w}, \mathbf{J})\, \langle \mathbf{w}|, \tag{4.1}$$

and the Liouville equation takes the form

$$\frac{\partial \rho_0(t, \mathbf{J})}{\partial t} = -i\mathfrak{L}(\mathbf{J}) \rho_0(t, \mathbf{J}). \tag{4.2}$$

For derivation of the generalized master equation in Paper I, the Liouville equation was projected into two parts with the projectors $\mathfrak{P}(\mathbf{0})$ and $\mathbf{1}[\mathbf{0}]$; $\mathfrak{P}(\mathbf{0})$ projects onto the "vacuum" state $|\mathbf{k} = \mathbf{0}\rangle$. The generalization to be obtained here utilizes $\mathbf{1}[\mathbf{k}]$, instead of $\mathbf{1}[\mathbf{0}]$. From the Liouville equation,

$$\frac{\partial \mathbf{1}[\mathbf{k}] \rho_0(t, \mathbf{J})}{\partial t} = -i\mathbf{1}[\mathbf{k}] \mathfrak{L} \rho_0(t, \mathbf{J}) = -i\mathbf{1}[\mathbf{k}] \mathfrak{L} \mathbf{1}[\mathbf{k}] \rho_0(t, \mathbf{J}) - i\mathfrak{L}_2 \mathfrak{P}(\mathbf{k}) \rho_0(t, \mathbf{J}), \tag{4.3}$$

according to (3.27). Using the notation

$$\mathfrak{L}[\mathbf{k}] = \mathbf{1}[\mathbf{k}] \mathfrak{L} \mathbf{1}[\mathbf{k}], \tag{4.4}$$

and noting that $\mathbf{1}[\mathbf{k}] = (\mathbf{1}[\mathbf{k}])^2$ since $\mathbf{1}[\mathbf{k}]$ is a projector, we obtain the differential equation

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}[\mathbf{k}]\right) \mathbf{1}[\mathbf{k}] \rho_0(t, \mathbf{J}) = -i\mathfrak{L}_2 \mathfrak{P}(\mathbf{k}) \rho_0(t, \mathbf{J}). \tag{4.5}$$

Operation from the left with the integrating factor $e^{it\mathfrak{L}[\mathbf{k}]}$ and integration with respect to time gives

$$\mathbf{1}[\mathbf{k}]\rho_0(t, \mathbf{J}) = \mathbf{1}[\mathbf{k}]\sigma_0(t, \mathbf{J}) - i\int_{-\infty}^{t} dt' e^{-i(t-t')\mathfrak{L}[\mathbf{k}]}\mathfrak{L}_2\mathfrak{P}(\mathbf{k})\rho_0(t', \mathbf{J}), \quad (4.6)$$

where

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}[\mathbf{k}]\right)\mathbf{1}[\mathbf{k}]\sigma_0(t, \mathbf{J}) = 0. \quad (4.7)$$

[The operator $\sigma_0(t, \mathbf{J})$ was denoted by $\rho_0^{\text{in}'}(t, \mathbf{J})$ in Paper I.] An expression for the interaction term $\mathfrak{L}_2\rho_0(t, \mathbf{J})$ of the Liouville equation results from (4.6) upon operation from the left with $\mathfrak{P}(\mathbf{k})\mathfrak{L}_2$ followed by integration over $\mathbf{k}$. From (3.28),

$$\mathfrak{L}_2\rho_0(t, \mathbf{J}) = \mathfrak{L}\sigma_0(t, \mathbf{J}) - i\int_{-\infty}^{t} dt' \mathfrak{G}(t - t', \mathbf{J})\rho_0(t', \mathbf{J}), \quad (4.8)$$

where

$$\mathfrak{G}(t, \mathbf{J}) \equiv \int d\mathbf{k}\mathfrak{P}(\mathbf{k})\mathfrak{L}_2 e^{-it\mathfrak{L}[\mathbf{k}]}\mathfrak{L}_2\mathfrak{P}(\mathbf{k}). \quad (4.9)$$

Accordingly, the Liouville equation becomes

$$\frac{\partial\rho_0(t, \mathbf{J})}{\partial t} + i\mathfrak{L}_1\rho_0(t, \mathbf{J}) = -i\mathfrak{L}_2\sigma_0(t, \mathbf{J}) - \int_{-\infty}^{t} dt' \mathfrak{G}(t - t', \mathbf{J})\rho_0(t', \mathbf{J}). \quad (4.10)$$

According to (3.10), the Fourier transform of the phase-space probability density $\rho(t, \mathbf{w}, \mathbf{J})$ is

$$\langle \mathbf{k}|\ \rho_0(t, \mathbf{J})\ |\mathbf{0}\rangle.$$

It obeys the equation, obtained from (4.10),

$$\frac{\partial\ \langle \mathbf{k}|\ \rho_0(t, \mathbf{J})\ |\mathbf{0}\rangle}{\partial t} + 2\pi i\mathbf{k}\cdot\boldsymbol{\nu}_1(\mathbf{J})\ \langle \mathbf{k}|\ \rho_0(t, \mathbf{J})\ |0\rangle = -i\ \langle \mathbf{k}|\ \mathfrak{L}_2\sigma_0(t, \mathbf{J})\ |0\rangle - \int_{-\infty}^{t} dt' g(t - t', \mathbf{k}, \mathbf{J})\ \langle \mathbf{k}|\ \rho_0(t', \mathbf{J})\ |\mathbf{0}\rangle, \quad (4.11)$$

where

$$g(t, \mathbf{k}, \mathbf{J}) = \text{Tr}\ [\mathfrak{G}(t, \mathbf{J})\mathfrak{P}(\mathbf{k})] = \langle \mathbf{k}|\ \mathfrak{L}_2 e^{-it\mathfrak{L}[\mathbf{k}]}\mathfrak{L}_2\ |\mathbf{k}\rangle. \quad (4.12)$$

It follows readily from (3.19) that

$$g^*(t, \mathbf{k}, \mathbf{J}) = g(t, -\mathbf{k}, \mathbf{J}). \quad (4.13)$$

Fourier transformation of (4.11) gives the time evolution of the phase-space probability density $\rho(t, \mathbf{w}, \mathbf{J})$:

$$\frac{\partial\rho(t, \mathbf{w}, \mathbf{J})}{\partial t} + \boldsymbol{\nu}_1(\mathbf{J})\cdot\frac{\partial\rho(t, \mathbf{w}, \mathbf{J})}{\partial \mathbf{w}} = -iL_2(\mathbf{w}, \mathbf{J})\sigma(t, \mathbf{w}, \mathbf{J}) - \int_{-\infty}^{t} dt' G(t - t', \mathbf{w}, \mathbf{J})\rho(t', \mathbf{w}, \mathbf{J}). \quad (4.14)$$

The phase-space operator $G(t, \mathbf{w}, \mathbf{J})$ is defined from $g(t, \mathbf{k}, \mathbf{J})$ as

$$G(t, \mathbf{w}, \mathbf{J}) = g\left(t, (2\pi i)^{-1}\frac{\partial}{\partial \mathbf{w}}, \mathbf{J}\right), \quad (4.15)$$

so that the Fourier transform of $g(t, \mathbf{k}, \mathbf{J})\ \langle \mathbf{k}|$ in (4.11) is

$$\int d\mathbf{k} e^{2\pi i\mathbf{w}\cdot\mathbf{k}} g(t, \mathbf{k}, \mathbf{J})\ \langle \mathbf{k}| = G(t, \mathbf{w}, \mathbf{J})\ \langle \mathbf{w}|$$

or

$$G(t, \mathbf{w}, \mathbf{J})\delta(\mathbf{w}' - \mathbf{w}) = \int d\mathbf{k} e^{2\pi i\mathbf{k}\cdot(\mathbf{w}-\mathbf{w}')} g(t, \mathbf{k}, \mathbf{J}). \quad (4.16)$$

According to (4.13), the operator $G(t, \mathbf{w}, \mathbf{J})$ is real.

Equation (4.11) in the $\mathbf{k}$ representation or (4.14) in phase space is a generalization of the generalized master equation. The generalized master equation which expresses the time evolution of the reduced distribution function for the momenta $\mathbf{J}$,

$$\rho(t, \mathbf{J}) = \int d\mathbf{w}\rho(t, \mathbf{w}, \mathbf{J}) = \langle \mathbf{0}|\ \rho_0(t, \mathbf{J})\ |\mathbf{0}\rangle, \quad (4.17)$$

is obtained simply by setting $\mathbf{k} = \mathbf{0}$ in (4.11):

$$\frac{\partial\rho(t, \mathbf{J})}{\partial t} = -i\ \langle \mathbf{0}|\ \mathfrak{L}_2\sigma_0(t, \mathbf{J})\ |\mathbf{0}\rangle - \int_{-\infty}^{t} dt' g(t - t', \mathbf{0}, \mathbf{J})\rho(t', \mathbf{J}). \quad (4.18)$$

Equation (4.14) is an alternative non-Markoffian form of the Markoffian phase-space Liouville equation itself. It expresses the change in probability density along the trajectories of the noninteracting system, the system governed by the Hamiltonian $H_1(\mathbf{J})$, in the presence of the interaction $H_2(\mathbf{w}, \mathbf{J})$. Multiplication by the displacement operator $\exp\ [t\boldsymbol{\nu}_1(\mathbf{J})\cdot\partial/\partial\mathbf{w}]$ along these trajectories, on the left-hand side of (4.14), gives

$$\frac{\partial\ \exp\ (t\boldsymbol{\nu}_1\cdot\partial/\partial\mathbf{w})\rho(t, \mathbf{w}, \mathbf{J})}{\partial t} = \frac{d\rho(t, \mathbf{w}(t), \mathbf{J})}{dt}, \quad (4.19)$$

where

$$\mathbf{w}(t) = \mathbf{w} + \boldsymbol{\nu}_1(\mathbf{J})t \quad (4.20)$$

is the coordinate along the trajectory, and d/dt is the total time derivative following the motion. Accordingly, (4.14) becomes, in the interaction picture,

$$\frac{d\rho(t, \mathbf{w}(t), \mathbf{J})}{dt} = -i\int d\mathbf{w}'\delta(\mathbf{w}(t) - \mathbf{w}')L_2(\mathbf{w}', \mathbf{J})\sigma(t, \mathbf{w}', \mathbf{J}) - \int_{-\infty}^{t} dt' \int d\mathbf{w}'\delta(\mathbf{w}(t) - \mathbf{w}') \times G(t - t', \mathbf{w}', \mathbf{J})\rho(t', \mathbf{w}', \mathbf{J}). \quad (4.21)$$

5. TIME EVOLUTION OF $\sigma_0(t, \mathbf{J})$

The operator $\sigma_0(t, \mathbf{J})$ appearing in the preceding section is specified by (4.7), which can be written

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}_1\right)\mathbf{1}[\mathbf{k}]\sigma_0(t, \mathbf{J}) = -i\mathfrak{L}_2[\mathbf{k}]\sigma_0(t, \mathbf{J}). \quad (5.1)$$

The formal solution of this equation is

$$\mathbf{1}[\mathbf{k}]\sigma_0(t, \mathbf{J}) = \mathbf{1}[\mathbf{k}]\sigma_0^{\text{in}}(t, \mathbf{J}) - i\int_{-\infty}^{t} dt' e^{-i(t-t')\mathfrak{L}_1}\mathfrak{L}_2[\mathbf{k}]\sigma_0(t', \mathbf{J}), \quad (5.2)$$

where $\sigma_0^{\text{in}}(t, \mathbf{J})$ is a solution of the Liouville equation without interaction

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}_1\right)\sigma_0^{\text{in}}(t, \mathbf{J}) = 0, \quad (5.3)$$

so that

$$\sigma_0^{\text{in}}(t, \mathbf{J}) = e^{(-i\mathfrak{L}_1 t)}\sigma_0^{\text{in}}(0, \mathbf{J}). \quad (5.4)$$

Here, $\sigma_0^{\text{in}}(t, \mathbf{J})$ is the asymptotic value of $\sigma_0(t, \mathbf{J})$ for $t \to -\infty$. For $t \to +\infty$, $\sigma_0(t, \mathbf{J})$ asymptotically becomes equal to $\sigma_0^{\text{out}}(t, \mathbf{J})$, where

$$\mathbf{1}[\mathbf{k}]\sigma_0^{\text{out}}(t, \mathbf{J}) = \mathbf{1}[\mathbf{k}]\sigma_0^{\text{in}}(t, \mathbf{J}) - i\int_{-\infty}^{\infty} dt' e^{-i(t-t')\mathfrak{L}_1}\mathfrak{L}_2[\mathbf{k}]\sigma_0(t', \mathbf{J}). \quad (5.5)$$

$\sigma_0^{\text{out}}(t, \mathbf{J})$ is also a solution of the Liouville equation without interaction:

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}_1\right)\sigma_0^{\text{out}}(t, \mathbf{J}) = 0,$$
$$\sigma_0^{\text{out}}(t, \mathbf{J}) = e^{-i\mathfrak{L}_1 t}\sigma_0^{\text{out}}(0, \mathbf{J}). \quad (5.6)$$

Multiplication of (5.5) by the displacement operator, along the trajectories of the noninteracting system $e^{i\mathfrak{L}_1 t}$ gives

$$\mathbf{1}[\mathbf{k}]\sigma_0^{\text{out}}(0, \mathbf{J}) = \mathbf{1}[\mathbf{k}]\sigma_0^{\text{in}}(0, \mathbf{J}) - i\int_{-\infty}^{\infty} dt' e^{it'\mathfrak{L}_1}\mathfrak{L}_2[\mathbf{k}]\sigma_0(t', \mathbf{J}) \quad (5.7)$$

independent of time (interaction picture).

Operation on (5.2) from the left with $\mathfrak{F}(\mathbf{k})\mathfrak{L}_2$ followed by integration over $\mathbf{k}$ gives

$$\mathfrak{L}_2\sigma_0(t, \mathbf{J}) = \mathfrak{L}_2\sigma_0^{\text{in}}(t, \mathbf{J}) - i\int_{-\infty}^{t} dt' \mathfrak{D}(t - t', \mathbf{J})\sigma_0(t', \mathbf{J}), \quad (5.8)$$

where

$$\mathfrak{D}(t, \mathbf{J}) \equiv \int d\mathbf{k}\mathfrak{F}(\mathbf{k})\mathfrak{L}_2 e^{-it\mathfrak{L}_1}\mathfrak{L}_2[\mathbf{k}]. \quad (5.9)$$

The terms in $\mathfrak{L}_2\sigma_0$ in (4.10), (4.11), (4.14), and (4.21) are specified by (5.8).

6. APPROACH TO A STATIONARY STATE

We have seen in the previous section that, as time passes from $t \to -\infty$ to $t \to +\infty$, $\sigma_0(t, \mathbf{J})$ changes from $\sigma_0^{\text{in}}(t, \mathbf{J})$ to $\sigma_0^{\text{out}}(t, \mathbf{J})$, where both σ_0^{in} and σ_0^{out} are solutions of the Liouville equations without interaction, and therefore are constants of the motion along the trajectories of the system without interaction. It was shown in Paper I that the same behavior is exhibited by the density operator $\rho_0(t, \mathbf{J})$ itself. Here we take into account the separation of the Hamiltonian according to (2.4), instead of the separation according to (2.1) used in Paper I.

When the Liouville equation is written as

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}_1\right)\rho_0(t, \mathbf{J}) = -i\mathfrak{L}_2\rho_0(t, \mathbf{J}), \quad (6.1)$$

the integrating factor $e^{i\mathfrak{L}_1 t}$ gives the formal solution

$$\rho_0(t, \mathbf{J}) = \rho_0^{\text{in}}(t, \mathbf{J}) - i\int_{-\infty}^{t} dt' e^{-i(t-t')\mathfrak{L}_1}\mathfrak{L}_2\rho_0(t', \mathbf{J}), \quad (6.2)$$

where $\rho_0^{\text{in}}(t, \mathbf{J})$, like $\sigma_0^{\text{in}}(t, \mathbf{J})$ in (5.4), is a solution of the Liouville equation without interaction

$$\rho_0^{\text{in}}(t, \mathbf{J}) = e^{-i\mathfrak{L}_1 t}\rho_0^{\text{in}}(0, \mathbf{J}). \quad (6.3)$$

In fact, comparison of (4.6), (5.2), and (6.2) shows that, for $t \to -\infty$, asymptotically $\rho_0(t, \mathbf{J}) \to \sigma_0(t, \mathbf{J})$ so that

$$\rho_0^{\text{in}}(t, \mathbf{J}) = \sigma_0^{\text{in}}(t, \mathbf{J}). \quad (6.4)$$

Here, $\rho_0^{\text{in}}(t, \mathbf{J})$ is the value reached asymptotically at $t \to -\infty$ by the density operator of the system. For $t \to +\infty$, this operator becomes equal to

$$\rho_0^{\text{out}}(t, \mathbf{J}) = \rho_0^{\text{in}}(t, \mathbf{J}) - i\int_{-\infty}^{\infty} dt' e^{-i(t-t')\mathfrak{L}_1}\mathfrak{L}_2\rho_0(t', \mathbf{J}). \quad (6.5)$$

Then, ρ_0^{out} is also a solution of the Liouville equation without interaction:

$$\rho_0^{\text{out}}(t, \mathbf{J}) = e^{-i\mathfrak{L}_1 t}\rho_0^{\text{out}}(0, \mathbf{J}). \quad (6.6)$$

Multiplication of (6.5) by $e^{\,i\mathfrak{L}_1}$ gives, in the interaction picture,

$$\rho_0^{\text{out}}(0, \mathbf{J}) = \rho_0^{\text{in}}(0, \mathbf{J}) - i\int_{-\infty}^{\infty} dt e^{it\mathfrak{L}_1}\mathfrak{L}_2\rho_0(t, \mathbf{J}), \quad (6.7)$$

independent of time.

Along the trajectories of the motion governed by $H_1(\mathbf{J})$, Liouville's theorem does not hold in the presence of the interaction $H_2(\mathbf{w}, \mathbf{J})$. The probability density is not constant: $\rho_0(t, \mathbf{J})$ changes asymptotically from $\rho_0^{\text{in}}(t, \mathbf{J}) = \sigma_0^{\text{in}}(t, \mathbf{J})$, for $t \to -\infty$, to $\rho_0^{\text{out}}(t, \mathbf{J})$, for $t \to \infty$, according to (6.2). In phase space the

asymptotic probability densities are

$$\rho^{\text{out}}(t, \mathbf{w}, \mathbf{J}) = e^{-itL_1(\mathbf{w},\mathbf{J})}\rho^{\text{out}}(0, \mathbf{w}, \mathbf{J}) = \rho^{\text{out}}(0, \mathbf{w} - \boldsymbol{\nu}_1(\mathbf{J})t, \mathbf{J}),$$
$$\rho^{\text{in}}(t, \mathbf{w}, \mathbf{J}) = \rho^{\text{in}}(0, \mathbf{w} - \boldsymbol{\nu}_1(\mathbf{J})t, \mathbf{J}). \quad (6.8)$$

These have the important property that the reduced distribution functions $\rho^{\text{out}}(t, \mathbf{J})$ and $\rho^{\text{in}}(t, \mathbf{J})$ for the generalized momenta $\mathbf{J}$ are independent of time; for example,

$$\rho^{\text{out}}(t, \mathbf{J}) \equiv \int d\mathbf{w}\rho^{\text{out}}(t, \mathbf{w}, \mathbf{J}) = \rho^{\text{out}}(0, \mathbf{J}). \quad (6.9)$$

Accordingly, the expectation values of all properties which are functions of $\mathbf{J}$ alone become independent of time for $t \to \pm\infty$. For example, for $F(\mathbf{J})$, when $t \to +\infty$,

$$\langle F\rangle_\infty = \int d\mathbf{w}\int d\mathbf{J}F(\mathbf{J})\rho^{\text{out}}(t, \mathbf{w}, \mathbf{J}) = \int d\mathbf{J}F(\mathbf{J})\rho^{\text{out}}(0, \mathbf{J}). \quad (6.10)$$

More generally, the expectation of any dynamical property with the functional form

$$F(t, \mathbf{w}, \mathbf{J}) = e^{-itL_1(\mathbf{w},\mathbf{J})}F(0, \mathbf{w}, \mathbf{J}) = F(0, \mathbf{w} - \boldsymbol{\nu}_1(\mathbf{J})t, \mathbf{J}) \quad (6.11)$$

becomes independent of time.

Since, for $t \to \pm\infty$,

$$\left(\frac{\partial}{\partial t} + i\mathfrak{L}_1\right)\rho_0(t, \mathbf{J}) \to 0 \quad (6.12)$$

asymptotically, therefore, from (4.10),

$$\mathfrak{L}_2\sigma_0(t, \mathbf{J}) \to i\int_{-\infty}^{t} dt'\mathfrak{G}(t - t', \mathbf{J})\rho_0(t', \mathbf{J}), \quad (6.13)$$

so that

$$\mathfrak{L}_2\sigma_0^{\text{in}}(t, \mathbf{J}) \to 0, \quad \text{for} \quad t \to -\infty, \quad (6.14)$$

$$\mathfrak{L}_2\sigma_0^{\text{out}}(t, \mathbf{J}) \to i\int_{-\infty}^{\infty} dt'\mathfrak{G}(t - t', \mathbf{J})\rho_0(t', \mathbf{J}), \quad \text{for} \quad t \to +\infty. \quad (6.15)$$

On the other hand, from (4.8),

$$\mathfrak{L}_2\rho_0^{\text{out}}(t, \mathbf{J}) \to 0, \quad \text{for} \quad t \to +\infty. \quad (6.16)$$

It is evident, of course, from the Liouville equation (6.1) that if (6.12) holds for $t \to \pm\infty$, then

$$\mathfrak{L}_2\rho_0(t, \mathbf{J}) \to 0, \quad \text{for} \quad t \to \pm\infty. \quad (6.17)$$

The preceding conclusions of Eqs. (6.1)–(6.11) concerning the asymptotic behavior of $\rho_0(t, \mathbf{J})$ follow directly from the Liouville equation in the form (6.1), but do not depend on the properties of $\mathfrak{L}_1$ and $\mathfrak{L}_2$ based on the separation of the Hamiltonian in (2.4). The solution of the Liouville equation can be written alternatively in the forms

$$\rho_0(t, \mathbf{J}) = e^{-it\mathfrak{L}}\rho_0(0, \mathbf{J}) \quad (6.18)$$

$$= e^{-it\mathfrak{L}_1}\left[\rho_0^{\text{in}}(0, \mathbf{J}) - i\int_{-\infty}^{t} dt'e^{it'\mathfrak{L}_1}\mathfrak{L}_2\rho_0(t', \mathbf{J})\right] \quad (6.19)$$

$$= \rho_0^{\text{in}}(\mathbf{J}) - i\int_{-\infty}^{t} dt'\mathfrak{L}\rho_0(t', \mathbf{J}). \quad (6.20)$$

In (6.19), which is equivalent to (6.2), $\mathfrak{L}_1$ and $\mathfrak{L}_2$ may be regarded in general as arbitrary, unrelated to the separation (2.4). The form (6.20) shows that, for $t \to -\infty$, $\rho_0(t, \mathbf{J}) \to \rho_0^{\text{in}}(\mathbf{J})$, which is independent of time. For $t \to +\infty$,

$$\rho_0(t, \mathbf{J}) \to \rho_0^{\text{in}}(\mathbf{J}) - i\int_{-\infty}^{\infty} dt\mathfrak{L}\rho_0(t, \mathbf{J}), \quad (6.21)$$

also independent of time. The probability distribution becomes stationary for $t \to \pm\infty$. Expectation values for all dynamical properties $F(\mathbf{w}, \mathbf{J})$ become independent of time [cf. (6.11)].

Similarly, the solution of (4.7) can be written as

$$\mathbf{1}[\mathbf{k}]\sigma_0(t, \mathbf{J}) = \mathbf{1}[\mathbf{k}]\sigma_0^{\text{in}}(\mathbf{J}) - i\int_{-\infty}^{t} dt'\mathfrak{L}[\mathbf{k}]\sigma_0(t', \mathbf{J}) \quad (6.22)$$

as well as in the form (5.2). Therefore, for $t \to +\infty$,

$$\sigma_0(t, \mathbf{J}) \to \sigma_0^{\text{in}}(\mathbf{J}) - i\int_{-\infty}^{\infty} dt\mathfrak{L}[\mathbf{k}]\sigma_0(t, \mathbf{J}), \quad (6.23)$$

independent of time. Accordingly, from (4.8) or (6.15),

$$\int_{-\infty}^{\infty} dt'\mathfrak{G}(t - t', \mathbf{J})\rho_0(t', \mathbf{J})$$

becomes independent of time for $t \to \infty$.

7. REDUCED DISTRIBUTION FUNCTIONS

If we write $\mathbf{w}$ as

$$\mathbf{w} = \mathbf{w}_r + \mathbf{w}_s, \quad (7.1)$$

where $\mathbf{w}_r$ represents the set of components $w_1, w_2, \cdots, w_r$, then the reduced probability density $\rho_r(t, \mathbf{w}_r, \mathbf{J})$ in phase space is defined as

$$\rho_r(t, \mathbf{w}_r, \mathbf{J}) \equiv \int d\mathbf{w}_s\rho(t, \mathbf{w}, \mathbf{J}) = \int d\mathbf{w}_s \operatorname{Tr}[\rho_0(t, \mathbf{J})|\mathbf{w}\rangle\langle\mathbf{w}|].$$

In Hilbert space the corresponding reduced density operator is

$$\rho_0^r(t, \mathbf{J}) = \int d\mathbf{w}|\mathbf{w}\rangle\rho_r(t, \mathbf{w}_r, \mathbf{J})\langle\mathbf{w}|. \quad (7.2)$$

From (3.7) and (3.10),

$$\rho_r(t, \mathbf{w}_r, \mathbf{J}) = \int d\mathbf{w}_s \langle \mathbf{w}| \rho_0(t, \mathbf{J}) |\mathbf{0}\rangle$$
$$= \int d\mathbf{w}_s \int d\mathbf{k} e^{2\pi i \mathbf{w}\cdot\mathbf{k}} \langle \mathbf{k}| \rho_0(t, \mathbf{J}) |\mathbf{0}\rangle$$
$$= \int d\mathbf{k}_r e^{2\pi i \mathbf{w}_r\cdot\mathbf{k}_r} \langle \mathbf{k}_r| \rho_0(t, \mathbf{J}) |\mathbf{0}\rangle, \quad (7.3)$$

where

$$\mathbf{k} = \mathbf{k}_r + \mathbf{k}_s, \quad |\mathbf{k}_r\rangle \equiv |\mathbf{k}_r, \mathbf{k}_s = \mathbf{0}\rangle. \quad (7.4)$$

Define

$$|\mathbf{w}_r\rangle = \int d\mathbf{k}_r e^{-2\pi i \mathbf{w}_r\cdot\mathbf{k}_r} |\mathbf{k}_r\rangle, \quad (7.5)$$

so that, according to (3.6),

$$|\mathbf{w}_r\rangle = \int d\mathbf{w}_s \int d\mathbf{k} e^{-2\pi i \mathbf{w}\cdot\mathbf{k}} |\mathbf{k}\rangle = \int d\mathbf{w}_s |\mathbf{w}\rangle. \quad (7.6)$$

Then, from (7.3) and (7.6),

$$\rho_r(t, \mathbf{w}_r, \mathbf{J}) = \langle \mathbf{w}_r| \rho_0(t, \mathbf{J}) |\mathbf{0}\rangle$$
$$= \mathrm{Tr}\, [\rho_0(t, \mathbf{J}) |\mathbf{w}_r\rangle \langle \mathbf{w}_r|]. \quad (7.7)$$

But also

$$\int d\mathbf{w}_s |\mathbf{w}\rangle \langle \mathbf{w}| = \int d\mathbf{w}_s \int d\mathbf{k} \int d\mathbf{k}' |\mathbf{k}\rangle e^{2\pi i \mathbf{w}\cdot(\mathbf{k}'-\mathbf{k})} \langle \mathbf{k}'|$$
$$= |\mathbf{w}_r\rangle \langle \mathbf{w}_r|, \quad (7.8)$$

so that, from (7.2),

$$\rho_0^r(t, \mathbf{J}) = \int d\mathbf{w}_r \int d\mathbf{w}_s |\mathbf{w}\rangle \rho_r(t, \mathbf{w}_r, \mathbf{J}) \langle \mathbf{w}|$$
$$= \int d\mathbf{w}_r |\mathbf{w}_r\rangle \rho_r(t, \mathbf{w}_r, \mathbf{J}) \langle \mathbf{w}_r|. \quad (7.9)$$

From (7.9),

$$\rho_r(t, \mathbf{w}_r, \mathbf{J}) = \mathrm{Tr}\, [\rho_0^r(t, \mathbf{J}) |\mathbf{w}_r\rangle \langle \mathbf{w}_r|]. \quad (7.10)$$

Accordingly, $\rho_0^r(t, \mathbf{J})$ is an operator in a reduced Hilbert space spanned by the set of vectors $\{|\mathbf{w}_r\rangle\}$ or $\{|\mathbf{k}_r\rangle\}$. Thus, we have

$$\int d\mathbf{w}_r |\mathbf{w}_r\rangle \langle \mathbf{w}_r| = \int d\mathbf{k}_r |\mathbf{k}_r\rangle \langle \mathbf{k}_r| = \mathbf{1}_r, \quad (7.11)$$

where $\mathbf{1}_r$ is the unit operator in the reduced Hilbert space, and

$$\langle \mathbf{k}_r' | \mathbf{k}_r\rangle = \delta(\mathbf{k}_r' - \mathbf{k}_r), \quad \langle \mathbf{w}_r' | \mathbf{w}_r\rangle = \delta(\mathbf{w}_r' - \mathbf{w}_r). \quad (7.12)$$

The unit operator $\mathbf{1}_r$ is also a projector onto the reduced Hilbert space, since

$$\mathbf{1}_r |\mathbf{w}\rangle = \int d\mathbf{k}_r |\mathbf{k}_r\rangle \langle \mathbf{k}_r | \mathbf{w}\rangle$$
$$= \int d\mathbf{k}_r |\mathbf{k}_r\rangle e^{-2\pi i \mathbf{w}_r\cdot\mathbf{k}_r} = |\mathbf{w}_r\rangle, \quad (7.13)$$

and, from Eqs. (7.7)–(7.9),

$$\mathbf{1}_r \rho_0(t, \mathbf{J}) \mathbf{1}_r = \int d\mathbf{w} |\mathbf{w}_r\rangle \mathrm{Tr}\, [\rho_0(t, \mathbf{J}) |\mathbf{w}\rangle \langle \mathbf{w}|] \langle \mathbf{w}_r|$$
$$= \int d\mathbf{w}_r |\mathbf{w}_r\rangle \mathrm{Tr}\, [\rho_0(t, \mathbf{J}) |\mathbf{w}_r\rangle \langle \mathbf{w}_r|] \langle \mathbf{w}_r|$$
$$= \rho_0^r(t, \mathbf{J}). \quad (7.14)$$

In agreement with (7.7) and (7.10), therefore,

$$\rho_r(t, \mathbf{w}_r, \mathbf{J}) = \mathrm{Tr}\, [\rho_0(t, \mathbf{J}) |\mathbf{w}_r\rangle \langle \mathbf{w}_r|]$$
$$= \mathrm{Tr}\, [\rho_0^r(t, \mathbf{J}) |\mathbf{w}_r\rangle \langle \mathbf{w}_r|]. \quad (7.15)$$

In (7.3), the Fourier transform of the reduced probability density,

$$\langle \mathbf{k}_r| \rho_0(t, \mathbf{J}) |\mathbf{0}\rangle = \langle \mathbf{k}_r| \rho_0^r(t, \mathbf{J}) |\mathbf{0}\rangle,$$

is obtained from $\langle \mathbf{k}| \rho_0(t, \mathbf{J}) |\mathbf{0}\rangle$, the Fourier transform of the total probability density, simply by setting $\mathbf{k} = \mathbf{k}_r$. Accordingly, from (4.11),

$$\frac{\partial}{\partial t} \langle \mathbf{k}_r| \rho_0^r(t, \mathbf{J}) |\mathbf{0}\rangle + 2\pi i \mathbf{k}_r \cdot \boldsymbol{\nu}_{1r}(\mathbf{J}) \langle \mathbf{k}_r| \rho_0^r(t, \mathbf{J}) |\mathbf{0}\rangle$$
$$= -i \langle \mathbf{k}_r| \mathfrak{L}_2 \sigma_0(t, \mathbf{J}) |\mathbf{0}\rangle$$
$$- \int_{-\infty}^{t} dt' g(t - t', \mathbf{k}_r, \mathbf{J}) \langle \mathbf{k}_r| \rho_0^r(t', \mathbf{J}) |\mathbf{0}\rangle. \quad (7.16)$$

For $\mathbf{k}_r = \mathbf{0}$, the generalized master equation (4.18) is recovered. Fourier transformation of (7.16) gives the time evolution equation of the reduced probability density $\rho_r(t, \mathbf{w}_r, \mathbf{J})$:

$$\frac{\partial \rho_r(t, \mathbf{w}_r, \mathbf{J})}{\partial t} + \boldsymbol{\nu}_{1r}(\mathbf{J}) \cdot \frac{\partial \rho_r(t, \mathbf{w}_r, \mathbf{J})}{\partial \mathbf{w}_r}$$
$$= -i \int d\mathbf{w}_s L_2(\mathbf{w}, \mathbf{J}) \sigma(t, \mathbf{w}, \mathbf{J})$$
$$- \int_{-\infty}^{t} dt' G(t - t', \mathbf{w}_r, \mathbf{J}) \rho_r(t', \mathbf{w}_r, \mathbf{J}). \quad (7.17)$$

It has already been noted that Eq. (4.14), in non-Markoffian form, is equivalent to a Markoffian equation, the Liouville equation itself. Similarly, the non-Markoffian equation (7.17) has an equivalent Markoffian form. The Liouville equation is

$$\frac{\partial \rho(t, \mathbf{w}, \mathbf{J})}{\partial t} + \boldsymbol{\nu}_1(\mathbf{J}) \cdot \frac{\partial \rho(t, \mathbf{w}, \mathbf{J})}{\partial \mathbf{w}}$$
$$= -iL_2(\mathbf{w}, \mathbf{J}) \rho(t, \mathbf{w}, \mathbf{J}), \quad (7.18)$$

but the interaction term, according to (4.8), is

$$-iL_2(\mathbf{w}, \mathbf{J}) \rho(t, \mathbf{w}, \mathbf{J})$$
$$= -iL_2(\mathbf{w}, \mathbf{J}) \sigma(t, \mathbf{w}, \mathbf{J})$$
$$- \int_{-\infty}^{t} dt' G(t - t', \mathbf{w}, \mathbf{J}) \rho(t', \mathbf{w}, \mathbf{J}). \quad (7.19)$$

Integration on $\mathbf{w}_s$ gives

$$\frac{\partial\rho(t, \mathbf{w}_r, \mathbf{J})}{\partial t} + \boldsymbol{\nu}_{1r}(\mathbf{J}) \cdot \frac{\partial\rho(t, \mathbf{w}_r, \mathbf{J})}{\partial \mathbf{w}_r} = -i\int d\mathbf{w}_s L_2(\mathbf{w}, \mathbf{J})\rho(t, \mathbf{w}, \mathbf{J}), \quad (7.20)$$

where

$$-i\int d\mathbf{w}_s L_2(\mathbf{w}, \mathbf{J})\rho(t, \mathbf{w}, \mathbf{J}) = -i\int d\mathbf{w}_s L_2(\mathbf{w}, \mathbf{J})\sigma(t, \mathbf{w}, \mathbf{J}) - \int_{-\infty}^{t} dt' G(t - t', \mathbf{w}_r, \mathbf{J})\rho_r(t', \mathbf{w}_r, \mathbf{J}). \quad (7.21)$$

The Markoffian equation (7.20) is equivalent to (7.17). In particular, the non-Markoffian generalized master equation (4.18) is equivalent to the Markoffian equation

$$\frac{\partial\rho(t, \mathbf{J})}{\partial t} = -i\int d\mathbf{w} L_2(\mathbf{w}, \mathbf{J})\rho(t, \mathbf{w}, \mathbf{J}) = \frac{\partial}{\partial \mathbf{J}} \cdot \int d\mathbf{w}\rho(t, \mathbf{w}, \mathbf{J}) \frac{\partial H_2(\mathbf{w}, \mathbf{J})}{\partial \mathbf{w}}, \quad (7.22)$$

since

$$-i\int d\mathbf{w} L_2(\mathbf{w}, \mathbf{J})\rho(t, \mathbf{w}, \mathbf{J}) = \frac{\partial}{\partial \mathbf{J}} \cdot \int d\mathbf{w}\sigma(t, \mathbf{w}, \mathbf{J}) \frac{\partial H_2(\mathbf{w}, \mathbf{J})}{\partial \mathbf{w}} - \int_{-\infty}^{t} dt' g(t - t', \mathbf{0}, \mathbf{J})\rho(t', \mathbf{J}). \quad (7.23)$$

Apart from the term in $\sigma_0(t, \mathbf{J})$, the non-Markoffian equations (7.16) and (7.17) are closed equations in the sense that in (7.16) only one Fourier coefficient $\langle \mathbf{k}_r | \rho_0^r(t, \mathbf{J}) | \mathbf{0} \rangle$ appears, and in (7.17) only one reduced distribution function $\rho_r(t, \mathbf{w}_r, \mathbf{J})$ appears; the equivalent Markoffian equation (7.20) contains the distribution function $\rho(t, \mathbf{w}, \mathbf{J})$, i.e., all Fourier coefficients, on the right-hand side. The term in $\sigma_0(t, \mathbf{J})$ in (7.16) and (7.17) is obtained directly from (5.8), and depends on all Fourier coefficients except $\langle \mathbf{k}_r | \sigma_0(t, \mathbf{J}) | \mathbf{0} \rangle$, initially. Asymptotically for $t \to \infty$, the interaction term of the Liouville equation vanishes, so that, as in (6.15),

$$\int d\mathbf{w}_s L_2(\mathbf{w}, \mathbf{J})\sigma(t, \mathbf{w}, \mathbf{J}) \to i\int_{-\infty}^{t} dt' G(t - t', \mathbf{w}_r, \mathbf{J})\rho_r(t', \mathbf{w}_r, \mathbf{J}). \quad (7.24)$$

In recent papers,[9] which have appeared since completion of this work, Muriel and Dresden have obtained a hierarchy of equations in the case of N particles interacting by central forces (and extended their results to include time-dependent outside fields). Their results agree with (7.17) when it is taken into account that their initial time is chosen at $t = 0$ rather than at $t = -\infty$. They emphasize that, in contrast to the BBGKY hierarchy, their hierarchy is decoupled in the coordinates. Their remarks apply equally to (7.17). The process of setting $\mathbf{k} = \mathbf{k}_r$, i.e., setting $\mathbf{k}_s = \mathbf{0}$, to obtain (7.16) is equivalent to integration over the coordinates $\mathbf{w}_s$ in the phase space. Integration over coordinates of the individual particles of their N-body system is the projection operation utilized by Muriel and Dresden. This operation should not be confused with the projection performed by the operator $\mathfrak{I}(k)$ of Eq. (3.22).

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Generalized Group-Theoretical Analysis of Spontaneous Symmetry Breaking*

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A group-theoretical analysis of spontaneous symmetry breaking is carried out in an extension of Glashow's work. A general theorem is proved which is then used to give several interesting results. Apart from a rederivation of Glashow's result, we are able to show, among other things, the following: If a hadronic triplet exists in nature which is nontrivially coupled to the rest of the hadrons, then octet enhancement immediately follows independently of any dynamical detail; in models containing the vector nonet, $\phi - \omega$ mixing can, in principle, occur as a particular form of spontaneous symmetry breaking in the octet pattern; and if octet enhancement holds, the very accurate mass formula $m_\phi^2 + m_\omega^2 = 2m_{k^*}^2$ is established without recourse to any dynamical detail. Under the same general assumption, a further relation is found relating the mass of the nonet with the mixing angle, which is $4m_{k^*}^2 - 3(\cos^2\theta m_\phi^2 + \sin^2\theta m_\omega^2) - m_\rho^2 = 0$.

1. INTRODUCTION

Let us suppose that for a specific problem in physics, we can write down a basic set of equations which is invariant under a certain symmetry group G. Then we would expect that solutions of these equations would reflect the full symmetry of the basic set of equations. If for some reason this is not the case, i.e., if there exists a solution which reflects some asymmetries with respect to the group G, then we say that a *spontaneous symmetry breaking* has occurred.

Such a possibility was discussed by Heisenberg and his coworkers.[1] They pointed out that the equations of quantum field theory are nonlinear operator equations. Since nonperturbative solutions to nonlinear equations do not, in general, possess the full symmetry of the equations themselves, it is conceivable that the field equations may be highly symmetric expressions, while their solutions may reflect the asymmetries of nature. Several calculations have been performed by various authors to confirm the above conjecture of Heisenberg *et al.* These calculations have been done with specific models. Jona-Losino and Nambu[2] considered a theory with a Lagrangian possessing γ_5 invariance and found that, although the basic Lagrangian contains no mass term $m\bar{\psi}\psi$ since such terms violate γ_5 invariance, a solution exists that admits fermions of finite mass. A calculation with similar conclusion was performed independently by Goldstone.[3] Baker and Glashow[4] considered a theory based on the Dyson equations, a set of coupled nonlinear equations relating the 1-particle Green's functions and the vertex functions for a set of particles, which were assumed to possess $SU(3)$ symmetry. They found that nonperturbative solutions exist that contain multiplets with respect to the symmetry group possessing nondegenerate masses. Their formulation of the problem is essentially a bootstrap requirement since they required that the physical masses are completely dynamical in origin. (Technically, this means setting the bare masses equal to zero.) Their conclusions, however, are not completely conclusive since, to overcome divergence difficulties, they had to employ cutoffs in some of the integrals and assume the dominance of a certain class of Feynman diagrams. Similar calculations have also been performed by other authors, some in the field-theoretical framework[5] others in terms of S-matrix theory.[6]

Glashow discussed, group-theoretically, a bootstrap problem of eight baryons interacting with each other with an interaction invariant under $SU(3)$.[7] He found that, if spontaneous mass splitting does occur under the condition that isospin and hypercharge are still conserved, then mass splitting must occur according to one of the following patterns:

(a) The mass-splitting matrix transforms as a unitary singlet: in this case, we do not have any mass splitting; the octet remains degenerate;

(b) The mass-splitting matrix transforms as the $I = 0$ and $Y = 0$ component of octet [the 8-dimensional irreducible representation of $SU(3)$]: in this case, we have the Gell-Mann–Okubo formula;

(c) The mass-splitting matrix transforms as the $I = 0$ and $Y = 0$ component of a 27-plet [the 27-dimensional irreducible representation of $SU(3)$]: in this case, we have a mass splitting where the masses satisfy the 27-plet formula[8]

$$m_N + m_\Xi = 3m_\Sigma - m_\Lambda .$$

In the rest of this paper, we shall present a generalization of Glashow's method, which, as we shall see, lends itself to a number of interesting applications. Incidentally, we shall present, as a by-product of a

more general theorem, a detailed proof of Glashow's results, which is almost totally absent in Glashow's extremely short article.

2. GENERALIZED GROUP-THEORETICAL TREATMENT

We consider a situation where the masses of a system of particles belonging to a number of $SU(3)$ multiplets are given dynamically by a set of equations. Such a set of equations may, for instance, come out of a bootstrap calculation. Let the set of equations be $SU(3)$ invariant.

For simplicity, we shall limit ourselves to the case where there are only two multiplets. If we expand the equations in terms of small deviations from $SU(3)$ symmetry and keep only linear terms, we have

$$\delta m_i^* = \sum_{j=1}^{m} F_{ji}\delta m_j^* + \sum_{\alpha=1}^{n} H_{\alpha i}\delta m_\alpha, \tag{1}$$

where δm_i^*, $i = 1, 2, \cdots, m$, and δm_α, $\alpha = 1, 2, \cdots, n$, denote mass splittings of the members of the two multiplets, respectively. [We have used the term "multiplet" here in a more general sense than usual, in that it does not have to correspond to an irreducible representation of $SU(3)$. It may correspond to a reducible representation such as the case of the vector "nonet." Our proof of the theorem is independent of the irreducibility of the multiplets.] All the detailed dynamics of the system, such as the coupling constants, has been relegated to the matrices (F_{ji}) and $(H_{\alpha i})$. Of course, to determine the various masses, equations involving δm_α on the left-hand side are also necessary and are also usually available in dynamical calculations. For the following discussion we only have to consider Eq. (1). To treat Eq. (1) group-theoretically, it turns out to be more convenient and fruitful to consider mass-splitting matrices instead. So we write, instead of (1),

$$\delta M_{ij} = \sum_{1\le l,k\le m} F_{lk,ij}\delta M_{lk} + \sum_{1\le\alpha,\beta\le n} H_{\alpha\beta,ij}\delta m_{\alpha\beta}. \tag{2}$$

We shall look upon (δM_{ij}) and $(\delta m_{\alpha\beta})$ as vectors in m^2- and n^2-dimensional vector spaces and $(F_{lk,ij})$ and $(H_{\alpha\beta,ij})$ as $m^2 \times m^2$ and $n^2 \times m^2$ matrices. Then, (2) can be written in the symbolic form

$$\delta M = \delta M \cdot \hat{F} + \delta m \cdot \hat{H}. \tag{3}$$

If we suppose that the two multiplets transform according to the $SU(3)$ unitary representations $\{m\}$ and $\{n\}$, respectively, it is easy to see the following:

$$\delta M \text{ transforms as } \{m\}^* \otimes \{m\}, \tag{4}$$

$$\delta m \text{ transforms as } \{n\}^* \otimes \{n\}, \tag{5}$$

where $\{m\}^*$ and $\{n\}^*$ are the adjoint representations of $\{m\}$ and $\{n\}$, respectively. The representations $\{m\}^* \otimes \{m\}$ and $\{n\}^* \otimes \{n\}$ are generally reducible. Let us assume, without loss of generality, that they can be reduced into the following form:

$$\{m\}^* \otimes \{m\} = D^{(1)} \oplus D^{(2)} \oplus D^{(3)} \oplus D^{(4)} \oplus D^{(5)}, \tag{6}$$

$$\{n\}^* \otimes \{n\} = D^{(1)} \oplus D^{(2)} \oplus D^{(3)} \oplus D^{(6)} \oplus D^{(7)}, \tag{7}$$

where the $D^{(i)}$ denote irreducible representations of $SU(3)$. The superscript (i) just labels the particular representation and has nothing to do with the dimensionality of the representation. Then, if Eq. (3) is invariant under $SU(3)$ and Eqs. (6) and (7) hold, then we can prove the following theorem.

Theorem: (I) If $D^{(i)}$ is not equivalent to $D^{(j)}$ for all $i \neq j$, then

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(2)}\hat{p}^{(2)} + \lambda^{(3)}\hat{p}^{(3)} + \lambda^{(4)}\hat{p}^{(4)} + \lambda^{(5)}\hat{p}^{(5)}, \tag{8}$$

$$\hat{H} = \mu^{(1)}\hat{\Pi}^{(1)} + \mu^{(2)}\hat{\Pi}^{(2)} + \mu^{(3)}\hat{\Pi}^{(3)}; \tag{9}$$

(II) If $D^{(3)}$ is equivalent to $D^{(4)}$, then

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(2)}\hat{p}^{(2)} + \lambda^{(3)}\hat{p}^{(3)} + \lambda^{(4)}\hat{p}^{(4)} + \lambda^{(5)}\hat{p}^{(5)} + \lambda^{(3,4)}\hat{p}^{(3,4)} + \lambda^{(4,3)}\hat{p}^{(4,3)}, \tag{10}$$

$$\hat{H} = \mu^{(1)}\hat{\Pi}^{(1)} + \mu^{(2)}\hat{\Pi}^{(2)} + \mu^{(3)}\hat{\Pi}^{(3)} + \mu^{(4,3)}\hat{\Pi}^{(4,3)}; \tag{11}$$

(III) If $D^{(3)}$ is equivalent to $D^{(6)}$, then

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(2)}\hat{p}^{(2)} + \lambda^{(3)}\hat{p}^{(3)} + \lambda^{(4)}\hat{p}^{(4)} + \lambda^{(5)}\hat{p}^{(5)}, \tag{12}$$

$$\hat{H} = \mu^{(1)}\hat{\Pi}^{(1)} + \mu^{(2)}\hat{\Pi}^{(2)} + \mu^{(3)}\hat{\Pi}^{(3)} + \mu^{(3,6)}\hat{\Pi}^{(3,6)}. \tag{13}$$

To define the symbols, let us denote the representation space of $\{m\}^* \otimes \{m\}$ by $S^{(m)}$, the representation space of $\{n\}^* \otimes \{n\}$ by $S^{(n)}$, the subspace of $S^{(m)}$ that generates the representation $D^{(j)}$ by $S^{(m,j)}$, and the subspace of $S^{(n)}$ that generates the representation $D^{(i)}$ by $S^{(n,i)}$. Then $\hat{p}^{(i)}$ $(S^{(m)} \to S^{(m)})$ is defined as the projection operator that projects the subspace $S^{(m,i)}$ onto itself, and $\hat{\Pi}^{(i)}$ $(S^{(n)} \to S^{(m)})$ is defined as that operator which maps any vector belonging to $S^{(n,i)}$ to that vector in $S^{(m,i)}$ with identical transformation properties and which maps the rest of $S^{(n)}$ to zero. In the case when $D^{(i)}$ is equivalent to $D^{(j)}$, $\hat{p}^{(i,j)}$ $(S^{(m)} \to S^{(m)})$ is the operator that maps any vector in $S^{(m,j)}$

to that vector in $S^{(m,i)}$ with identical transformation properties and maps the rest of $S^{(m)}$ to zero. In the case when $D^{(k)}$ is equivalent to $D^{(l)}$, $\hat{\Pi}^{(k,l)}$ is the operator that maps any vector in $S^{(n,l)}$ to that vector in $S^{(m,k)}$ with identical transformation properties and that maps the rest of $S^{(n)}$ to zero. $\lambda^{(i)}$, $\lambda^{(i,j)}$, $\mu^{(l)}$, and $\mu^{(l,k)}$ are all numerical constants.

Proof: Let us look at Eq. (3) under the $SU(3)$ transformation:

$$\delta M \to \delta M' = \delta M(U^* \otimes U), \tag{14}$$

$$\delta m \to \delta m' = \delta m(V^* \otimes V), \tag{15}$$

where U and V are representation matrices in $\{m\}$ and $\{n\}$, respectively, induced by the same group element in $SU(3)$. For (3) to be invariant under $SU(3)$, we must have

$$\delta M' = \delta M' \cdot \hat{F} + \delta m' \hat{H}. \tag{16}$$

Substituting (14) and (15) into (16), one gets

$$\delta M = \delta M(U^* \otimes U)\hat{F}(U^* \otimes U)^{-1} + \delta m(V^* \otimes V)\hat{H}(U^* \otimes U)^{-1}. \tag{17}$$

Comparing (3) and (17), one gets

$$(U^* \otimes U)\hat{F} = \hat{F}(U^* \otimes U), \tag{18}$$

$$(V^* \otimes V)\hat{H} = \hat{H}(U^* \otimes U). \tag{19}$$

From (6) and (7), we see that

$$U^* \otimes U = J^{-1}UJ, \tag{20}$$

$$V^* \otimes V = K^{-1}VK, \tag{21}$$

where J and K are unitary matrices and

$$U = \begin{Vmatrix} U_1 & & & & 0 \\ & U_2 & & & \\ & & U_3 & & \\ & & & U_4 & \\ 0 & & & & U_5 \end{Vmatrix}, \tag{22}$$

$$V = \begin{Vmatrix} U_1 & & & & 0 \\ & U_2 & & & \\ & & U_3 & & \\ & & & V_6 & \\ 0 & & & & V_7 \end{Vmatrix}. \tag{23}$$

It should be emphasized at this point that J and K are independent of the particular group element in $SU(3)$ which U and V represent. U_i and V_j are representation matrices belonging to the representations $D^{(i)}$ and $D^{(j)}$, respectively. Substituting (20) and (21) into (19), we have

$$V\tilde{H} = \tilde{H}U, \tag{24}$$

where

$$\tilde{H} = K\hat{H}J^{-1}. \tag{25}$$

Substituting (20) into (18), we have

$$U\tilde{F} = \tilde{F}U, \tag{26}$$

where

$$\tilde{F} = J\hat{F}J^{-1}. \tag{27}$$

Writing

$$U_x = \begin{Vmatrix} U_4 & 0 \\ 0 & U_5 \end{Vmatrix}, \quad V_x = \begin{Vmatrix} V_6 & 0 \\ 0 & V_7 \end{Vmatrix}, \tag{28}$$

we can divide $\tilde{H}$ into appropriate blocks in the form

$$\tilde{H} = \begin{Vmatrix} H_{11} & H_{12} & H_{13} & H_{1x} \\ H_{21} & H_{22} & H_{23} & H_{2x} \\ H_{31} & H_{32} & H_{33} & H_{3x} \\ H_{x1} & H_{x2} & H_{x3} & H_{xx} \end{Vmatrix} \tag{29}$$

and $\tilde{F}$ into

$$\tilde{F} = \begin{Vmatrix} F_{11} & F_{12} & F_{13} & F_{14} & F_{15} \\ F_{21} & F_{22} & F_{23} & F_{24} & F_{25} \\ F_{31} & F_{32} & F_{33} & F_{34} & F_{35} \\ F_{41} & F_{42} & F_{43} & F_{44} & F_{45} \\ F_{51} & F_{52} & F_{53} & F_{54} & F_{55} \end{Vmatrix}. \tag{30}$$

We have, from (24),

$$\begin{Vmatrix} U_1H_{11} & U_1H_{12} & U_1H_{13} & U_1H_{1x} \\ U_2H_{21} & U_2H_{22} & U_2H_{23} & U_2H_{2x} \\ U_3H_{31} & U_3H_{32} & U_3H_{33} & U_3H_{3x} \\ V_xH_{x1} & V_xH_{x2} & V_xH_{x3} & V_xH_{xx} \end{Vmatrix} = \begin{Vmatrix} H_{11}U_1 & H_{12}U_2 & H_{13}U_3 & H_{1x}U_x \\ H_{21}U_1 & H_{22}U_2 & H_{23}U_3 & H_{2x}U_x \\ H_{31}U_1 & H_{32}U_2 & H_{33}U_3 & H_{3x}U_x \\ H_{x1}U_1 & H_{x2}U_2 & H_{x3}U_3 & H_{xx}U_x \end{Vmatrix} \tag{31}$$

and, also, from (26),

$$\left\|\begin{array}{ccccc} U_1F_{11} & U_1F_{12} & U_1F_{13} & U_1F_{14} & U_1F_{15} \\ U_2F_{21} & U_2F_{22} & U_2F_{23} & U_2F_{24} & U_2F_{25} \\ U_3F_{31} & U_3F_{32} & U_3F_{33} & U_3F_{34} & U_3F_{35} \\ U_4F_{41} & U_4F_{42} & U_4F_{43} & U_4F_{44} & U_4F_{45} \\ U_5F_{51} & U_5F_{52} & U_5F_{53} & U_5F_{54} & U_5F_{55} \end{array}\right\| = \left\|\begin{array}{ccccc} F_{11}U_1 & F_{12}U_2 & F_{13}U_3 & F_{14}U_4 & F_{15}U_5 \\ F_{21}U_1 & F_{22}U_2 & F_{23}U_3 & F_{24}U_4 & F_{25}U_5 \\ F_{31}U_1 & F_{32}U_2 & F_{33}U_3 & F_{34}U_4 & F_{35}U_5 \\ F_{41}U_1 & F_{42}U_2 & F_{43}U_3 & F_{44}U_4 & F_{45}U_5 \\ F_{51}U_1 & F_{52}U_2 & F_{53}U_3 & F_{54}U_4 & F_{55}U_5 \end{array}\right\|. \tag{32}$$

From $H_{ij}U_j = U_iH_{ij}$, $1 \leq i, j \leq 3$, in (31), we have, using Schur's lemma,[9]

$$H_{ij} = \delta_{ij}\mu^{(i)}I_{(i)}, \quad i,j = 1,2,3, \tag{33}$$

and, from $F_{kl}U_l = U_kF_{kl}$, $k, l = 1, 2, 3, 5$,

$$F_{kl} = \delta_{kl}\lambda^{(k)}I_{(k)}, \quad k,l = 1,2,3,5, \tag{34}$$

where δ_{ij} and δ_{kl} are Kronecker δ symbols, $\mu^{(i)}$ and $\lambda^{(k)}$ are unknown numerical constants, and $I_{(i)}$ and $I_{(k)}$ are identity matrices of appropriate dimensions. We shall now specialize to the various cases.

(I) *$D^{(i)}$ is not equivalent to $D^{(j)}$ for all unequal i, j.* From (31), we have

$$U_iH_{ix} = H_{ix}U_x, \quad i = 1,2,3. \tag{35}$$

Let ξ be a vector that transforms like $D^{(1)}$. Then, under the group operation in question, $\xi \to \xi U_1$. The vector

$$\xi H_{1x} \to (\xi U_1)H_{1x} = (\xi H_{1x})U_x, \tag{36}$$

where we have made use of the fact that H_{1x} does not transform under $SU(3)$ and also the equality (35). Hence, the vector ξH_{1x} transforms according to $D^{(x)} = D^{(4)} \oplus D^{(5)}$. If ξH_{1x} is nontrivial, there exists a vector subspace of the representation space of $D^{(1)}$ that transforms like $D^{(x)}$, which is in contradiction with our assumption. Hence $\xi H_{1x} = 0$, for all ξ, which requires that

$$H_{1x} = 0. \tag{37}$$

Similarly, we can prove $H_{x1} = H_{x2} = H_{2x} = H_{x3} = H_{3x} = 0$. A similar argument can be applied to the equation $H_{xx}U_x = V_xH_{xx}$, with the result that $H_{xx} = 0$.

Hence, we have, for this case,

$$\tilde{H} = \left\|\begin{array}{cccc} \mu^{(1)}I_{(1)} & 0 & 0 & 0 \\ 0 & \mu^{(2)}I_{(2)} & 0 & 0 \\ 0 & 0 & \mu^{(3)}I_{(3)} & 0 \\ 0 & 0 & 0 & 0 \end{array}\right\|. \tag{38}$$

The equalities in (33) and (34) can be extended in this case to $1 \leq k, l \leq 5$, resulting in

$$\tilde{F} = \left\|\begin{array}{ccccc} \lambda^{(1)}I_{(1)} & & & & \\ & \lambda^{(2)}I_{(2)} & & 0 & \\ & & \lambda^{(3)}I_{(3)} & & \\ & 0 & & \lambda^{(4)}I_{(4)} & \\ & & & & \lambda^{(5)}I_{(5)} \end{array}\right\|. \tag{39}$$

Equations (38) and (39) establish our assertions (8) and (9) for Case (I).

(II) *$D^{(3)}$ is equivalent to $D^{(4)}$.* In this case, J can be chosen so that $U_3 = U_4$. Then

$$U_x = \left\|\begin{array}{cc} U_3 & 0 \\ 0 & U_5 \end{array}\right\|. \tag{40}$$

From (35), we have

$$U_3H_{3x} = H_{3x}U_x; \tag{41}$$

we write

$$H_{3x} = \|H_{3x}^{(1)} \mid H_{3x}^{(2)}\|. \tag{42}$$

Then, from (41),

$$\|U_3H_{3x}^{(1)} \mid U_3H_{3x}^{(2)}\| = \|H_{3x}^{(1)}U_3 \mid H_{3x}^{(2)}U_5\| \tag{43}$$

and, hence,

$$H_{3x}^{(1)} = \mu^{(4,3)}I_{(3)}, \quad H_{3x}^{(2)} = 0. \tag{44}$$

All the other conclusions about the H-submatrices are the same as in Case (I). Thus, we have, in this case,

$$\tilde{H} = \left\|\begin{array}{ccccc} \mu^{(1)}I_{(1)} & & & & 0 \\ & \mu^{(2)}I_{(2)} & & & \\ & & \mu^{(3)}I_{(3)} & \mu^{(4,3)}I_{(3)} & 0 \\ 0 & & 0 & 0 & 0 \end{array}\right\|. \tag{45}$$

We can also easily show that

$$\tilde{F} = \left\| \begin{array}{ccccc} \lambda^{(1)}I_{(1)} & & & & 0 \\ & \lambda^{(2)}I_{(2)} & & & \\ & & \lambda^{(3)}I_{(3)} & \lambda^{(4,3)}I_{(3)} & \\ & & \lambda^{(3,4)}I_{(3)} & \lambda^{(4)}I_{(3)} & \\ 0 & & & & \lambda^{(5)}I_{(5)} \end{array} \right\|. \tag{46}$$

(III) $D^{(3)}$ *is equivalent to* $D^{(6)}$. In this case, the only equality obtainable from (31) which will give rise to conclusions different from Case (I) is

$$V_x H_{x3} = H_{x3} U_3. \tag{47}$$

Since

$$V_x = \left\| \begin{array}{c|c} U_3 & 0 \\ \hline 0 & V_7 \end{array} \right\|, \tag{48}$$

we shall now write

$$H_{x3} = \left\| \begin{array}{c} H_{x3}^{(1)} \\ \hline H_{x3}^{(2)} \end{array} \right\| \tag{49}$$

and get, from (48),

$$\left\| \begin{array}{c} U_3 H_{x3}^{(1)} \\ \hline V_7 H_{x3}^{(2)} \end{array} \right\| = \left\| \begin{array}{c} H_{x3}^{(1)} U_3 \\ \hline H_{x3}^{(2)} U_3 \end{array} \right\|. \tag{50}$$

Hence,

$$H_{x3}^{(1)} = \mu^{(3,6)} I_{(3)}, \quad H_{x3}^{(2)} = 0.$$

Therefore,

$$\tilde{H} = \left\| \begin{array}{ccccc} \mu^{(1)}I_{(1)} & & & & 0 \\ & \mu^{(2)}I_{(2)} & & & \\ & & \mu^{(3)}I_{(3)} & & \\ & & \mu^{(3,6)}I_{(3)} & & \\ 0 & & & & 0 \end{array} \right\|. \tag{51}$$

It is also straightforward to show that

$$\tilde{F} = \left\| \begin{array}{ccccc} \lambda^{(1)}I_{(1)} & & & & \\ & \lambda^{(2)}I_{(2)} & & & \\ & & \lambda^{(3)}I_{(3)} & & \\ & & & \lambda^{(4)}I_{(4)} & \\ & & & & \lambda^{(5)}I_{(5)} \end{array} \right\|. \tag{52}$$

QED

3. APPLICATIONS OF THE GENERAL RESULTS

A. Glashow's Results

We shall reproduce Glashow's results[7] on the bootstrapping of an octet of baryons. There we have the equation

$$\delta m_i^* = \sum_{j=1}^{8} F_{ji} \delta m_j^*. \tag{53}$$

Comparing this with (1), we have $\hat{H} = 0$. Now $\{m\} = \{8\}$ and, hence, the mass matrix (δM_{ij}) will transform according to

$$\{8\}^* \otimes \{8\} = \{1\} \oplus \{8_D\} \oplus \{8_F\} \oplus \{10\} \oplus \{10\}^* \oplus \{27\}, \tag{54}$$

where $\{8_D\}$ and $\{8_F\}$ are equivalent. Then using the theorem for case (II), we have

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(10)}\hat{p}^{(10)} + \lambda^{(10^*)}\hat{p}^{(10^*)} + \lambda^{(27)}\hat{p}^{(27)} + \lambda^{(D)}\hat{\hat{p}}^{(D)} + \lambda^{(F)}\hat{p}^{(F)} + \lambda^{(F,D)}\hat{p}^{(F,D)} + \lambda^{(D,F)}\hat{\hat{p}}^{(D,F)}, \tag{55}$$

where the λ's are numerical constants and the $\hat{p}$ operators have the meanings assigned to them in the general theorem.

We shall now make the following assumptions:

(A) *The mass-splitting matrix transforms as a single irreducible tensor of SU(3) and*

(B) *the spontaneous symmetry breaking does not disrupt isospin and hypercharge conservation.*

As we have seen, the matrix (δM) transforms as $\{8\}^* \otimes \{8\}$, which can be decomposed according to (54). From (54) we can now pick out all the possible states that are invariant under isospin transformations and hypercharge gauge transformation. Having picked out these states, which are represented by 8×8 matrices, these matrices can be calculated by using the $SU(3)$ CG coefficients.[8,10] These matrices with respect to the basis $(p, n, \Sigma^+, \Sigma^0, \Sigma^-, \Lambda, \Xi^0, \Xi^-)$ are given as follows:

$$\delta M \approx |\{8_D\}, \quad I = 0, \quad Y = 0\rangle \sim 1/\sqrt{20}\ \text{diag}\{-1, -1, 2, 2, 2, -2, -1, -1\}, \tag{56}$$

$$\delta M \sim |\{8_F\}, \quad I = 0, \quad Y = 0\rangle \sim \tfrac{1}{2}\ \text{diag}\{-1, -1, 0, 0, 0, 0, +1, +1\}. \tag{57}$$

If the mass splitting transforms as a linear superposition of (56) and (57), i.e., if it transforms like a general octet component, then

$$\delta m_N = -\alpha - \beta, \quad \delta m_\Sigma = 2\alpha, \quad \delta m_\Lambda = -2\alpha, \quad \delta m_\Xi = -\alpha + \beta. \tag{58}$$

Eliminating α and β from (58), we can easily show that

the GMO formula

$$\tfrac{1}{2}(\delta m_N + \delta m_\Xi) = \tfrac{3}{4}\delta m_\Lambda + \tfrac{1}{4}\delta m_\Sigma \tag{59}$$

must be satisfied. We have

$$\delta M \sim |\{27\},\quad I=0,\quad Y=0\rangle$$
$$\sim \sqrt{\tfrac{3}{40}}\ \text{diag}\,\{1, 1, -\tfrac{1}{3}, -\tfrac{1}{3}, -\tfrac{1}{3}, -3, 1, 1\}. \tag{60}$$

It can be similarly shown that the above mass splitting satisfies the formula

$$\delta m_N + \delta m_\Xi = 3\delta m_\Sigma - \delta m_\Lambda \tag{61}$$

which was given by De Swart.[8] It is well known that this so-called 27-plet formula is not satisfied experimentally. Also, we note that Eq. (61) is a weaker requirement than (60). We have

$$\delta M \sim |\{1\},\quad I=0,\quad Y=0\rangle$$
$$\sim 1/\sqrt{8}\ \text{diag}\,\{1, 1, 1, 1, 1, 1, 1, 1\}, \tag{62}$$

in which case we have no mass splitting.

B. Bootstrap Involving the Baryon Decuplet and the Baryon Octet (the B–Δ Bootstrap)

Let δm_i^* denote the mass splitting of the decuplet and δm_α denote the mass splitting of the octet:

$$\delta m_i^* = \sum_{j=1}^{10} F_{ji}\delta m_j^* + \sum_{\alpha=1}^{8} H_{\alpha i}\delta m_\alpha. \tag{63}$$

Now, since

$$\{10\}^* \otimes \{10\} = \{1\} \oplus \{8\} \oplus \{27\} \oplus \{64\},$$
$$\{8\}^* \otimes \{8\} = \{1\} \oplus \{8_D\} \oplus \{8_F\} \oplus \{10\} \oplus \{10\}^* \oplus \{27\}. \tag{64}$$

We can quote Case III of our general theorem to write

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(8)}\hat{p}^{(8)} + \lambda^{(27)}\hat{p}^{(27)} + \lambda^{(64)}\hat{p}^{(64)}, \tag{65}$$

$$\hat{H} = \mu^{(1)}\hat{\Pi}^{(1)} + \mu^{(8,D)}\hat{\Pi}^{(8,D)} + \mu^{(8,F)}\hat{\Pi}^{(8,F)} + \mu^{(27)}\hat{\Pi}^{(27)}, \tag{66}$$

where the notations are by now self-explanatory. Let (δM) denote the 10×10 mass-splitting matrix of the decuplet and (δm) the 8×8 mass-splitting matrix of the octet. We make now the following further assumption:

(C) *All multiplets that have been taken into the bootstrap are nontrivially coupled.* In other words, any mass splitting in one particular multiplet is going to have nonzero effect on the masses of the other multiplets involved in the bootstrap problem.

Then, since $\hat{H}$ only connects mass matrices with identical transformation properties, we conclude that, if (δm) transforms like a certain $SU(3)$ irreducible tensor, then (δM) will also transform like the same irreducible tensor. In particular,

(a) If (δm) transforms as a linear combination of (56) and (57), i.e., if the baryon octet satisfies the GMO formula, then (δM) must be proportional to diag $\{1, 1, 1, 1, 0, 0, 0, -1, -1, -2\}$. That is, we have the equal-spacing rule for the decuplet, which is very well satisfied experimentally.

(b) If (δm) transforms as in (60), then (δM) must be proportional to diag $\{3, 3, 3, 3, -5, -5, -5, -3, -3, -9\}$ which gives rise to the mass formula

$$\tfrac{1}{8}[m(N^*) - m(Y^*)] = -\tfrac{1}{2}[m(Y^*) - m(\Xi^*)] = \tfrac{1}{6}[m(\Xi^*) - m(\Omega^-)], \tag{67}$$

which is not at all in agreement with experiment.

(c) If (δm) transforms as in (62), i.e., if there is no mass-splitting in the octet, then (δM) must be proportional to diag $\{1, 1, 1, 1, 1, 1, 1, 1, 1, 1\}$. In other words, there is also no mass splitting in the decuplet.

C. Existence of a Unitary Triplet and Octet Enhancement

Suppose there exists a triplet which is nontrivially coupled to the rest of the hadrons, by which we mean that the mass splitting of the triplet has nonzero effect on the other multiplets. For simplicity, but without loss of actual generality, we shall assume that the triplet is only coupled to an octet of baryons. Then we have

$$\delta m_i^* = \sum_{j=1}^{8} F_{ji}\delta m_j^* + \sum_{\alpha=1}^{3} H_{\alpha i}\delta m_\alpha, \tag{68}$$

where δm_i^* denotes mass splitting within the octet and δm_α denotes the mass splitting in the triplet, respectively. Then, because of

$$\{3\}^* \otimes \{3\} = \{1\} \oplus \{8\} \tag{69}$$

and the decomposition (54), we have

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(10)}\hat{p}^{(10)} + \lambda^{(10*)}\hat{p}^{(10*)} + \lambda^{(27)}\hat{p}^{(27)} + \lambda^{(D)}\hat{p}^{(D)} + \lambda^{(F)}\hat{p}^{(F)} + \lambda^{(F,D)}\hat{p}^{(F,D)} + \lambda^{(D,F)}\hat{p}^{(D,F)}, \tag{70}$$

$$\hat{H} = \mu^{(1)}\hat{\Pi}^{(1)} + \mu^{(D,8)}\hat{\Pi}^{(D,8)} + \mu^{(F,8)}\hat{\Pi}^{(F,8)}. \tag{71}$$

We see that $\hat{H}$, apart from $\hat{H}^{(1)}$ which does not connect actual mass splittings among the multiplets, involves only "projection operators" which connect irreducible matrices transforming like a component of $\{8\}$. From our assumption (C) that the triplet is nontrivially coupled to the octet and (A) that the mass splitting of each multiplet transforms like a single irreducible tensor, it obviously follows that the mass splitting of the baryon octet must transform like a component of an octet and, hence, must obey the Gell-Mann–Okubo formula.

Hence, we have obtained octet enhancement independently of any detailed dynamics as soon as we assume the existence of a triplet which is nontrivially coupled to the hadrons. In the above argument, we do

not have to assume that this triplet of particles are quarks, i.e., fundamental building blocks of all matter. We know that the GMO formula can be deduced from quark models[11]: but all these derivations depend on a greater or lesser extent to some drastic dynamical approximations. The foregoing group-theoretical argument, however, is independent of any dynamical detail or assumption.

Since triplets have not yet been discovered, we cannot attribute the phenomenon of octet enhancement lightly to the influence of triplets.

It is interesting to note that, if there are no triplets or other multiplets with nonzero triality, then we cannot carry out an argument similar to the above to account for octet enhancement, no matter how many "tensorial" multiplets we put into our bootstrap. [Triality is defined, for the representation $\{n\} = D(p, q)$ as $t \equiv (p - q) \bmod (3)$. Tensorial representations are those with $t = 0$. All known hadronic multiplets to date fall into tensorial representations.] This is because, for all tensorial representations $\{n\}$ (except $\{1\}$),

$$\{n\}^* \otimes \{n\} = \{1\} \oplus \{8\} \oplus \{27\} \oplus \cdots . \quad (72)$$

The $\{27\}$ always appears in the CG series.

We can show this most easily by using Speiser method for obtaining the CG series (see J. J. De Swart, Ref. 8, pp. 326–327). We have to find the CG series of $D(q, p) \otimes D(p, q)$ [since $D(q, p) = D(p, q)^*$], for all p and q such that $p \equiv q \pmod 3$, and see whether they all contain the $\{27\} = D(2, 2)$. It turns out that, if we put the eigenvalue diagram of $D(q, p)$ on top of the point (p, q) in the lattice diagram (Figs. 5 and 6 in De Swart, Ref. 8) in the way specified by the Speiser method, we can show by simple geometry that, for all $p \equiv q \pmod 3$, the eigenvalue diagram always covers the point (2, 2) in the first sextant of the lattice, but never the image points of (2, 2) in the other sextants. By Speiser's rule, this shows that $D(q, p) \otimes D(p, q)$ always contains the $\{27\} = D(2, 2)$ in the CG decomposition.

D. Spontaneous ϕ–ω Mixing

Let us consider a bootstrap problem where an octet of vector mesons and a singlet vector meson are involved. It may be necessary in practice to put in more particles in order to complete the bootstrap, say, the pseudoscalar octet: but the conclusions to be discussed below will be essentially unchanged. We must bear in mind also that, when we say "mass matrix," it is actually the mass-squared matrix that we are referring to since we are concerned here with bosons. Let us write the mass matrix of the nonet in the basis $(K^{*+}, K^{*0}, \rho^+, \rho^0, \rho^-, \bar{K}^{*0}, K^{*-}, \omega^8, \omega')$, where $|\omega^8\rangle$ transforms as the eighth component of an octet and $|\omega'\rangle$ is a unitary singlet. The nonet of vector mesons transform as

$$\{1\} \oplus \{8\}. \quad (73)$$

Note that now we have a reducible representation of $SU(3)$. This does not matter since, as we have stressed in Sec. 2, our theorem applies equally well to reducible multiplets. Because of (73), the mass-splitting matrix (δM_{ij}) transforms as

$$\begin{aligned}(\{1\} \oplus \{8\})^* \otimes (\{1\} \oplus \{8\}) \\ = \{1\} \oplus \{1\}' \oplus \{8_D\} \oplus \{8_F\} \oplus \{8_x\} \oplus \{8_y\} \oplus \{10\} \\ \oplus \{10\}^* \oplus \{27\}, \quad (74)\end{aligned}$$

where $\{1\}$ and $\{1\}'$ are equivalent to each other. $\{8_D\}$, $\{8_F\}$, $\{8_x\}$, and $\{8_y\}$ are all equivalent. If mass splitting should occur spontaneously, they would be proportional to either of the following matrices if isospin and hypercharge still are conserved:

(a) $\Delta M \sim |\{8_D\},\ I = 0,\ Y = 0\rangle$
$\sim 1/\sqrt{20}\ \mathrm{diag}\{-1, -1, 2, 2, 2, -1, -1, -2, 0\}$,

(b) $\Delta M \sim |\{8_F\},\ I = 0,\ Y = 0\rangle$
$\sim \frac{1}{2}\ \mathrm{diag}\{-1, -1, 0, 0, 0, 1, 1, 0, 0\}$,

(c) $\Delta M \sim |\{27\},\ I = 0,\ Y = 0\rangle$
$\sim \sqrt{\frac{3}{40}}\ \mathrm{diag}\{1, 1, -\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}, 1, 1, -3, 0\}$,

(d) $\Delta M \sim |\{8_x\};\ I = 0,\ Y = 0\rangle$

$$\sim 1/\sqrt{2} \left\| \begin{array}{c|cc} 0 & 0 & \\ \hline 0 & 0 & 1 \\ & 1 & 0 \end{array} \right\|,$$

(e) $\Delta M \sim |\{8_y\},\ I = 0,\ Y = 0\rangle$

$$\sim 1/\sqrt{2} \left\| \begin{array}{c|cc} 0 & 0 & \\ \hline 0 & 0 & -i \\ & i & 0 \end{array} \right\|,$$

(f) $\Delta M \sim |\{1\},\ I = 0,\ Y = 0\rangle$
$\sim 1/\sqrt{8}\ \mathrm{diag}\{1, 1, 1, 1, 1, 1, 1, 1, 0\}$,

(g) $\Delta M \sim |\{1\}',\ I = 0,\ Y = 0\rangle$
$\sim \mathrm{diag}\{0, 0, 0, 0, 0, 0, 0, 0, 1\}$.

For our particular mesonic system, the possibility of (b) can be ruled out because of charge conjugation invariance. This is because, if a mass splitting occurs in accordance with (b), then the K^* and its antiparticle $\bar{K}^*$ will have mass shifts with opposite signs, resulting in $m(K^*) \neq m(\bar{K}^*)$, in contradiction with charge conjugation invariance or more generally with CPT invariance.[12]

We shall make the assumption that *the nonet is degenerate to start with.* That is, we shall neglect mass splittings coming from (f) and (g).

We shall illustrate how spontaneous mixing sets in by considering the very simple case where symmetry breaking occurs in accordance with (d). Then, to find the mass of the physical states, it is necessary to diagonalize (d) by the orthogonal transformation:

$$\begin{Vmatrix} 1 & & & & & & & & \\ & 1 & & & & & & 0 & \\ & & 1 & & & & & & \\ & & & 1 & & & & & \\ & & & & 1 & & & & \\ & & & & & 1 & & & \\ & & & & & & 1 & & \\ & & & & & & & 1/\sqrt{2} & 1/\sqrt{2} \\ & & 0 & & & & & -1/\sqrt{2} & 1/\sqrt{2} \end{Vmatrix}. \tag{75}$$

That is, the physical states are, instead of $|\omega^8\rangle$ and $|\omega'\rangle$,

$$\begin{aligned} |\phi\rangle &= \cos\theta\,|\omega^8\rangle + \sin\theta\,|\omega'\rangle, \\ |\omega\rangle &= -\sin\theta\,|\omega^8\rangle + \cos\theta\,|\omega'\rangle, \end{aligned} \tag{76}$$

where $\theta = 45°$. Hence, the ϕ and ω mesons are equal mixtures of $|\omega^8\rangle$ and $|\omega'\rangle$.

We shall see now what happens when we *impose the general condition of octet enhancement.* That is, we shall assume that there are no symmetry breakings except those which transform like a component of an octet. In other words, we shall assume that the mass-splitting matrix is proportional to a general linear combination of the various "8-matrices" (a), (d), and (e) and that, in particular, mass splitting in accordance with (c), which transforms like a component of the 27-plet, cannot occur. In that case, the mass matrix looks like

$$\begin{Vmatrix} 1+\beta & & & & & & & & \\ & 1+\beta & & & & & & 0 & \\ & & 1-2\beta & & & & & & \\ & & & 1-2\beta & & & & & \\ & & & & 1-2\beta & & & & \\ & & & & & 1+\beta & & & \\ & & & & & & 1+\beta & & \\ & & 0 & & & & & 1+2\beta & \gamma-i\delta \\ & & & & & & & \gamma+i\delta & 1 \end{Vmatrix}. \tag{77}$$

This matrix can be diagonalized into the form

$$\begin{aligned} \operatorname{diag}\{&1+\beta, 1+\beta, 1-2\beta, 1-2\beta, 1-2\beta, \\ &1+\beta, 1+\beta, 1+\beta+(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}, \\ &1+\beta-(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}\}, \end{aligned} \tag{78}$$

with the transformation

$$\begin{aligned} |\phi\rangle &= \cos\theta\,|\omega^8\rangle + \sin\theta e^{i\chi}\,|\omega'\rangle, \\ |\omega\rangle &= -e^{-i\chi}\sin\theta\,|\omega^8\rangle + \cos\theta\,|\omega'\rangle, \end{aligned} \tag{79}$$

where

$$\begin{aligned} \sin\theta &= \frac{(\gamma^2+\delta^2)^{\frac{1}{2}}}{\{2(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}[(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}+\beta]\}^{\frac{1}{2}}}, \\ \cos\theta &= \frac{\beta+(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}}{\{2(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}[(\beta^2+\gamma^2+\delta^2)^{\frac{1}{2}}+\beta]\}^{\frac{1}{2}}}, \\ \chi &= \arctan(-\delta/\gamma). \end{aligned} \tag{80}$$

If we define

$$\begin{aligned} |\tilde{\omega}'\rangle &= e^{i\chi}\,|\omega'\rangle, \\ |\tilde{\omega}\rangle &= e^{i\chi}\,|\omega\rangle, \end{aligned} \tag{81}$$

we have

$$\begin{aligned} |\phi\rangle &= \cos\theta\,|\omega^8\rangle + \sin\theta\,|\tilde{\omega}'\rangle, \\ |\tilde{\omega}\rangle &= -\sin\theta\,|\omega^8\rangle + \cos\theta\,|\tilde{\omega}'\rangle. \end{aligned} \tag{82}$$

If we had used $|\tilde{\omega}'\rangle$ instead of $|\omega'\rangle$ all along in our basis, we would have avoided the appearance of δ in (77). Since we are free to do this, we shall assume that this proper choice of phase has been made and from now on we are going to look at (77), (78), and (80) with the understanding that $\delta = 0$.

Then we have, from (78),

$$\begin{aligned} m_{K^*} &= m_{\bar{K}^*} = 1+\beta, \\ m_\rho &= 1-2\beta, \\ m_\phi &= 1+\beta+(\beta^2+\gamma^2)^{\frac{1}{2}}, \\ m_\omega &= 1+\beta-(\beta^2+\gamma^2)^{\frac{1}{2}}. \end{aligned} \tag{83}$$

It follows easily from (88) that

$$m_\phi + m_\omega = 2m_{K^*}. \tag{84}$$

This result is independent of the mixing angle and is good to within 2% experimentally. From Eqs. (80)

and (83), we can establish the further relation

$$4m_{K^*} - 3(\cos^2\theta m_\phi + \sin^2\theta m_\omega) - m_\rho = 0. \quad (85)$$

This result, as an afterthought, is hardly surprising since it is exactly the GMO formula, if one considers $\cos^2\theta m_\phi + \sin^2\theta m_\omega$ to be the mass of the eighth component of an octet, whose other components consist of the isotriplet ρ, the doublet K^*, and its antiparticles $\bar{K}^*$.

Let us summarize our results here. Starting from a nonet of vector mesons which we assume to possess (accidentally) degenerate mass, we find that mixing between the two $I = 0$ and $Y = 0$ mesons can, in principle, occur as a particular form of spontaneous symmetry breaking. The mass-splitting matrices corresponding to such symmetry violations transform as the eighth component of an octet, thus suggesting that ϕ–ω mixing is just another manifestation of octet enhancement in symmetry breaking. Conversely, assuming octet enhancement in symmetry breaking in its most general form, we find that spontaneous symmetry breaking in the vector nonet can only occur in such a way as to satisfy Eqs. (84) and (85).

We have no way, in this group-theoretical discussion, of determining the mixing angle θ. To get some feeling about the kind of mixing angle that would emerge from (85), let us put

$$m_\omega = m_\rho, \quad (86)$$

which is well satisfied experimentally. We get, after substituting this into (84) and (85), that

$$\cos^2\theta = \tfrac{2}{3} \cong 67\%. \quad (87)$$

In other words, the meson is a member of an octet 67% of the time and a singlet 33% of the time.

It is interesting to compare our results with those of other authors who "computed" mass formulas and mixing angles in more specific models.

i. Triplet Models

To be specific, we shall describe Zweig's model.[11] In this model, the vector mesons are considered as quark–antiquark bound states. More precisely,

$$|\rho^+\rangle = |a^2a_1\rangle, \quad |k^{*+}\rangle = |a^3a_1\rangle,$$
$$|\phi\rangle = -|a^3a_3\rangle, \quad |\omega\rangle = 1/\sqrt{2}\{|a^1a_1\rangle + |a^2a_2\rangle\}. \quad (88)$$

Now, we know that the states

$$|\omega^8\rangle = 1/\sqrt{6}\{|a^1a_1\rangle + |a^2a_2\rangle - 2|a^3a_3\rangle\},$$
$$|\omega'\rangle = 1/\sqrt{3}\{|a^1a_1\rangle + |a^2a_2\rangle + |a^3a_3\rangle\} \quad (89)$$

transform as the eighth component of an octet and a unitary singlet, respectively, as can be checked by direct computation based on the assumed transformation properties of $|a^i\rangle$ and $|a_j\rangle$. The last two states in (88) can be written as linear combinations of states in (89) as follows:

$$|\phi\rangle = \cos\theta\,|\omega^8\rangle + \sin\theta\,|\omega'\rangle,$$
$$|\omega\rangle = -\sin\theta\,|\omega^8\rangle + \cos\theta\,|\omega'\rangle, \quad (90)$$

where

$$\cos\theta = \sqrt{\tfrac{2}{3}}, \quad \sin\theta = \sqrt{\tfrac{1}{3}}. \quad (91)$$

Using formula (88), we can compute the masses of the nine vector mesons in terms of the masses of their constituent quarks. This gives the formula (86) and

$$4m_{K^*} - 2m_\phi - m_\omega - m_\rho = 0, \quad (92)$$

which can be recognized as a special case of (85) by setting $\cos\theta = \sqrt{\frac{2}{3}}$. It is important to emphasize that even in this specific model of dubious validity (e.g., the existence of quarks!), nothing more is really derived than in the general group theoretical discussion. As we have shown, octet enhancement is a consequence of the "existence" of a unitary triplet. The accidental degeneracy of the nonet is implicit in the definition of all the nine vector mesons as the same kind of quark–antiquark states. The mixing angle is actually introduced already in the definition of $|\phi\rangle$ and $|\omega\rangle$ as shown in the last two equations of (88). It is only after all these assumptions have been made that Eqs. (86) and (92) follow. In other words, in the quark model, Eq. (92) follows from an assumption on the value of the mixing angle. This obviously is true also in the general group-theoretical discussion—one simply has to substitute $\cos\theta = \sqrt{\frac{2}{3}}$ into Eq. (85). By defining the mixing angle at the outset, the independence of (84) on the amount of mixing was not recognized in the context of the quark model.

ii. Okubo's Model

Okubo[13] wrote down an esthetically simple form for the mass term of a Lagrangian involving the vector nonet which treats the ω' on the same footing as the other vector mesons (and, of course, assuming octet transformation property of the Lagrangian). He obtained (84) and (85) with the same value for the mixing angle. In his model, the assumption about the mass term in the Lagrangian is of a very *ad hoc* nature and the mass formulas and mixing angle are immediate consequences of it. So we tend to go along with Gasiorowicz[14] in believing that the "... observation of Okubo must be viewed as a curiosity."

Sakurai[15] has studied phenomenologically the consequences of a mixing like that shown in (90) and found a connection between the masses of the physical vector nonet and the mixing angle. Although he has not written down the connection in a compact form, it actually can be summarized by Eq. (85). He substituted the experimental masses of the vector nonet and found that $\cos\theta = 60\%$. Since he has concentrated on the mixing angle, he has not found (84).

E. Bootstrapping of ϕ–ω Mixing and Mass Splittings in the Octet Pattern

Consider the specific example of a bootstrap involving the vector nonet and the pseudoscalar octet, where we can write down the equations

$$\delta m_i^* = \sum_{j=1}^{9} F_{ji}\delta m_j^* + \sum_{\alpha=1}^{8} H_{\alpha i}\delta m_\alpha, \tag{93}$$

where the δm_i^* are the mass shifts of the vector nonet and δm_α of the pseudoscalar octet. Since

$$(\{1\}\oplus\{8\})^*\otimes(\{1\}\oplus\{8\}) = \{1\}\oplus\{1\}'\oplus\{8_D\} \oplus\{8_F\}\oplus\{8_x\}\oplus\{8_y\}\oplus\{10\}\oplus\{10\}^*\oplus\{27\}, \tag{94}$$

$$\{8\}^*\otimes\{8\} = \{1\}\oplus\{8_D\}\oplus\{8_F\}\oplus\{10\} \oplus\{10\}^*\oplus\{27\}, \tag{95}$$

the operators $\hat{F}$ and $\hat{H}$ can be written, according to the general theorem, as

$$\hat{F} = \lambda^{(1)}\hat{p}^{(1)} + \lambda^{(2)}\hat{p}^{(2)} + \lambda^{(D)}\hat{p}^{(D)} + \cdots + \lambda^{(D,x)}\hat{p}^{(D,x)} + \lambda^{(x,D)}\hat{p}^{(x,D)} + \cdots, \tag{96}$$

$$\hat{H} = \mu^{(1,1)}\hat{\Pi}^{(1,1)} + \mu^{(1',1)}\hat{\Pi}^{(1',1)} + \mu^{(D)}\hat{\Pi}^{(D)} + \cdots + \mu^{(x,D)}\hat{\Pi}^{(x,D)} + \cdots. \tag{97}$$

We are interested in terms like $\hat{p}^{(D,x)}$, $\hat{p}^{(x,D)}$ in (96) and $\hat{\Pi}^{(x,D)}$ in (97). $\hat{p}^{(D,x)}$ connects the mass splitting matrix of the vector nonet that gives rise to ϕ–ω mixing to a mass splitting matrix that corresponds to mass shifts in accordance with the GMO formula. Thus, if $\lambda^{(D,x)}$ is nonzero, any ϕ–ω mixing that occurs is going to further enhance the "normal" mass splittings in the octet pattern. Similarly, if $\lambda^{(x,D)}$ is nonzero, any "normal" mass splitting in the octet pattern will tend to give ϕ–ω mixing a further boost. In an analogous manner, terms like $\hat{\Pi}^{(x,D)}$ in (97) connect mass splittings of the pseudoscalar octet in the octet pattern with ϕ–ω mixing in the vector nonet. Hence, we see that a bootstrapping between ϕ–ω mixing and the "normal" mass splittings in the octet pattern can, in principle, occur. Whether it really does occur depends, of course, on the values of the coefficients $\lambda^{(D,x)}$, $\lambda^{(x,D)}$, $\mu^{(x,D)}$, $\cdots$, which in turn depend on the detailed dynamics. Until we have some more information about these coefficients, it seems more natural to consider ϕ–ω mixing in the vector mesons and the mass splitting according to GMO formula in the pseudoscalar octet, say, on the same footing—that either of these is the cause and consequence of the other. Dynamically, it may turn out to be more profitable to look for both of these effects in a bootstrap model instead of assuming that one is more fundamental than the other. We tend to believe, therefore, that any attempt to "derive" mass formulas from ϕ–ω mixing can, at best, be partly valid.

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Current Algebras, the Sugawara Model, and Differential Geometry

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The Lie algebra defined by the currents in the Sugawara model is defined in a way that is natural from the point of view of Lie transformation theory and differential geometry. Previous remarks that the Sugawara model is associated with a field-theoretical dynamical system on a Lie group manifold are made more precise and presented in a differential geometric setting.

1. INTRODUCTION

This work is a sequel to that in Refs. 1 and 2, although we attempt to keep this material as independent as possible of this earlier work.

In general, our aim is to study the "current algebras" that arise in quantum field theory from the point of view of contemporary Lie group theory and differential geometry. An immediate problem is that of identifying the "current algebras" as natural mathematical objects, and showing how these objects appear independently of the quantum field theory context in which they first arose in physics.

Now, one is accustomed in physics to seeing "currents" labeled as $V_\mu^a(x)$. Here μ is a "space–time" index $0 \leq \mu \leq 3$; a is an "internal symmetry" index $1 \leq a \leq n$. Typically, the index a labels a basis of an internal symmetry Lie algebra **G**, such as the Lie algebra of $SU(2)$, $SU(3)$, or $SU(3) \times SU(3)$. Also, $x = (x_i)$, $1 \leq i \leq 3$, denotes a point of R^3, i.e., Euclidean 3-space.

In addition, the "currents" $V_\mu^a(x)$ are to satisfy "commutation relations." The simplest of those relations is the following[3]:

$$[V_0^a(x), V_0^b(y)] = c_{abc}V_0^c(x)\delta(x - y), \tag{1.1}$$

where the c_{abc} are the structure constants of the Lie algebra **G**. In addition, the following relation seems natural[4]:

$$[V_0^a(x), V_i^b(y)] = c_{abc}V_i^c(x) + \partial_j^x V_{ij}^{ab}(x, y). \tag{1.2}$$

In (1.2), the V_{ij}^{ab} are "new" mathematical objects whose properties must be investigated further. In the Sugawara model,[2,5,6] these objects are not, in fact, "new," but are given in the form

$$V_{ij}^{ab}(x, y) = \delta_{ij}h_{ab}\delta(x - y), \tag{1.3}$$

where h_{ab} is the constant matrix of a bilinear form on **G**. Now, consistency between (1.1) and (1.2) and the Jacobi identity requires that this form be invariant under the adjoint group of **G**. In case **G** is a compact, semisimple Lie algebra,[7] it is known that the basis for **G** can be chosen so that h_{ab} takes the form $h_{ab} = \delta_{ab}$. It is this form that one finds in Sugawara's paper.[5] Further, in this model the following relations hold:

$$[V_i^a(x), V_j^b(y)] = 0. \tag{1.4}$$

Now, relations (1.1)–(1.4) define a certain infinite-dimensional Lie algebra. If one knew detailed mathematical information about the representations of this algebra by operators on Hilbert spaces presumably one would be in a position to begin to study physical processes, using the model as a tool. (Of course, in essence, this is Gell-Mann's program for studying elementary particle physics from the "current algebra" point of view.) Unfortunately, nothing very substantial is known from even a pure mathematics point of view about the representations of such Lie algebras. Our aim in this paper is the more modest one of describing a natural algebraic and geometric process for generating commutation relations of form (1.1) and (1.2).

We now convert the commutation relations (1.1) and (1.2) as given in the physicist's way, into more proper mathematical objects that make definite algebraic sense. Let F be the set of real valued, infinitely differential functions $f: x \to f(x)$ of a real 3-vector x. Since such functions can be added, multiplied, and multiplied by real scalars, F forms a commutative, associative algebra over the real numbers.

For $f \in F$, introduce the formal symbol

$$V_\mu^a(f) = \int V_\mu^a(x)f(x)\,dx,$$

$$V_{ij}^{ab}(f_1, f_2) = \int V_{ij}^{ab}(x, y)f_1(x)f_2(y)\,dx\,dy. \tag{1.5}$$

Then, following the usual rules for calculations with Dirac δ functions, relations (1.1)–(1.2) imply the rules

$$[V_0^a(f_1), V_0^b(f_2)] = c_{abc}V_0^c(f_1f_2), \tag{1.6}$$

$$[V_0^a(f_1), V_i^b(f_2)] = c_{abc}V_i^e(f_1f_2) - V_{ij}^{ab}(\partial_j(f_1), f_2). \tag{1.7}$$

We now attempt to realize these "abstract" commutation relations by assigning to them linear operators in a vector space W. We suppose that W is an F-module, and look for representations of the $V_\mu^a(f)$ by means of linear transformations: $W \to W$ that are also F-linear.

Let us try to realize the relations (1.6) in the form

$$\begin{aligned} V_0^a(f) &= fD_a + \partial_j(f)D_{aj}, \\ V_i^a(f) &= fE_{ai}, \end{aligned} \tag{1.8}$$

where D_a, D_{ai}, and E_{ai} are F-linear maps $W \to W$. The following conditions on these operators are then necessary and sufficient that (1.6) be satisfied:

$$\begin{aligned} [D_a, D_b] &= c_{abc}D_c, \\ [D_{ai}, D_{bj}] &= 0, \\ [D_a, D_{bi}] &= c_{abc}D_{ci}. \end{aligned} \tag{1.9}$$

Now, let us try to satisfy (1.7):

$$[f_1D_a + \partial_j(f_1)D_{aj}, f_2E_{bi}] = c_{abc}f_1f_2E_{ci} - V_{ij}^{ab}[\partial_j(f_1), f_2].$$

In order to satisfy this relation, we must then have

$$\begin{aligned} [D_a, E_{bi}] &= c_{abc}E_{ci}, \\ V_{ij}^{ab}(f_1, f_2) &= f_1f_2[D_{aj}, E_{bi}]. \end{aligned} \tag{1.10}$$

We can now read off the condition (1.3), i.e., that the Schwinger term be a c number. Namely, $[D_{aj}, E_{bi}]$ commutes with D_a, D_{aj}, and E_{aj}. It would perhaps be interesting to investigate the most general of these possible conditions. However, we do not attempt this here, but instead present a specific way of realizing these abstract relations, that is motivated—as explained in Sec. 4—by canonical, Lagrangian quantum field theory.

2. CURRENTS DEFINED IN TERMS OF PROLONGATIONS OF VECTOR FIELDS

We introduce the range of indices $1 \leq \alpha, \beta, \gamma \leq m$, together with the summation convention. Let $\varphi = (\varphi_\alpha)$ denote the coordinates of a manifold M of dimension m. (We try to keep the knowledge of manifold theory required for the sequel to a primitive level. See Refs. 7 and 8 for an explanation of that which is needed.)

Suppose $\mathbf{G}$ is a Lie algebra of vector fields[8,9] on M. Thus, each $X \in \mathbf{G}$ can be realized as a first-order linear differential operator M,

$$X = A_\alpha \partial_\alpha, \tag{2.1}$$

where the A_α are functions of the φ's, and $\partial_\alpha = \partial/\partial\varphi_\alpha$.

Introduce a "new" space of variables x, φ_α, and $\varphi_{\alpha i}$, denoted by M'. (In terms of the jargon,[9] M' is to be identified with the space of 1-jets of mappings: $R^3 \to M$.) Let F denote the ring of C^∞ real-valued functions $f: x \to f(x)$, on R^3.

Associate with X of form (2.1), $f \in F$, the vector field on M'

$$V_0^X(f) = fA_\alpha\partial_\alpha + (\partial_i(f)A_\alpha + f\partial_\beta(A_\alpha)\varphi_{\beta i})\partial_{\alpha i}. \tag{2.2}$$

[$V_0^X(f)$ may be identified with the "prolongation" of the vector field on X on $R^3 \times M$ to the "1-jet" space M'. See Refs. 1, 9, and 10.]

Suppose that X and Y are the vector fields of form (2.1). Suppose that $Z = [X, Y]$, the Jacobi bracket of X and Y, i.e., Z is the commutator of the differential operators of form (2.1). Then, one proves readily that

$$[V_0^X(f_1), V_0^Y(f_2)] = V_0^{[X,Y]}(f_1f_2), \quad \text{for} \quad f_1, f_2 \in F. \tag{2.3}$$

This is the geometric analog of the current-commutator relation (1.1) or (1.6).

In terms of the F-module language, let W be the space of the functions of the x, φ_α, and $\varphi_{\alpha i}$. Then, in terms of formula (1.8),

$$\begin{aligned} D_X &= A_\alpha\partial_\alpha + \partial_\beta(A_\alpha)\varphi_{\beta i}\partial_{\alpha i}, \\ D_{X,i} &= A_\alpha\partial_{\alpha i}. \end{aligned} \tag{2.4}$$

Let us now attempt to choose E_{ai} as differential operators to satisfy (1.10). We do not attempt to investigate the most general sort of choice of E_{ai}, but look for the E's as zeroth-order differential operators, of the form

$$E_{X,i} = h_{ai}^X\varphi_{ai}, \tag{2.5}$$

where the h_{ai}^X are functions of φ alone. Thus,

$$V_i^X(f) = fh_{ai}^X\varphi_{ai}. \tag{2.6}$$

Then, condition (1.10) takes the form

$$\begin{aligned} [D_X, E_{Y,i}] &= (A_\alpha\partial_\alpha + \partial_\beta(A_\alpha)\varphi_\beta, \partial_{\alpha i})(h_{\gamma_j}^Y\varphi_{\gamma_j}) \\ &= A_\alpha\partial_\alpha(h_{\gamma_j}^Y)\varphi_{\gamma_j} + \partial_\beta(A_\alpha)\varphi_{\beta i}h_{\alpha i}^Y \\ &= E_{[X,Y],i} = h_{\alpha i}^{[X,Y]}\varphi_{\alpha i}. \end{aligned} \tag{2.7}$$

Now, if $h(\varphi)$ is a function of φ alone, i.e., a function on the manifold M, and if X is a vector field on M of form (2.1), define—as in Ref. 8—the "Lie derivative" of h by X as

$$X(h) = A_\alpha\partial_\alpha(h).$$

Similarly, if

$$\omega = h_\alpha\, d\varphi_\alpha$$

is a 1-differential form on M, define its Lie derivative by X as

$$\begin{aligned} X(\omega) &= X(h_\alpha)\, d\varphi_\alpha + h_\alpha\, d(X(\varphi_\alpha)) \\ &= A_\beta\partial_\beta(h_\alpha)\, d\varphi_\alpha + h_\alpha\partial_\beta(A_\alpha)\, d\varphi_\beta. \end{aligned} \tag{2.8}$$

The geometric meaning of this Lie derivative operation is discussed in detail in Ref. 8. For example, ω is invariant under the 1-parameter transformation group on M generated by X if and only if $X(\omega) = 0$.

Note now that Eqs. (2.7) imply the relations

$$X(h^Y_{\beta i}) = -\partial_\beta(A_\alpha)h^Y_{\alpha i} + h^{[X,Y]}_{\beta i}. \tag{2.9}$$

Equation (2.9) can be recast into a more interesting form. Introduce 1-differential forms on M as follows:

$$\omega^Y_i = h^Y_{\beta i}\, d\varphi_\beta. \tag{2.10}$$

With the "Lie derivative" of 1-forms defined by (2.8), we see that Eqs. (2.9) are equivalent to

$$X(\omega^Y_i) = \omega^{[X,Y]}_i, \quad \text{for} \quad X \text{ and } Y \in \mathbf{G}. \tag{2.11}$$

In turn, condition (2.8) can be interpreted as follows. Let $F^1(M)$ denote the vector space of 1-differential forms on M. The action of Lie derivative defines a representation of $\mathbf{G}$ by operators on $F^1(M)$. Then, for fixed i, the map $Y \to \omega^Y_i$ is a linear map of $G \to F^1(M)$ that intertwines the action of G on both these spaces.

This interpretation immediately enables us to construct such a system of currents. Indeed, suppose that B: $V(M) \times V(M) \to F(M)$ is an $F(M)$-bilinear map, i.e., B is a covariant 2-tensor on M. Suppose also that B is invariant under the action of G, i.e.,

$$X(B(Y, Z)) = B([X, Y], Z) + B(Y, [X, Z]), \tag{2.12}$$

for Y, $Z \in V(M)$ and $X \in \mathbf{G}$. [For example, if B defines a Riemannian metric[8] on M, then (2.8) is the condition that X generate a 1-parameter group of isometries on M, i.e., that X be a Killing vector field.] Then, one can define ω^Y_i as

$$\omega^Y_i(X) = c_i B(Y, X) \tag{2.13}$$

for all $X \in V(M)$, where c_i is a real scalar.

As an example, one can choose $M = G$, where G is a compact, semisimple Lie group whose Lie algebra is $\mathbf{G}$, and where $\mathbf{G}$ is identified[8] with the Lie algebra of right-invariant vector fields on G itself. B may be defined as the bi-invariant Riemannian metric on G defined by the Killing form of $\mathbf{G}$. It may be readily checked that this construction then specializes to the Lagrangian model of the Sugawara algebra given previously.[2,6]

Let us now investigate further the necessary conditions that must be satisfied to give a c-number Schwinger term.

3. CONDITIONS THAT THE SCHWINGER TERM BE A c NUMBER

We keep the notations of Sec. 2. The "Schwinger term" can be read off from (1.10) as

$$V^{X,Y}_{ij}(f_1, f_2) = f_1 f_2[D_{X,j}, E_{Y,i}] = f_1 f_2 A_\alpha h^Y_{\alpha j}.$$

The condition that the Schwinger term be independent of the φ's (or that it be a "c number," in quantum mechanical language) is then that

$$A_\alpha h^Y_{\alpha j} = \text{const}, \quad \text{for} \quad X, Y \in \mathbf{G}. \tag{3.1}$$

In terms of the 1-forms ω^Y_i given by (2.10), Eq. (3.1) takes the form

$$\omega^Y_i(X) = \text{const}, \quad \text{for} \quad X, Y \in \mathbf{G}, \tag{3.2}$$

where the left-hand side of (3.2) is the inner product between the differential form and vector field. (See Ref. 8 for this operation.)

In addition to (3.2), let us suppose that $\mathbf{G}$ acts transitively on M; that is, the following condition is satisfied: If ω is a 1-form on M, such that $\omega(X) = 0$ for all $X \in \mathbf{G}$, then $\omega = 0$.

Let us return to the investigation of condition (3.2). Then, for X, Y, and $Z \in \mathbf{G}$,

$$\begin{aligned} d\omega^Y_i(X, Z) &= X(\omega^Y_i(Z)) - Z(\omega^Y_i(X)) - \omega^Y_i([X, Z]) \\ &= -\omega^Y_i([X, Z]), \end{aligned} \tag{3.3}$$

where d is the exterior derivative operation.[8]

In particular, suppose that X_a is a basis for $\mathbf{G}$, with

$$[X_a, X_b] = c_{abc}X_c, \tag{3.4}$$

and let

$$\omega^a_i = \omega^{X_a}_i. \tag{3.5}$$

Then, (3.3) is equivalent to the conditions

$$d\omega^a_i = c_{bca}\omega^b_i \wedge \omega^c_i \quad \text{(no summation on } i), \tag{3.6}$$

where $\wedge$ is the exterior product operation.

The most general possible solution to these conditions can now be read off from (3.6). Let G be a Lie group whose Lie algebra is $\mathbf{G}$. Let ω^a denote the right-invariant 1-forms (the "Cartan–Maurer forms") on G, corresponding to the basis ω^a. They satisfy

$$d\omega^a = c_{bca}\omega^b \wedge \omega^c. \tag{3.7}$$

By the Frobenius complete-integrability theorem,[8] there are then maps $\psi_i: M \to G$ such that

$$\omega^a_i = \psi^*_i(\omega^a), \tag{3.8}$$

where ψ^*_i denotes the pull-back map or forms generated by ψ_i. The Sugawara model corresponds to the case

where $M = G$, and the ψ_i are the identity map. Thus, it is in some sense a "universal model" for current algebras of this type.

4. CONNECTIONS WITH QUANTUM FIELD THEORY

In Ref. 2 we point out that there is a connection between the formal operational rules of canonical Lagrangian field theory and the sort of algebraic–differential geometric considerations presented in this paper. In this section, we present a few further brief remarks in this direction, a full discussion is presented in Ref. 9.

Let us now use x to denote a 4-vector x_μ, an element of R^4. Suppose that $\varphi_\alpha(x)$ are a set of spin-zero, boson quantum fields. Now, we consider a Lagrangian of the form

$$L = \tfrac{1}{2} g_{\mu\nu} h_{\alpha\beta}(\varphi) \partial_\mu \varphi_\alpha \partial_\nu \varphi_\beta . \tag{4.1}$$

In (4.1), $g_{\mu\nu}$ is the Lorentz metric tensor, while $h_{\alpha\beta}(\varphi)$ are, for the moment, any set of functions on M_n which depend symmetrically on α and β. Let

$$L_{\alpha\mu} = g_{\mu\nu} h_{\alpha\beta} \partial_\nu \varphi_\beta , \tag{4.2}$$

$$L_\alpha = \tfrac{1}{2} g_{\mu\nu} \partial_\alpha (h_{\beta\gamma}) \partial_\mu \varphi_\beta \partial_\nu \varphi_\gamma ,$$

$$\pi_\alpha = L_{\alpha 0} = h_{\alpha\beta} \partial_0 \varphi_\beta . \tag{4.3}$$

We say that the field theory defined by L is *canonical* if Eqs. (4.3) can be inverted (at the classical level), expressing the time derivative $\partial_0 \varphi_\beta$ on terms of the π_α. With the specific choice (4.1) of the Lagrangian, this amounts to requiring that the determinant of the matrix $h_{\alpha\beta}$ be nonzero, i.e., that the symmetric quadratic differential form

$$ds^2 = h_{\alpha\beta}\, d\varphi_\alpha\, d\varphi_\beta \tag{4.4}$$

define a pseudo-Riemannian metric[8] for M. In fact, we also suppose that the form (4.4) is positive definite, so that it defines a Riemannian metric[8] for M. Then, one would expect that the Riemannian geometry of M would play a role in the properties of the quantum fields constructed from L. (Of course, L is one of a type of what physicists call "phenomenological Lagrangians.")

The equations of motion constructed from L can be written down using (4.2) and (4.3):

$$\partial_\mu (g_{\mu\nu} h_{\alpha\beta}(\varphi(x)) \partial_\nu \varphi_\beta(x)) = \tfrac{1}{2} g_{\mu\nu} \partial_\alpha (h_{\beta\gamma})(\varphi(x)) \partial_\mu \varphi_\beta(x) \partial_\nu \varphi_\gamma(x). \tag{4.5}$$

It is interesting to note that at the classical level, Eqs. (4.5) define what Eels and Sampson call[11] *harmonic maps* $R^4 \to M$, where R^4 has the Lorentz metric and M has the metric form (4.4).

Let us now rewrite (4.5) as

$$g_{\mu\nu}[h_{\alpha\beta} \partial_\mu \partial_\nu \varphi_\beta + \partial_\gamma (h_{\alpha\beta}) \partial_\mu \varphi_\gamma \partial_\nu \varphi_\beta] = \tfrac{1}{2} g_{\mu\nu} \partial_\alpha (h_{\beta\gamma}) \partial_\mu \varphi_\beta \partial_\nu \varphi_\gamma . \tag{4.6}$$

Notice that (4.6) enables us to determine the time derivatives $\partial_0 \pi_\alpha$. Thus, there are no formal "algebraic" contradictions involved in introducing the canonical, equal-time commutation relations

$$[\pi_\alpha(x), \varphi_\beta(y)]_{x_0 = y_0 = 0} = \delta_{\alpha\beta} \delta(x - y),$$
$$0 = [\pi_\alpha(x), \pi_\beta(y)]_{x_0 = y_0 = 0} = [\varphi_\alpha(x), \varphi_\beta(y)]_{x_0 = y_0 = 0} . \tag{4.7}$$

These commutation relations, together with the equation of motion (4.6), then determine the "quantized" field theory, at least in a formal algebraic way. For example, one could use power-series expansions for the $h_{\alpha\beta}$ about their "free-field" values,

$$h_{\alpha\beta}(\varphi) = h_{\alpha\beta}(0) + h_{\alpha\beta\gamma} \varphi_\gamma + h_{\alpha\beta\gamma\gamma}\, \varphi_\gamma \varphi_\gamma , + \cdots , \tag{4.8}$$

and follow the usual rules for quantizing products of functions as "operators."

Now, suppose that X is a vector field on M given by formula (2.1). Let $X\,(ds^2)$ be the Lie derivative of the metric form (4.2) by this vector field.[8] Suppose it is of the form

$$X(ds^2) = h^X_{\alpha\beta}\, d\varphi_\alpha\, d\varphi_\beta . \tag{4.9}$$

Let L^X be the Lagrangian defined analogously to (4.1) from the form

$$L^X = \tfrac{1}{2} g_{\mu\nu} h^X_{\alpha\beta} \partial_\mu \varphi_\alpha \partial_\nu \varphi_\beta . \tag{4.10}$$

Construct the "vector current" associated with X, by the usual formula

$$V^X_\mu = L_{\alpha\mu} A_\alpha = g_{\mu\nu} A_\alpha h_{\alpha\beta} \partial_\nu \varphi_\beta . \tag{4.11}$$

Then, at the classical level, "Noether's theorem" specializes to the formula

$$\partial_\mu V^X_\mu = L^X. \tag{4.12}$$

This relation may also be expected to hold at a quantum level, if things are done right. In particular, the current is "conserved," i.e., the left-hand side of (4.12) is zero, if $L^X = 0$, which translates geometrically via (4.9) into the condition that X be a Killing vector field, i.e., that the 1-parameter group of transformations on M generated by X leave invariant the metric determined by ds^2. If, more generally, one wants (as in PCAC type theories) the left-hand side of (4.12) to be a "new" field transforming in a certain way, one would require that the metric form (4.5) be one of a family of metrics on M transforming under the transformation group G whose Lie algebra contains X. In turn, if G acts

transitively on M, the possibilities for such families can be read off from the vector-bundle version of the Frobenius reciprocity theorem.[7]

One can now use (4.11) to convert the currents V_μ^X into elements of the Lie algebra generated by the fields $\varphi_\alpha(x)$, $\pi_\alpha(x)$ their derivatives, and "functions" of the fields defined by formal power series of type (4.8). In particular, one can purely algebraically compute commutation relations of the form

$$[V_\mu^X(x), V_\nu^Y(y)]_{x_0=y_0} = 0.$$

In this way, one can calculate, at a purely algebraic level, commutation relations of the type (1.1), (1.2), or (1.4). In turn, the usual rules for quantizing objects like $\varphi_\alpha(x)$, $h(\varphi_\alpha(x))$, and $\partial_i\varphi_\alpha(x)$ suggest the particular types of "representations" of the "integrated" currents $V_\mu^X(f)$ used in previous sections. Of course, the point is that, once having written down, or guessed, "abstract" commutation relations for the currents, one can forget the quantum field theory background, and work in a well-defined mathematical way. Further work on this purely algebraic direction can be found in Refs. 9 and 12.

Finally, we may note that putting these remarks together determines the choice of metric form (4.5) which leads to the Sugawara-type of commutation relations for the currents. Namely, M is G itself, and the metric form (4.5) is the unique metric invariant under right and left translations. From the mathematical point of view, this is the most interesting property yet investigated of the current commutation relations, since it seems to say (if indeed the current commutation relations are at all basic in physics) that the geometry of the Lie group manifold itself [corresponding to a given symmetry group of the elementary particles, e.g., $G = SU(2)$, $SU(2) \times SU(2)$, and $SU(3)$ or $SU(3) \times SU(3)$] plays a fundamental role in the physics of elementary particles. It would also be interesting to investigate analogous relations, starting off with fields $\varphi_\alpha(x)$ of higher spin and/or different statistics, e.g., fermions.

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[1] R. Hermann, *Lie Algebras and Quantum Mechanics* (W. A. Benjamin, Inc., N.Y., to be published).

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[4] I owe this suggestion to C. Itzykson and I. Todorov.

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Numerical Analysis of an Integral Equation with a δ Function in the Kernel*

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(Received 15 January 1969)

An integral equation which has a two-part kernel, where one part contains a δ function, is analyzed with respect to its analytic structure in the λ plane and with respect to numerical approximations to it. The analytic structure of the approximate solution is also investigated. It is found that there is no difficulty in approximating the Dirac δ function by a Kronecker δ; even though the approximate kernel does not approach the true kernel, the solution corresponding to the approximate kernel does approach the true solution. In keeping with the fact that the kernel does not meet the Fredholm conditions, we find that the solution has branch cuts in the λ plane. A form for the solution analogous to Fredholm's solution which emphasizes the analytic structure (i.e., a branch cut) is obtained.

I. INTRODUCTION

A few years ago, it became feasible to study the quantum 3-body problem with separable potentials by using Faddeev theory for reduction of the problem to a 1-dimensional integral equation with a Fredholm kernel. It has been the impression of many workers and observers of the field that the fundamental contribution of the Faddeev equations was to yield an integral equation which had a Fredholm (i.e., completely continuous) kernel and that the solution of integral equations with kernels not enjoying this property is practically impossible.

transitively on M, the possibilities for such families can be read off from the vector-bundle version of the Frobenius reciprocity theorem.[7]

One can now use (4.11) to convert the currents V_μ^X into elements of the Lie algebra generated by the fields $\varphi_\alpha(x)$, $\pi_\alpha(x)$ their derivatives, and "functions" of the fields defined by formal power series of type (4.8). In particular, one can purely algebraically compute commutation relations of the form

$$[V_\mu^X(x), V_\nu^Y(y)]_{x_0=y_0} = 0.$$

In this way, one can calculate, at a purely algebraic level, commutation relations of the type (1.1), (1.2), or (1.4). In turn, the usual rules for quantizing objects like $\varphi_\alpha(x)$, $h(\varphi_\alpha(x))$, and $\partial_i\varphi_\alpha(x)$ suggest the particular types of "representations" of the "integrated" currents $V_\mu^X(f)$ used in previous sections. Of course, the point is that, once having written down, or guessed, "abstract" commutation relations for the currents, one can forget the quantum field theory background, and work in a well-defined mathematical way. Further work on this purely algebraic direction can be found in Refs. 9 and 12.

Finally, we may note that putting these remarks together determines the choice of metric form (4.5) which leads to the Sugawara-type of commutation relations for the currents. Namely, M is G itself, and the metric form (4.5) is the unique metric invariant under right and left translations. From the mathematical point of view, this is the most interesting property yet investigated of the current commutation relations, since it seems to say (if indeed the current commutation relations are at all basic in physics) that the geometry of the Lie group manifold itself [corresponding to a given symmetry group of the elementary particles, e.g., $G = SU(2)$, $SU(2) \times SU(2)$, and $SU(3)$ or $SU(3) \times SU(3)$] plays a fundamental role in the physics of elementary particles. It would also be interesting to investigate analogous relations, starting off with fields $\varphi_\alpha(x)$ of higher spin and/or different statistics, e.g., fermions.

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Numerical Analysis of an Integral Equation with a δ Function in the Kernel*

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An integral equation which has a two-part kernel, where one part contains a δ function, is analyzed with respect to its analytic structure in the λ plane and with respect to numerical approximations to it. The analytic structure of the approximate solution is also investigated. It is found that there is no difficulty in approximating the Dirac δ function by a Kronecker δ; even though the approximate kernel does not approach the true kernel, the solution corresponding to the approximate kernel does approach the true solution. In keeping with the fact that the kernel does not meet the Fredholm conditions, we find that the solution has branch cuts in the λ plane. A form for the solution analogous to Fredholm's solution which emphasizes the analytic structure (i.e., a branch cut) is obtained.

I. INTRODUCTION

A few years ago, it became feasible to study the quantum 3-body problem with separable potentials by using Faddeev theory for reduction of the problem to a 1-dimensional integral equation with a Fredholm kernel. It has been the impression of many workers and observers of the field that the fundamental contribution of the Faddeev equations was to yield an integral equation which had a Fredholm (i.e., completely continuous) kernel and that the solution of integral equations with kernels not enjoying this property is practically impossible.

For example, Weinberg, while discussing integral equations with δ functions in the kernel, has stated,[1] "The solution of such linear integral equations is known to be straightforward if (and really only if) the kernel . . . is of the 'completely continuous' type." And Lovelace has stated,[2] "Now all numerical methods for solving integral equations depend on reducing them to matrix equations. This means that the kernel is replaced by an operator of finite rank . . . . Thus, unless the kernel of an integral equation is a compact operator it cannot be approximated by a matrix equation and there is therefore little hope of solving it numerically." The implication of these authors' statements seems to be that an integral equation which involves a δ function in the kernel cannot be solved by matrix methods (at least as it stands, i.e., without some algebraic manipulation beforehand). We wish to show that δ functions in the kernel do not prevent the direct solution of the equation by matrix methods even though the kernel is not Fredholm.

Before proceeding, we wish to distinguish two types of problems which appear in the reduction of the Lippman–Schwinger integral equation to a form which can be shown to be of the Fredholm type. The Lippmann–Schwinger equation for three bodies with separable 2-body potentials can be put in a form

$$\phi(x) = f(x) + \lambda \int_a^b [K(x, y) + k(x)\delta(x - y)]\phi(y)\, dy, \tag{1}$$

where x and y are real variables, $k(x)$ is a finite continuous complex function of the real variable x, and $K(x, y)$ and $f(x)$ are complex functions of the real variables x, y. λ is a complex parameter which we have introduced to correspond to Fredholm's theory. The kernel here is made up of two parts. The second part is one which corresponds to disconnected diagrams in perturbation theory and for this reason contains the δ function. This δ function has been called a "dangerous δ function" by Weinberg. The problem of how this δ function can be handled is what we are concerned with in this paper. The second problem, which should not be confused with this one, concerns the first part of the kernel in Eq. (1). This part comes from the completely connected 3-body diagrams in perturbation theory. It can have singularities when the momenta (which are related to the variables x and y) correspond to values for which classical 3-body collisions can take place.[3] The latter singularities have been studied by Faddeev,[4] who has shown that an equation with this kind of singularity (but without the δ-function singularity) has the Fredholm solution. Furthermore, these singularities do not appear if the energy of the 3-body system is negative so that no classical scattering can take place. We ignore this singularity and assume $K(x, y)$ to be finite and continuous[5] on the range of the real variables x and y.

It is generally stated that the reason no matrix approximation to Eq. (1) will work is that, if the kernel K is not completely continuous, no finite approximation to it, K_N exists such that $\lim \|K - K_N\| \to 0$, as $N \to \infty$. We show in Sec. III that, although this is true, there does exist a sequence of kernels K_N such that their solutions ϕ_N approach ϕ, as $N \to \infty$. In Sec. II we show, by means of a technique almost identical to that used to rid the Faddeev equations of the "dangerous" δ functions, that Eq. (1) has solutions for all λ except for (a) $1/\lambda$ on a continuous line in the complex plane and (b) poles in the λ plane which are analogous to zeros of the Fredholm denominator. In the 3-body problem, the continuous line of singularities (a) corresponds to scattering states with two bodies bound and the poles (b) correspond to 3-body bound states.

II. SOLUTION OF EQUATION

If we carry out the integration over the δ function in Eq. (1), we have

$$\phi(x)[1 - \lambda k(x)] = f(x) + \lambda \int_a^b K(x, y)\phi(y)\, dy. \tag{2}$$

We would like to divide Eq. (2) by the quantity $1 - \lambda k(x)$ in order to obtain a Fredholm equation of the second kind. We can do this division with no difficulty provided $1 - \lambda k(x) \neq 0$, for all x on the interval $[a, b]$. Now, $k(x)$, being continuous, maps the interval $[a, b]$ on the real axis into a line L in the complex plane. If $1/\lambda$ is not on L, then $[1 - \lambda k(x)] \neq 0$. Hereafter, we take λ such that $1/\lambda$ is not on L. Then

$$\phi(x) = \frac{f(x)}{1 - \lambda k(x)} + \lambda \int_a^b \frac{1}{1 - \lambda k(x)} K(x, y)\phi(y)\, dy. \tag{3}$$

This is just the equation used to obtain numerical solutions in Faddeev theory. The integral Eq. (3) is of the Fredholm type, since $K(x, y)$ is continuous and finite and since $1/[1 - \lambda k(x)]$ is also continuous and finite. We will introduce a parameter Λ, which may be set equal to λ later, and rewrite Eq. (3) as

$$\phi(x) = F(x; \lambda) + \Lambda \int_a^b K(x, y; \lambda)\phi(y)\, dy, \tag{4}$$

where

$$F(x, \lambda) = \frac{f(x)}{1 - \lambda k(x)},$$

$$K(x, y; \lambda) = \frac{1}{1 - \lambda k(x)} K(x, y),$$

and where λ is a parameter of the problem, and Λ becomes the usual Fredholm parameter.

This step (i.e., using the correct λ) is crucial since it allows the solution to be meromorphic in the Λ plane, because Λ multiplies only a completely continuous part of the kernel. It seems to be somewhat common mathematical practice to always introduce λ in such a way that it multiplies only the completely continuous part of a singular kernel in order to obtain simple behavior in the λ plane.[6]

The solution of Eq. (4) is unique and is

$$\phi(x) = F(x, \lambda) + \int_a^b \frac{C(x, y; \lambda; \Lambda)}{D(\lambda; \Lambda)} F(y; \lambda)\, dy, \quad (5)$$

where C and D are given by Fredholm theory.[7] It is Fredholm's result that $C(x, y; \lambda; \Lambda)$ and $D(\lambda; \Lambda)$ are entire functions of Λ for every value of λ, $1/\lambda$ not on L. Furthermore, each term in the expansions for C and D is analytic in λ except for $1/\lambda$ on L. Therefore, the solution of Eq. (1) is

$$\phi(x) = F(x, \lambda) + \int_a^b \frac{C(x, y; \lambda; \lambda)}{D(\lambda; \lambda)} F(y; \lambda)\, dy, \quad (6)$$

where $C(x, y; \lambda; \lambda)$ and $D(\lambda, \lambda)$ and $F(x, \lambda)$ are analytic in λ except for $1/\lambda$ on L. Thus, $\phi(x, \lambda)$ is analytic in λ for $1/\lambda$ not on L except for isolated poles where $D(\lambda, \lambda) = 0$. Therefore, in distinction to the situation existing for kernels obeying the Fredholm conditions, we have a *branch cut* as well as poles in the λ plane.

III. MATRIX SOLUTION

Consider the linear equation problem

$$\phi_N(x_i) = f(x_i) + \lambda \sum_{j=1}^{N} \left(K(x_i, x_j) + k(x_i) \frac{\delta_{ij}}{\Delta} \right) \phi_N(x_j) \Delta, \quad (6)$$

where $x_j = a + j\Delta$, and where $\Delta = (b - a)/N$. Thus, for $1/\lambda$ not on L we have $[1 - \lambda k(x_j)] \neq 0$. Here, $\Delta = (b - a)/N$. Thus, Eq. (6) is a direct numerical treatment of the integral Eq. (1). We show in this section that the solutions of Eq. (6) in the limit of large N approach the solutions of Eq. (1).

The solution of Eq. (6) is given by

$$\phi_N(x_i) = \sum_{j=1}^{N} (M_N^{-1})_{ij} f(x_j), \quad (7)$$

where

$$(M_N)_{ij} = \delta_{ij}[1 - \lambda k(x_i)] - \lambda \Delta K(x_i, x_j).$$

In the same way that Eq. (1) was converted into Eq. (3), we may convert Eq. (6) into

$$\phi_N(x_i) = \frac{1}{1 - \lambda k(x_i)} f(x_i) + \lambda \sum_{j=1}^{N} \frac{1}{1 - \lambda k(x_i)} K(x_i, x_j) \phi_N(x_j). \quad (8)$$

But this equation clearly approaches Eq. (3) as $N \to \infty$. In fact, the kernel of Eq. (8) approaches the kernel of Eq. (3) as $N \to \infty$. Thus, $\phi_N(x_i)$ approaches $\phi(x)$ as $N \to \infty$. But, $\phi_N(x_i)$ is given perfectly adequately by Eq. (7) for any finite N. Thus, while the kernel of Eq. (6) does not approach the kernel of Eq. (1) as N approaches infinity, the solution of Eq. (6) does approach the solution of Eq. (1), since it is the same as the solution of Eq. (3) provided the conditions on λ are met.

IV. ANALYTIC PROPERTIES OF THE APPROXIMATE SOLUTION

It is interesting to examine the analytic properties in λ of the solution of Eq. (6) for finite N.

In order to proceed, we assume that there exists an M such that for all x, y, and z

$$\max \left\{ \left| \frac{K(z, y) - K(z, x)}{k(x) - k(y)} \right|, \ |K(x, y)| \right\} < M.$$

This bounds $K(x, y)$ on the one hand and, if the slope (in x) of $K(z, x)$ does not go to zero anywhere, it also places a lower bound on the slope of $k(x)$. At points where the slope of $K(z, x)$ is zero, the condition on $k(x)$ is weaker, however. The kernels in the 3-body equations and the kernel in the worked example in the Appendix satisfy this condition. We expand Eq. (6) in a manner similar to that used in Fredholm theory. Thus, if we solve Eq. (6) as a set of linear equations, we have Eq. (7). The inverse of $(M_N)_{ij}$ is

$$(M_N^{-1})_{ij} = C_{ij}/D,$$

where $C_{ij} = (-1)^{i+j}$ [minor of the (j, i)th element of M_N] and where $D = \det(M_N)$. We may write the determinant D as an expansion in powers of Δ, and we obtain

$$D = \prod_i (1 - \lambda k_i) + \Delta \sum_j \left(\prod_{(i \neq j)} (1 - \lambda k_i) \right) (-\lambda) K_{ij} + \frac{\Delta^2}{2!} \sum_{j,k} \left(\prod_{i(\neq j,k)} (1 - \lambda k_i) \right) (-\lambda)^2 \times \begin{vmatrix} K_{ij} & K_{jk} \\ K_{kj} & K_{kk} \end{vmatrix} + \cdots,$$

where we have used the notation k_i for $k(x_i)$ and K_{ij} for $K(x_i, x_j)$. We may factor out the product of the diagonal elements of the determinant and obtain

$$D = \left(\prod_i (1 - \lambda k_i) \right) \left(1 - \lambda \Delta \sum_j \frac{1}{1 - \lambda k_j} K_{jj} + \frac{\lambda^2 \Delta^2}{2!} \sum_{jk} \frac{1}{(1 - \lambda k_j)(1 - \lambda k_k)} \times \begin{vmatrix} K_{jj} & K_{jk} \\ K_{kj} & K_{kk} \end{vmatrix} + \cdots \right).$$

Then, we may use partial fractions on each of the factors $1/[(1-\lambda k_j)\cdots(1-\lambda k_n)]$ so that

$$D=\left(\prod_i(1-\lambda k_i)\right)\left(1-\Delta\sum_j\frac{1}{\frac{1}{\lambda}-k_j}F_j\right), \quad (9)$$

where

$$F_j=K_{jj}-\Delta\sum_k\frac{1}{k_j-k_k}\begin{vmatrix}K_{jj}&K_{jk}\\K_{kj}&K_{kk}\end{vmatrix}+\cdots+(-1)^n\frac{\Delta^n}{n!}$$
$$\times\sum_{j_1\cdots j_n}\frac{1}{(k_j-k_{j_1})(k_j-k_{j_2})\cdots(k_j-k_{j_n})}$$
$$\times\begin{vmatrix}K_{jj}&K_{jj_1}&\cdots&K_{jj_n}\\K_{j_1j}&K_{j_1j_1}&\cdots&K_{j_1j_n}\\\cdot&\cdot&&\cdot\\\cdot&\cdot&&\cdot\\\cdot&\cdot&&\cdot\\K_{j_nj}&K_{j_nj_1}&\cdots&K_{j_nj_n}\end{vmatrix}+\cdots. \quad (10)$$

To investigate the convergence of this series for F_j, we may subtract the first column from each of the succeeding columns in the determinant in the nth term. Then we may write the part of the nth term under the summation sign as

$$\begin{vmatrix}K_{jj}&\frac{K_{jj_1}-K_{jj}}{k_j-k_{j_1}}&\cdots\\K_{j_1j}&\frac{K_{j_1j_1}-K_{j_1j}}{k_j-k_{j_1}}&\cdots\\\cdot&\cdot&\\\cdot&\cdot&\\\cdot&\cdot&\end{vmatrix},$$

but each element of this determinant is assumed to be bounded by M and, therefore,[7] we find that the nth term is bounded by $M^n n^{\frac{1}{2}n}(b-a)^{n-1}/(n-1)!$. Therefore, the series is convergent.

Thus, there exists some analytic function $F(x)$ such that for all ϵ there exists an integer M such that for all N greater than M and for all j, $1\leq j\leq N$, we have $|F(x_j)-F_j|<\epsilon$.

Thus, for some N the summation term in Eq. (9) may be considered

$$g(1/\lambda)=\Delta\sum_j\frac{1}{(1/\lambda)-k(x_j)}F(x_j), \quad (11)$$

where $F(x)$ is an analytic function of x.

But in any neighborhood (in the $1/\lambda$ plane) of the line $1/\lambda$ on L we may find an M large enough so that for all $N>M$ the expression (11) is equal to any value whatever inside that neighborhood. In particular, it is equal to 1 somewhere in that neighborhood so that the zeros of D must be distributed along the line $1/\lambda$ on L. It is easily shown by considering the integral

$$\frac{1}{2\pi i}\int_c\frac{g'(z)}{1-g(z)}\,dz$$

on a contour c completely enclosing the branch cut that the number of zeros on L can differ from the number of poles on L only by a finite number. Thus, we expect the solution of Eq. (6) to have poles in the main along the line $1/\lambda$ on L with other isolated poles possible.

V. THE CONTINUOUS LIMIT

If the numerator function C_{ij} is treated in a way similar to the way we treated the denominator function and if the continuous limit is taken, then the solution to Eq. (1) may be written

$$\phi(x)=\int\frac{C(x,y;\lambda)}{D(\lambda)}f(y)\,dy+f(x)\frac{1}{1-\lambda k(x)}, \quad (11')$$

where

$$C(x,y;\lambda)=\frac{1}{1-\lambda k(x)}\frac{1}{1-\lambda k(y)}\lambda\left(K(x,y)-\int_a^b\frac{1}{(1/\lambda)-k(z)}F(x,y;z)\,dz\right), \quad (12)$$

$$D(\lambda)=1-\int_a^b\frac{1}{(1/\lambda)-k(z)}F(z)\,dz, \quad (13)$$

and where the "spectral functions" $F(z)$ and $F(x,y;z)$ are

$$F(z)=K(z,z)-\int_a^b\frac{1}{k(z)-k(x)}\begin{vmatrix}K(x,x)&K(x,z)\\K(z,x)&K(z,z)\end{vmatrix}dx$$
$$+\cdots+\frac{(-1)^n}{n!}\int_a^b dx_1\cdots\int_a^b dx_n\left(\prod_i\frac{1}{k(z)-k(x_i)}\right)\begin{vmatrix}K(z,z)&K(z,x_1)&\cdots&K(z,x_n)\\K(x_1,z)&K(x_1,x_1)&\cdots&\\\cdot&\cdot&&\cdot\\\cdot&\cdot&&\cdot\\\cdot&\cdot&&\cdot\\K(x_n,z)&\cdots&&K(x_n,x_n)\end{vmatrix}+\cdots, \quad (14)$$

and

$$F(x, y; z) = \begin{vmatrix} K(x, y) & K(x, z) \\ K(z, y) & K(z, z) \end{vmatrix} - \int_a^b \frac{dx_1}{k(z) - k(x_1)} \begin{vmatrix} K(x, y) & K(x, z) & K(x, x_1) \\ K(z, y) & K(z, z) & K(z, x_1) \\ K(x_1, y) & K(x_1, z) & K(x_1, x_1) \end{vmatrix}$$

$$+ \cdots + (-1)^n \frac{1}{n!} \int_a^b dx_1 \cdots \int_a^b dx_n \left(\prod_i \frac{1}{k(z) - k(x_i)} \right)$$

$$\times \begin{vmatrix} K(x, y) & K(x, z) & K(x, x_1) & \cdots & K(x, x_n) \\ K(z, y) & K(z, z) & K(z, x_1) & \cdots & \\ K(x_1, y) & K(x_1, z) & K(x_1, x_1) & \cdots & \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ K(x_n, y) & & \cdots & & K(x_n, x_n) \end{vmatrix} + \cdots . \tag{15}$$

Interestingly, the only appearance of λ is in Eqs. (11′), (12), and (13) with no appearance of λ in the series expressions for $F(z)$ and $F(x, y; z)$.

VI. CONCLUSION

Thus, we expect that a direct matrix approach to the Lippman–Schwinger equation should prove quite satisfactory in the region below the threshold for scattering with two bodies bound so that λ is not on the branch cut. Such a calculation has actually been reported by Borysowicz and Dabrowski.[8] It was a calculation of the bound state of the 3-nucleon system for which quite reasonable results were obtained. The calculation was actually carried[9] into the region of the n–d cut and evidence was found of the zeros of the denominator function mentioned in Sec. 4. In retrospect, it is not surprising that the solution of Eq. (1) has branch cuts in the λ plane since the kernel of Eq. (1) is not Fredholm, as the main Fredholm result implies that the solution has only isolated poles in λ. It is also not surprising that the numerical approach to a branch cut be via a row of poles having residues inversely proportional to the density of poles on the line. It is also true that *on the line of singularities itself* the numerical solution does not approach the solution of Eq. (1), since for all N there is a row of poles in the λ plane along the branch line of the solution (1), but on the other hand the solution of Eq. (1) is not defined at all on such a line.

The question finally arises as to how any numerical method can give the solution of the integral equation along the branch cut in the λ plane. This can be done by letting the numerical procedure depend on λ. Numerical procedures can be found so that for any N the solution is analytic in λ along the branch cut and for any λ on the branch cut $\phi_N(\lambda) \to \phi^+(\lambda)$ as $N \to \infty$, where the superscript plus sign indicates the value of $\phi(\lambda)$ on a particular side of the branch cut. In that case, however, it does not seem convenient to start with Eq. (1), but with a form derived from Eq. (3). That is, we define

$$\phi(x) = [1 - \lambda k(x)]^{-1} \psi(x);$$

Eq. (3) then becomes

$$\psi(x) = f(x) + \lambda \int_a^b K(x, y) \frac{1}{1 - \lambda k(y)} \psi(y)\, dy. \tag{16}$$

Thus, the singularity in the integrand at $y =$ solution of $1 - \lambda k(y) = 0$ is made manifest, and the numerical evaluation of the integral can be accomplished by taking a principal value plus $i\pi\delta$ for the denominator. As noted, the numerical procedure for such an integration must depend on the location of the singularity, and thus on λ. This is a practical procedure used by several workers in the solution of Fadeev's equations.[10]

Some workers[11] have used a rotation of momentum axis in the Fadeev equations in order to avoid singularities in the integrands. This method has the advantage that a fixed set of points in the integration procedure may be used. In this case, of course, it does not matter whether one starts from Eq. (1) or Eq. (16), since they are algebraically equivalent.

APPENDIX

Consider the homogeneous equation

$$E\phi(\mathbf{k}) = \frac{k^2}{2m} \phi(\mathbf{k}) + \Lambda v(\mathbf{k}) \int v(\mathbf{k}') \phi(\mathbf{k}') \frac{d\mathbf{k}'}{(2\pi)^3}.$$

This is just the Schrödinger equation for a separable potential in momentum space. If v is spherically

symmetric so that only s waves occur, we have

$$\phi(k) = \frac{1}{E}\int_0^\infty \left(\frac{k^2}{2m}\,\delta(k-k') + \Lambda v(k)v(k')\frac{k'^2}{2\pi^2}\right)\phi(k')\,dk'. \quad \text{(A1)}$$

This equation is just a homogeneous form of Eq. (1), where $1/E$ corresponds to λ. To find the eigenvalues of this equation, we may write $D(E)$ and find its zeros. We use the forms given in Eqs. (13) and (14) to evaluate $D(E)$. We treat the special case $v(k) = 1$ for $k \leq k_a$ and $v(k) = 0$ for $k > k_a$. First, we consider the continuous limit, then the case of a discrete approximation. $F(z)$ in Eq. (14) becomes

$$F(z) = \Lambda z^2/2\pi^2,$$

so that D becomes

$$D(E) = 1 - \int_0^{k_a} \frac{\Lambda}{2\pi^2}\frac{z^2\,dz}{E - z^2/2m}.$$

Introducing the dimensionless variables $\kappa = z/k_a$ and $\gamma^2 = 2mE/k_a^2$, we have

$$D(E) = 1 - \frac{\Lambda m k_a}{\pi^2}\int_0^1 \frac{\kappa^2\,d\kappa}{\gamma^2 - \kappa^2} = 1 + \frac{\Lambda m k_a}{\pi^2}\left[1 + \tfrac{1}{2}\gamma \ln\left(\frac{\gamma - 1}{\gamma + 1}\right)\right]. \quad \text{(A2)}$$

The "physical cut" in E, which arises here from the non-Fredholm character of our equations, is the branch cut of the logarithm.

In the discrete case $F(z)$ becomes $\Lambda z_j^2/2\pi^2$, where $z_j = k_a(j - \frac{1}{2})/N$, so that $D(E)$ becomes

$$D(E) = 1 - \Delta\sum_{j=1}^{N} \frac{\Lambda}{2\pi^2}\frac{z_j^2}{E - z_j^2/2m}. \quad \text{(A3)}$$

Carrying out the summation, we obtain

$$D(E) = 1 + (\Lambda m k_a/\pi^2) \times \left\{1 + \frac{\gamma}{2}[\psi(-\tfrac{1}{2} - \gamma N + N) - \psi(-\tfrac{1}{2} - \gamma N - N)]\right\}, \quad \text{(A4)}$$

where $\psi(x)$ is the logarithmic derivative of the factorial function. Here the branch cut of Eq. (A2) is replaced by a line of poles.

The values of E chosen by $E = z_j^2/2m$ are similar to the unperturbed levels in a periodic or box normalization of finite size, while the zeros of $D(E)$ in Eq. (A4) are similar to the perturbed values of such energy levels.

It is easily shown that $D(E)$ as given by Eq. (A4) approaches $D(E)$ as given by Eq. (A2) in the limit $N \to \infty$, for any λ not on the physical cut.

To go further, this problem can be solved for the case of the inhomogeneous integral equation but most of the features of analyticity are contained in $D(E)$.

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Interpretation of the Symmetry of the Clebsch–Gordan Coefficients Discovered by Regge

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An interpretation is proposed for the intriguing symmetry of the Clebsch–Gordan coefficients discovered in 1958 by Regge. The interpretation is based on the observation that, in the reduction of the Kronecker product of two irreducible representations of an $SU(2)$ group, there appears in a natural way another $SU(2)$ group, which is almost independent of the original one. The Regge symmetry is interpreted as the symmetry under the interchange of these two $SU(2)$ groups. In more picturesque language, the Regge symmetry is the symmetry under the interchange of the "two-ness" of the *two* angular momenta being added with the "two-ness" of $SU(2)$. It follows from this interpretation that a symmetry of the same nature is present in the generalized Clebsch–Gordan coefficient that appears in the reduction of the Kronecker product of n (and not two, except when $n = 2$) irreducible representations of $SU(n)$.

INTRODUCTION

In the study of the quantum theory of angular momentum, a central role is played by the Clebsch–Gordan (CG) coefficient or 3-j symbol. The concept of this coefficient was introduced[1] nearly half a century ago, and its properties were studied and described in great detail in the years immediately following. In particular, it was thought that its symmetries were well understood and it came as quite a surprise when, as late as 1958, Regge[2] demonstrated the existence of a new, and rather bizarre, symmetry of the CG coefficient.

Whereas the previously known symmetries had a natural physical or geometrical interpretation, the symmetry discovered by Regge appeared not to have any such explanation. To quote from Regge's original paper: "Thus far we cannot justify these symmetries using simple physical arguments."[2] This unexplained symmetry has led Bargmann[3] to conjecture that the rotation group has special properties not shared by other groups. We are referring here to the Racah–Wigner calculus of the group and the fact that many properties of the appropriately generalized 3-j symbols, 6-j symbols, etc., are common to many groups. At the same time, however, Shelepin and Karasev[4] constructed a Racah–Wigner calculus for $SU(n)$ group by considering the so-called $(n + 1) \times (n + 1)$ symbol, which is a direct generalization of the 3×3 symbol introduced by Regge. As will be seen from the interpretation of the Regge symmetry we propose, the contradiction between Bargmann's conjecture and the work of Shelepin and Karasev is only apparent.

Shelepin and Karasev contributed to the theory of the Racah–Wigner calculus. On a more practical side one should mention the work of Shimpuku,[5] who looked into the simplifications, due to the Regge symmetry, in numerical computations of 3-j symbols. The magic square feature of the Regge 3×3 symbol was exploited by Giovannini and Smith[6] in their study of the 3-j symbol.

It is natural to expect that the Regge symmetry for the 3-j symbol should have implications for the 6-j symbol, 9-j symbol, etc. It was shown by Regge[7] and by Jahn and Howell[8] that the 6-j symbol, or Racah coefficient, indeed possesses additional symmetries.

Although we do not claim to have quoted here every contribution to the subject of Regge symmetry, we believe that our list of references is representative. None of these contributions offer an explanation for the Regge symmetry. In a paper by Ponzano and Regge,[9] published as recently as 1968, we find the following statement: "The geometrical and physical content of these symmetries is still to be understood and they remain a puzzling feature of the theory of angular momenta."

After stating the symmetries of the $SU(2)$ CG coefficient in Sec. 1, we show in Sec. 2 the existence of another $SU(2)$ group by employing the calculus of boson operators.[10] The importance of this other group for the Racah–Wigner calculus of $SU(n)$ has been emphasized by Biedenharn and coworkers.[11] We next demonstrate that the exchange of quantum numbers involved in the Regge symmetry corresponds to the exchange of these two $SU(2)$ groups. Even though this completes our explanation of the Regge symmetry, we give another version in Sec. 3 to make the meaning clearer. In this version, we introduce a new generating function for the CG coefficients and give a new proof of the Regge symmetries. As a final insight into the problem, we discuss in Sec. 4 the relation between CG coefficients and the representation functions insofar as it is relevant to the Regge symmetries. We

present here an expression[12] for the CG coefficient which makes manifest the fact that the CG coefficient is the quantized analog of the representation function.[13]

In the Conclusion, we make remarks about extension to $SU(n)$ and explain in what sense the $SU(2)$ group both is and is not different from $SU(n)$ groups, $n \neq 2$, as far as Regge symmetries are concerned.

1. SYMMETRIES OF THE CG COEFFICIENTS

The physical meaning of the CG coefficient is made immediately apparent in the bra and ket notation of Dirac. Thus,

$$\langle j_1 m_1 j_2 m_2 \,|\, jm \rangle \tag{1}$$

is the probability amplitude that, in the addition of the angular momentum whose square and z component are $j_1(j_1+1)$ and m_1 to the angular momentum $j_2(j_2+1)$ and m_2, one obtains the angular momentum $j(j+1)$ and m. It is clear from this definition that the CG coefficient should be invariant, except possibly for a phase, under the interchange of the subscripts one and two. Less trivial is the remark that the CG coefficient has symmetries under the permutation of all three angular momenta $\mathbf{J}_1$, $\mathbf{J}_2$, and $\mathbf{J}$. To make this symmetry apparent, the six numbers appearing in Eq. (1) are arranged in a two-rowed array called the 3-j symbol:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3}(2j_3+1)^{-\frac{1}{2}}\langle j_1 m_1 j_2 m_2 \,|\, j_3 - m_3 \rangle. \tag{2}$$

The 3-j symbol is invariant, up to a phase, under a permutation of its columns. The origin of this invariance is the fact that the addition of two angular momenta, $\mathbf{J}_1 + \mathbf{J}_2 = \mathbf{J}$, can be viewed as the addition of three angular momenta $\mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3 = 0$, because the negative of an angular momentum operator is, in a certain sense, also an angular momentum operator.[14] Therefore, it also follows that the 3-j symbol is invariant, up to a phase under the replacement

$$m_1 m_2 m_3 \rightarrow -m_1 - m_2 - m_3,$$

corresponding to the reversal of all three angular momenta.

Thus, we have as the symmetry group of the 3-j symbol the 3! permutations and the reversal of the three angular momenta—a symmetry group of 12 elements. These symmetries will be referred to as classical symmetries; their physical origin is clear.

Now, in fact, the symmetry group of the 3-j symbol consists of 72 elements. These can be generated by combining the classical symmetries with the Regge symmetries. To make all these symmetries apparent in the notation, one replaces the 3-j symbol by an array of nine numbers, the so-called Regge symbol or 3 × 3 symbol:

$$\begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} = \begin{vmatrix} j_1+j_2-j_3 & j_1-j_2+j_3 & -j_1+j_2+j_3 \\ j_3-m_3 & j_2-m_2 & j_1-m_1 \\ j_3+m_3 & j_2+m_2 & j_1+m_1 \end{vmatrix}. \tag{3}$$

The $72 = 3! \times 3! \times 2$ elements are the permutation of columns, the permutation of rows and transposition of the 3 × 3 symbol. Clearly, all these elements can be generated from the following fundamental ones: (a) permutation of the columns, (b) permutation of the 2nd and 3rd rows, (c) transposition. The (a) and (b) symmetries are seen to be the classical symmetries; (c) is a Regge symmetry. Other Regge symmetries result from combining (c) with (a) and/or (b). In the following, we concentrate on the transposition symmetry (c) and refer to it as *the* Regge symmetry; clearly, it is sufficient to find an explanation for it.

It is our thesis that the Regge symmetry reflects the fact that we are dealing with the reduction of the Kronecker product of *two* irreducible representations of $SU(2)$. Therefore, the notation that treats all three angular momenta symmetrically is not a help but a hindrance. Therefore, we set $j_3 = j$ and use the fact that $m_3 = -m_1 - m_2$ to write the Regge symbol as

$$\begin{vmatrix} j_1+j_2-j & j_1-j_2+j & -j_1+j_2+j \\ j+m_1+m_2 & j_2-m_2 & j_1-m_1 \\ j-m_1-m_2 & j_2+m_2 & j_1+m_1 \end{vmatrix}. \tag{4}$$

Thus, the transposition is equivalent to the interchange $m_1 + m_2 \leftrightarrow j_1 - j_2$, while $m_1 - m_2$, $j_1 + j_2$, and j are left unchanged.

2. THE "OTHER" $SU(2)$ GROUP

We start by constructing angular momentum operators, using the boson calculus realization of the angular momentum algebra. Let a, b, c, and d be four independent (commuting) boson annihilation operators

$$[a, \bar{a}] = [b, \bar{b}] = [c, \bar{c}] = [d, \bar{d}] = 1, \tag{5}$$

all other commutators being zero.

Let

$$L_1^{(1)} = \tfrac{1}{2}(\bar{a}b + \bar{b}a),$$
$$L_2^{(1)} = -\tfrac{1}{2}i(\bar{a}b - \bar{b}a), \quad (6)$$
$$L_3^{(1)} = \tfrac{1}{2}(\bar{a}a - \bar{b}b),$$

or

$$\mathbf{L}^{(1)} = \bar{\phi}\tfrac{1}{2}\boldsymbol{\sigma}\phi,$$

where ϕ is the 1-column matrix $\binom{a}{b}$ and the $\boldsymbol{\sigma}$ are the Pauli 2×2 matrices. Then, the three objects $L_1^{(1)}$, $L_2^{(1)}$, $L_3^{(1)}$ are isomorphic to the Cartesian components of an angular momentum, and we say that they generate a group called $SU(2)$.

We may construct another set, completely independent, by using the c and d operators

$$\mathbf{L}^{(2)} = \bar{\chi}\tfrac{1}{2}\boldsymbol{\sigma}\chi, \quad (7)$$

where χ is the 1-column matrix $\binom{c}{d}$. Since $\mathbf{L}^{(1)}$ and $\mathbf{L}^{(2)}$ commute, they generate together the group $SU(2) \times SU(2)$.

Now, aside from the above, we may construct another, isomorphic, set

$$\mathbf{U}^{(1)} = \bar{\zeta}\tfrac{1}{2}\boldsymbol{\sigma}\zeta, \quad \mathbf{U}^{(2)} = \bar{\eta}\tfrac{1}{2}\boldsymbol{\sigma}\eta, \quad (8)$$

where $\zeta = \binom{a}{c}$, $\eta = \binom{b}{d}$. $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$ also generate an $SU(2) \times SU(2)$ group. In fact, several other sets, such as the $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$ sets, can be obtained from the $\mathbf{L}^{(1)}$ and $\mathbf{L}^{(2)}$ set by permutation of the boson operators a, b, c, and d. This is a manifestation of the fact that the appropriate framework for the discussion of the reduction of the Kronecker product of two irreducible representations of the $SU(2)$ group is the $SU(4)$ group. This group has several $SU(2) \times SU(2)$ subgroups, examples of which are the group generated by $\mathbf{L}^{(1)}$ and $\mathbf{L}^{(2)}$ and the group generated by $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$. Although all these groups are mathematically identical, we can, of course, assign different physical meanings to them.

To emphasize the $SU(4)$ framework, it is convenient to use 4×4 matrices. We may write

$$\mathbf{L}^{(1)} = \bar{\Phi}\tfrac{1}{2}\boldsymbol{\tau}\tfrac{1}{2}(\rho_4 + \rho_3)\Phi, \quad (9)$$
$$\mathbf{L}^{(2)} = \bar{\Phi}\tfrac{1}{2}\boldsymbol{\tau}\tfrac{1}{2}(\rho_4 - \rho_3)\Phi, \quad (10)$$
$$\mathbf{U}^{(1)} = \bar{\Phi}\tfrac{1}{2}(\tau_4 + \tau_3)\tfrac{1}{2}\boldsymbol{\rho}\Phi, \quad (11)$$
$$\mathbf{U}^{(2)} = \bar{\Phi}\tfrac{1}{2}(\tau_4 - \tau_3)\tfrac{1}{2}\boldsymbol{\rho}\Phi, \quad (12)$$

where τ_α and ρ_β are 2×2 matrices whose direct product spans the space of 4×4 matrices $\tau_\alpha\rho_\beta$, $\alpha, \beta = 1, 2, 3, 4$, $\tau_\alpha = (\boldsymbol{\tau}, \tau_4)$, $\rho_\beta = (\boldsymbol{\rho}, \rho_4)$, with $\boldsymbol{\tau}$ and $\boldsymbol{\rho}$ copies of the Pauli $\boldsymbol{\sigma}$, and τ_4 and ρ_4 copies of the identity. Lastly,

$$\Phi = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}. \quad (13)$$

It is easily seen in this notation that

$$\mathbf{L} = \mathbf{L}^{(1)} + \mathbf{L}^{(2)} = \bar{\Phi}\tfrac{1}{2}\boldsymbol{\tau}\rho_4\Phi \quad (14)$$

and

$$\mathbf{U} = \mathbf{U}^{(1)} + \mathbf{U}^{(2)} = \bar{\Phi}\tfrac{1}{2}\tau_4\boldsymbol{\rho}\Phi \quad (15)$$

commute with each other. However, the $SU(2)$ groups generated by $\mathbf{L}$ and $\mathbf{U}$ are not completely independent because, as a little algebra shows,

$$\mathbf{L}^2 = \mathbf{U}^2. \quad (16)$$

Thus, $\mathbf{L}$ and $\mathbf{U}$ generate the so-called orbital $SU(2) \times SU(2)$ group, for which the notation $SU(2) * SU(2)$ has been proposed.[11] If we interpret $\mathbf{L}^{(1)}$ and $\mathbf{L}^{(2)}$ as the angular momentum operators of two independent physical subsystems, then $\mathbf{L}$ is clearly to be interpreted as the total angular momentum of the system and the "physical" $SU(2)$ groups are those generated by $\mathbf{L}^{(1)}$, $\mathbf{L}^{(2)}$, and $\mathbf{L}$. The "other" $SU(2)$ groups are those generated by $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, and $\mathbf{U}$. In the work of Biedenharn and coworkers[11] the "physical" groups correspond to the lower and the "other" groups correspond to the upper Gel'fand patterns in the diamond-shaped structure describing their boson polynomial.

This then demonstrates, as stated in the Introduction, the natural occurrence of "another" $SU(2)$ group in the discussion of the Racah–Wigner calculus of the "physical" $SU(2)$ group. We now proceed to show that the interchange of quantum numbers involved in the Regge symmetry is equivalent to the interchange of the $SU(2)$ groups generated by $\mathbf{L}^{(1)}$, $\mathbf{L}^{(2)}$, and $\mathbf{L}$ with those generated by $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, and $\mathbf{U}$.

As is well known, the boson operators can be used to provide explicit realization of angular momentum eigenvectors. Thus,

$$|j_1m_1\rangle = [(j_1 + m_1)!\,(j_1 - m_1)!]^{-\frac{1}{2}}\bar{a}^{j_1+m_1}\bar{b}^{j_1-m_1}|\,\rangle \quad (17)$$

is a properly normalized eigenvector of the angular momentum $\mathbf{L}^{(1)}$:

$$L_3^{(1)}\,|j_1m_1\rangle = m_1\,|j_1m_1\rangle,$$
$$(\mathbf{L}^{(1)})^2\,|j_1m_1\rangle = j_1(j_1 + 1)\,|j_1m_1\rangle, \quad (18)$$

with $|\,\rangle$ the vacuum state, i.e., the state annihilated by any annihilation operator a, b, c, d.

Similarly,

$$|j_2m_2\rangle = [(j_2 + m_2)!\,(j_2 - m_2)!]^{-\frac{1}{2}}\bar{c}^{j_2+m_2}\bar{d}^{j_2-m_2}|\,\rangle, \quad (19)$$

$$L_3^{(2)}\,|j_2m_2\rangle = m_2\,|j_2m_2\rangle,$$
$$(\mathbf{L}^{(2)})^2\,|j_2m_2\rangle = j_2(j_2 + 1)\,|j_2m_2\rangle. \quad (20)$$

The quantum numbers j_i and m_i, $i = 1, 2$, are integers or half-integers satisfying

$$-j_i \leq m_i \leq j_i, \quad j_i = 0, \tfrac{1}{2}, 1, \cdots. \quad (21)$$

This, then, defines all the quantum numbers that appear in the Regge symbol, Eq. (4), except for j, which is defined by

$$\mathbf{L}^2 \,|jm\rangle = j(j+1)\,|jm\rangle,$$
$$m = m_1 + m_2 \tag{22}$$

and is an integer (half-integer) if $j_1 + j_2$ is an integer (half-integer) and satisfies

$$|j_1 - j_2| \leq j \leq j_1 + j_2. \tag{23}$$

The state $|jm\rangle$ is, of course, given by

$$|jm\rangle = \sum_{m_1 m_2} |j_1 m_1 j_2 m_2\rangle \langle j_1 m_1 j_2 m_2 \,|\, jm\rangle, \tag{24}$$

with

$$|j_1 m_1 j_2 m_2\rangle$$
$$= [(j_1 + m_1)!\,(j_1 - m_1)!\,(j_2 + m_2)!\,(j_2 - m_2)!]^{-\frac{1}{2}} \times \tilde{a}^{j_1+m_1} \tilde{b}^{j_1-m_1} \tilde{c}^{j_2+m_2} \tilde{d}^{j_2-m_2} \,|\, \rangle, \tag{25}$$

where Eq. (24) defines the CG coefficient.

Now, we may consider the set of all states of the form (25), for all m_i and j_i satisfying Eq. (21) and restricted by

$$2(j_1 + j_2) = N, \tag{26}$$

where N is some integer. Clearly, the number of such states is

$$\sum_{j_1 + j_2 = \frac{1}{2}N} (2j_1 + 1)(2j_2 + 1)$$
$$= \sum_{j_1 = 0, \frac{1}{2}, 1, \cdots, \frac{1}{2}N} (2j_1 + 1)[2(\tfrac{1}{2}N - j_1) + 1]$$
$$= \sum_{k = 0, 1, \cdots, N} (k+1)(N - k + 1)$$
$$= \tfrac{1}{6}(N+1)(N+2)(N+3). \tag{27}$$

This number is equal to $\binom{N+3}{N}$, which is the dimension of the completely symmetric representation of $SU(4)$ specified by the Young diagram of one row and N columns. This means that the representation of $SU(2) \times SU(2)$, Eq. (25), can be imbedded in a *multiplicity-free* way in the symmetric representation of $SU(4)$.

But that is not all. The state $|jm\rangle$, Eq. (24), should actually carry the labels j_1 and j_2, since it is an eigenstate of $(\mathbf{L}^{(1)})^2$ and $(\mathbf{L}^{(2)})^2$. Instead, using Eq. (26) and defining

$$\mu = j_1 - j_2, \tag{28}$$

we may label this state

$$|N\mu jm\rangle. \tag{29}$$

It follows from Eq. (23) that μ obeys

$$-j \leq \mu \leq +j, \tag{30}$$

just like m. We can now ask the question: How many states of the form (29) are there for fixed N and all allowed values of j, μ, and m? The calculation depends on whether N is even or odd. For $N = 2p$, we have

$$\sum_{j=0}^{p} (2j+1)^2 = \frac{(2p+1)(2p+2)(2p+3)}{6}$$
$$= \binom{N+3}{N}, \tag{31}$$

while, for $N = 2p + 1$, we have

$$\sum_{j=\frac{1}{2}}^{p+\frac{1}{2}} (2j+1)^2 = \sum_{l=0}^{p} (2l+1+1)^2$$
$$= \frac{4(p+1)(p+2)(2p+3)}{6}$$
$$= \binom{N+3}{N}. \tag{32}$$

This means that the state $|N\mu jm\rangle$ can also be imbedded in a multiplicity-free way in the symmetric representation of $SU(4)$.[15] These states are, in fact, a representation of the $SU(2) * SU(2)$ generated by $\mathbf{L}$ and $\mathbf{U}$. To see this, we only need to observe that we have

$$\mathbf{L}^2 \,|N\mu jm\rangle = \mathbf{U}^2 \,|N\mu jm\rangle = j(j+1)\,|N\mu jm\rangle,$$
$$L_3 \,|N\mu jm\rangle = m\,|N\mu jm\rangle, \tag{33}$$
$$U_3 \,|N\mu jm\rangle = \mu\,|N\mu jm\rangle.$$

If we recall that the transposition (4) of the Regge symbol amounted to leaving j, $j_1 + j_2$ and $m_1 - m_2$ unchanged, while interchanging $m_1 + m_2$ with $j_1 - j_2$, then in our present notation this means leaving j, N, and $m_1 - m_2$ unchanged while interchanging m and μ. It is clear from Eq. (33) that interchanging $\mathbf{L}$ and $\mathbf{U}$ interchanges m and μ, leaving j and N invariant. Moreover, $m_1 - m_2$ is the eigenvalue of $L_3^{(1)} - L_3^{(2)}$ and this operator, as is clear from Eqs. (9)–(12), is equal to $U_3^{(1)} - U_3^{(2)}$. This completes the proof that the interchange of quantum numbers involved in the transposition of the Regge symbol corresponds to the interchange of the "physical" groups generated by $\mathbf{L}^{(1)}$, $\mathbf{L}^{(2)}$, and $\mathbf{L}$ with the "other" groups generated by $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, and $\mathbf{U}$. More precisely, we have shown that the effect on the quantum numbers that appear in the Regge symbol of interchanging the "physical" and "other" groups is the same as transposing the Regge symbol.

Our final task is to deduce the abstract significance of the interchange of the "physical" and "other" groups. In the boson operator realization, we have the four objects a, b, c, and d. The interchange under discussion is achieved by exchanging b and c. All four objects a, b, c, and d are mathematically identical; however, they were ascribed different physical meanings. Thus, a and b were paired to realize the angular momentum of subsystem 1, and c and d were paired to realize the angular momentum of subsystem 2. We need pairs of operators because we are dealing with $SU(2)$. The exchange of b and c means that we propose to arrange the two pairings differently and are, in effect, exchanging the two-ness of $SU(2)$ with the two-ness of the two subsystems. To put it one more way, we may relabel the boson operators

$$a = a_1^1, \quad b = a_2^1, \quad c = a_1^2, \quad d = a_2^2. \tag{34}$$

The object a_i^j has a two-valued lower index referring to "spin up" and "spin down." It has a two-valued upper index referring to the two subsystems whose spins are being added. The Regge symmetry involves interchanging upper and lower indices.

3. A GENERATING FUNCTION FOR THE CG COEFFICIENT

In this section, we derive the symmetries of the CG coefficient in a new way, different from both the derivation given by Regge[2] and that given by Bargmann.[3] We hope that this will help to clarify our interpretation of the Regge symmetries. In the process, we present a generating function for the CG coefficient, which we believe to be new.

From the multinomial theorem and the definition (25) we have

$$\begin{aligned}&(A\bar{a} + B\bar{b} + C\bar{c} + D\bar{d})^N \mid \rangle \\ &= N! \sum \frac{A^{j_1+m_1} B^{j_1-m_1} C^{j_2+m_2} D^{j_2-m_2}}{[(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!]^{\frac{1}{2}}} \\ &\quad \times |j_1 m_1 j_2 m_2\rangle,\end{aligned} \tag{35}$$

where A, B, C, and D are arbitrary c numbers, and the summation is over all j_1, j_2, m_1, and m_2 satisfying Eqs. (21) and (26).

Equation (35), is, of course, nothing but an explicit realization of the statement that the representations of the $SU(2) \times SU(2)$, generated by $\mathbf{L}^{(1)}$ and $\mathbf{L}^{(2)}$, can be imbedded in the symmetric representation of $SU(4)$. As we know from the previous section, a similar imbedding is possible for the representations of the orbital $SU(2) * SU(2)$ generated by $\mathbf{L}$ and $\mathbf{U}$. The explicit realization of this imbedding depends on whether N is even or odd. For N even, we have

$$\begin{aligned}&[E(F\bar{a} + G\bar{b} + G^{-1}\bar{c} + F^{-1}\bar{d})^2 + H(\bar{a}\bar{d} - \bar{b}\bar{c})]^{\frac{1}{2}N} \mid \rangle \\ &= (\tfrac{1}{2}N)! \sum \frac{(2j)!}{j!} \left(\frac{(\frac{1}{2}N + j + 1)!}{(2j+1)(\frac{1}{2}N - j)!} \right)^{\frac{1}{2}} \\ &\quad \times \frac{E^j F^{m+\mu} G^{m-\mu} H^{\frac{1}{2}N-j}}{[(j+m)!\,(j-m)!\,(j+\mu)!\,(j-\mu)!]^{\frac{1}{2}}} |N\mu j m\rangle,\end{aligned} \tag{36a}$$

where E, F, G, and H are arbitrary c numbers and the summation is over all integer values of j, m, and μ satisfying

$$-j \le m \le j, \quad -j \le \mu \le j, \quad 0 \le j \le \tfrac{1}{2}N. \tag{37a}$$

For N odd we have, instead,

$$\begin{aligned}&[E(F\bar{a} + G\bar{b} + G^{-1}\bar{c} + F^{-1}\bar{d})^2 + H(\bar{a}\bar{d} - \bar{b}\bar{c})]^{\frac{1}{2}(N-1)} \\ &\quad \times E^{\frac{1}{2}}(F\bar{a} + G\bar{b} + G^{-1}\bar{c} + F^{-1}\bar{d}) \mid \rangle \\ &= \left(\frac{N-1}{2}\right)! \sum \frac{(2j)!}{(j-\frac{1}{2})!} \left[\frac{(\frac{1}{2}N + j + 1)!}{(2j+1)(\frac{1}{2}N - j)!} \right]^{\frac{1}{2}} \\ &\quad \times \frac{E^j F^{m+\mu} G^{m-\mu} H^{\frac{1}{2}N-j}}{[(j+m)!\,(j-m)!\,(j+\mu)!\,(j-\mu)!]^{\frac{1}{2}}} |N\mu j m\rangle,\end{aligned} \tag{36b}$$

the summation being over all half-integer values of j, m, and μ satisfying

$$-j \le m \le j, \quad -j \le \mu \le j, \quad \tfrac{1}{2} \le j \le \tfrac{1}{2}N. \tag{37b}$$

Equation (36) is a direct consequence of the multinomial theorem, provided that the properly normalized eigenvector $|N\mu j m\rangle$ is given in terms of the boson operators by

$$\begin{aligned}&|N\mu j m\rangle \\ &= \left(\frac{(2j+1)(j+m)!\,(j-m)!\,(j+\mu)!\,(j-\mu)!}{(\frac{1}{2}N - j)!\,(\frac{1}{2}N + j + 1)!} \right)^{\frac{1}{2}} \\ &\quad \times \sum_k \frac{\bar{a}^k \bar{b}^{j+\mu-k} \bar{c}^{j+m-k} \bar{d}^{k-m-\mu}}{k!\,(j+\mu-k)!\,(j+m-k)!\,(k-m-\mu)!} \\ &\quad \times (\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j} \mid \rangle.\end{aligned} \tag{38}$$

The proof of Eq. (38) is left to Appendix A.

If we form the scalar product of the left-hand sides of Eq. (35) and (36a) we obtain (assuming, for simplicity, that E, F, G, and H are real)

$$\begin{aligned}\langle \mid [E(Fa + Gb + G^{-1}c + F^{-1}d)^2 + H(ad - bc)]^{\frac{1}{2}N} \\ \times (A\bar{a} + B\bar{b} + C\bar{c} + D\bar{d})^N \mid \rangle \\ = [E(FA + GB + G^{-1}C + F^{-1}D)^2 \\ + H(AD - BC)]^{\frac{1}{2}N} N!.\end{aligned} \tag{39}$$

Equation (39) applies when N is even; a similar expression holds when N is odd. The proof of Eq. (39) is given in Appendix B.

The result of these operations is a generating function for the CG coefficient

$$[E(FA + GB + G^{-1}C + F^{-1}D)^2 + H(AD - BC)]^{\frac{1}{2}N} = \left(\frac{N}{2}\right)! \sum \frac{(2j)!}{j!}\left[\frac{(\frac{1}{2}N + j + 1)!}{(2j+1)(\frac{1}{2}N - j)!}\right]^{\frac{1}{2}} \langle N\mu jm \mid j_1 m_1 j_2 m_2\rangle \times \frac{A^{j_1+m_1}B^{j_1-m_1}C^{j_2+m_2}D^{j_2-m_2}E^{j}F^{\mu+m}G^{\mu-m}H^{\frac{1}{2}N-j}}{[(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!\,(j+m)!\,(j-m)!\,(j+\mu)!\,(j-\mu)!]^{\frac{1}{2}}}, \quad (40)$$

where the sum extends over all the quantum numbers specified in Eqs. (21), (26), and (37a). Again, a slightly different expression results when N is odd.

Symmetry properties of the CG coefficient follow from the invariance of the generating function to particular substitutions. Thus, the substitution

$$A \leftrightarrow B, \quad C \leftrightarrow D, \quad F \leftrightarrow G, \quad E \to E, \quad H \to -H \quad (41)$$

proves the classical symmetry

$$\langle N\mu jm \mid j_1 m_1 j_2 m_2\rangle = (-)^{\frac{1}{2}N-j}\langle N\mu j - m \mid j_1 - m_1 j_2 - m_2\rangle, \quad (42)$$

whereas the substitution

$$A \to A, \quad B \leftrightarrow C, \quad D \to D, \quad E \to E, \quad F \to F, \quad G \to G^{-1}, \quad H \to H \quad (43)$$

proves the Regge symmetry, i.e., invariance of the CG coefficient under $m \leftrightarrow \mu$, with j, $j_1 + j_2$, and $m_1 - m_2$ left unchanged.

The classical symmetry under the permutation of $j_1 m_1$ with $j_2 m_2$ is also easily inferred from the invariance under the substitution

$$A \leftrightarrow C, \quad B \leftrightarrow D, \quad F \leftrightarrow G^{-1}, \quad E \to E, \quad H \to -H. \quad (44)$$

The classical symmetry under the permutation of jm with either $j_1 m_1$ or $j_2 m_2$ is not as readily apparent. What we are seeing here is the complement of the statement that a notation which treats all three angular momenta $\mathbf{J}_1$, $\mathbf{J}_2$, and $\mathbf{J}$ symmetrically is not helpful in understanding the Regge symmetry: the generating function, Eq. (40) clarifies the Regge symmetry but obscures the symmetry under the permutation of $\mathbf{J}$ with either $\mathbf{J}_1$ or $\mathbf{J}_2$.

How do we use the generating function (40) to clarify the Regge symmetry? Consider first a classical symmetry, say the symmetry under reversal of all angular momenta. According to Eq. (41), we must interchange A and B, C and D, F and G, leave E alone, and change the sign of H. A look at Eqs. (35) and (36) makes it clear that, in terms of the boson operators, this is equivalent to the interchange of a with b and c with d. Mathematically, there is no difference between a and b, but when we wrote Eq. (6) we assigned to $\bar{a}$ the physical meaning of the creation operator that creates "spin up" and to $\bar{b}$ the physical meaning of the creation operator that creates "spin down"—interchanging a and b corresponds, therefore, to the reversal of angular momentum $\mathbf{J}_1$. The same argument applies to c and d and $\mathbf{J}_2$.

Guided by the above, we see that the substitution (43) is equivalent in terms of boson operators to the interchanging of b and c (with a and d left unchanged) and, therefore, the Regge symmetry corresponds to this particular permutation of boson operators. From here on, we may repeat verbatim the arguments appearing at the end of the preceding section.

For the reader who may wonder what precisely was the purpose of this section, we point out that we produced here a generating function from which we can prove the Regge symmetries *and* obtain the same interpretation of these symmetries as proposed in the previous section. This could not be done with the generating function given by Schwinger[10] or Regge.[2]

4. CG COEFFICIENTS, REPRESENTATION FUNCTIONS, AND THE REGGE SYMMETRY

As is well known, in the so-called classical limit, the CG coefficient approaches the representation function; i.e., the matrix element of a finite rotation. The relation in question may be written as follows:

$$\langle jm\, JM \mid J + \mu, M + m\rangle \to (-1)^{j-m} D^{j}_{m\mu}(0, \beta, 0), \quad J \gg |M| \gg j, \quad \cos\beta = M/J. \quad (45)$$

The Regge 3×3 symbol corresponding to this CG coefficient may be written as

$$\begin{array}{|lll|} \hline 2J+\mu-j & j+\mu & j-\mu \\ j+m & J+M & J-M+\mu-m \\ j-m & J-M & J+M+\mu+m \\ \hline \end{array} \quad (46)$$

so that its transposition requires the following transformation of quantum numbers:

$$J \to J + \tfrac{1}{2}(\mu - m), \quad M \to M - \tfrac{1}{2}(\mu - m), \quad m \leftrightarrow \mu, \quad j \to j. \tag{47}$$

Consequently, *in the classical limit*, the Regge symmetry of the CG coefficient is equivalent to the symmetry under the interchange $m \leftrightarrow \mu$ of the representation function $D^j_{m\mu}$. This latter interchange can be given the physical interpretation of interchanging "body-fixed" and "space-fixed" coordinate systems when the D functions are identified with the eigenfunctions of the Schrödinger equation for a symmetric top.

Thus, in the classical limit for the CG coefficient, the Regge symmetry may be viewed as the symmetry under the interchange of "body-fixed" and "space-fixed" frames of reference. More precisely, we again have here two angular momenta—the angular momentum in the body-fixed and in the space-fixed frames—which commute with each other and have equal magnitudes, i.e., which generate the orbital $SU(2) * SU(2)$. And, again, the Regge symmetry is the symmetry under the interchange of the two $SU(2)$ groups.

However, this result is unsatisfactory since it really expresses a property of the representation function—which is equal to the CG coefficient only in the classical limit—whereas, the Regge symmetry refers to the CG coefficient itself.

However, the above asymptotic relation (45) provides a clue. If one considers the geometrical construction[16] used in deriving Eq. (45), one arrives at the following geometrical interpretation. The object $\langle jm\, JM \mid \tilde{J}\tilde{M}\rangle$ is the probability amplitude that a quantized vector $\mathbf{j}$, which has a component m along an axis specified by a classical vector $\mathbf{z}$, will then have the component $\mathbf{j}\cdot\tilde{\mathbf{J}}/\tilde{J}$ along a *quantized* vector $\tilde{\mathbf{J}}$. The object $D^j_{\mu m}(0, \beta, 0)$, on the other hand, is the probability amplitude that the quantized vector $\mathbf{j}$, which has the component m along an axis specified by a classical vector $\mathbf{z}$, will then have the component μ along a *classical* vector $\tilde{\mathbf{z}}$, where $\cos\beta = \mathbf{z}\cdot\tilde{\mathbf{z}}/z\tilde{z}$. Thus, the CG *coefficient constitutes the quantized analog of the representation function.*

The above relationship between the CG coefficient and the representation function may be displayed in a striking fashion by making use of the concept of generalized power.[17] We may define

$$x^{[a]} \equiv x!/(x-a)!, \tag{48}$$

where the factorial is to be understood as the Γ function when the argument is noninteger. It follows from Eq. (48) that

$$\frac{\Delta x^{[a]}}{\Delta x} = a x^{[a-1]}, \tag{49}$$

where the difference operator $\Delta/\Delta x$ is defined in the usual way, i.e.,

$$\frac{\Delta f(x)}{\Delta x} = f(x+1) - f(x). \tag{50}$$

When we compare Eq. (49) with

$$\frac{dx^a}{dx} = a x^{a-1}, \tag{51}$$

we see that *the generalized power is the difference analog of the conventional power.*

Let us now take the expression for the CG coefficient as given, for example, by Edmonds [Eq. (3.6.11)][18]

$$\begin{aligned}[(2P+1)/(2P+\mu-j+1)]^{\frac{1}{2}}&\langle jm\, JM \mid J+\mu, M+m\rangle \\ &= [(j-\mu)!\,(j+\mu)!\,(j-m)!\,(j+m)!\,(2P-2j)!/(2P)!]^{\frac{1}{2}} \\ &\quad\times \sum_s (-1)^s \frac{[(P+Q)!\,(P+Q+m+\mu)!\,(P-Q-j-\mu)!\,(P-Q-j-m)!]^{\frac{1}{2}}}{s!\,(j-\mu-s)!\,(j-m-s)!\,(m+\mu+s)!\,(P+Q-s)!\,(P-Q-2j+s)!},\end{aligned} \tag{52}$$

where

$$P+Q \equiv J+M, \quad P-Q \equiv J-M+j+\mu, \tag{53}$$

and rewrite it,[12] using the definition of generalized power, as[19]

$$\begin{aligned}\left(\frac{2P+1}{2P+\mu-j+1}\right)^{\frac{1}{2}}&\langle jm\, JM \mid J+\mu, M+m\rangle = \left(\frac{(j-\mu)!\,(j+\mu)!\,(j-m)!\,(j+m)!}{(2P)^{[2j]}(P+Q)^{[-m-\mu]}(P-Q)^{[j+\mu]}(P-Q)^{[j+m]}}\right)^{\frac{1}{2}} \\ &\times \sum_s (-1)^s \frac{(P+Q)^{[s]}(P-Q)^{[2j-s]}}{s!\,(j-m-s)!\,(j-\mu-s)!\,(m+\mu+s)!}.\end{aligned} \tag{54}$$

On the other hand, starting from Edmonds [Eq. (4.1.15)], we have

$$(-1)^{j-m}D^{j}_{m\mu}(0,\beta,0) = [(j-\mu)!\,(j+\mu)!\,(j-m)!\,(j+m)!]^{\frac{1}{2}} \times \sum_s (-1)^s \frac{(\cos\tfrac{1}{2}\beta)^{2s+m+\mu}(\sin\tfrac{1}{2}\beta)^{2j-2s-m-\mu}}{s!\,(j-m-s)!\,(j-\mu-s)!\,(m+\mu+s)!}$$
$$= [(j-\mu)!\,(j+\mu)!\,(j-m)!\,(j+m)!]^{\frac{1}{2}} \times \sum_s (-1)^s \frac{[(P+Q)/2P]^{s+\frac{1}{2}(m+\mu)}[(P-Q)/2P]^{j-s-\frac{1}{2}(m+\mu)}}{s!\,(j-m-s)!\,(j-\mu-s)!\,(m+\mu+s)!}, \tag{55}$$

where

$$Q/P \equiv \cos\beta. \tag{56}$$

But Eq. (55) can, of course, be written as

$$(-1)^{j-m}D^{j}_{m\mu}(0,\beta,0) = \left(\frac{(j-\mu)!\,(j+\mu)!\,(j-m)!\,(j+m)!}{(2P)^{2j}(P+Q)^{-m-\mu}(P-Q)^{j+\mu}(P-Q)^{j+m}}\right)^{\frac{1}{2}} \times \sum_s (-1)^s \frac{(P+Q)^s(P-Q)^{2j-s}}{s!\,(j-m-s)!\,(j-\mu-s)!\,(m+\mu+s)!}. \tag{57}$$

When we compare Eqs. (57) and (54), we see that the representation function and CG coefficient bear to each other the same relation as the normal power to the generalized power. This, then, is the mathematical version of the statement that the CG coefficient is the quantized analog of the representation function.

In this fashion, we remove the objection mentioned earlier to the interpretation of the Regge symmetry in terms of the interchange of "body-fixed" and "space-fixed" frames of reference. It may be worth pointing out that the transformation (47) leaves P and Q invariant so that in terms of the quantum numbers used in Eq. (54) the Regge transformation is $m \leftrightarrow \mu$, with all other quantities unchanged as is necessary for consistency.

CONCLUSION

In conclusion, and as a final insight into the problem, we consider the generalization of the Regge symmetry from $SU(2)$ to $SU(n)$. The realization of the $SU(n)$ algebra in terms of boson operators requires the introduction of n boson annihilation operators a_i, $i = 1, 2, \cdots, n$. The discussion of the Racah–Wigner calculus of $SU(n)$ requires the use of n copies of $SU(n)$. Thus, we introduce the n^2 boson annihilation operators a^j_i, with $i = 1, 2, \cdots, n$ and $j = 1, \cdots, n$. [Compare with Eq. (34) for $SU(2)$.] We see clearly the natural appearance of two kinds of $SU(n)$ groups: the "physical" $SU(n)$ involving transformations on the lower index of a^j_i, and the "other" $SU(n)$ involving transformations on the upper index of a^j_i.

Next, we define CG coefficients of rank[20] k as elements of the unitary matrix which reduces the Kronecker product of k irreducible representations of $SU(n)$. When $k > n$, these objects can be expressed in terms of those of rank k' where $k' \leq n$ [it is clear that the concept of this rank is not useful in $SU(2)$].

Given these definitions, we can state the Regge symmetry for $SU(n)$: The CG coefficient of rank n, arising in the reduction of n completely *symmetric* irreducible representations, is invariant under the transformation of quantum numbers that results from the interchange of the "physical" and "other" $SU(n)$ groups.

It is now also clear from this generalization how the rotation group [i.e., $SU(2)$] at the same time does and does not differ from $SU(n)$ groups, $n > 2$. It differs because the conventional (i.e., of rank 2) CG coefficient possesses the Regge symmetry in $SU(2)$ and does not in $SU(n)$, $n > 2$. It does not differ because the CG coefficient of rank n possesses the Regge symmetry for all $SU(n)$ including $n = 2$.

It has been pointed out to the author that the equality of the two sets of invariants of $U(n) * U(n)$ [cf. our Eq. (16)] has been established in the work of Louck[21] and that the work of Biedenharn[22] (in which limits of certain Racah coefficients are related to CG coefficients) raises the possibility of a geometrical interpretation of the Regge symmetry by exploring the tetrahedral structure of the Racah coefficient.

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APPENDIX A

In this appendix, we show that the properly normalized eigenvector $|N\mu jm\rangle$ is given in terms of the boson operators by Eq. (38). It follows from the definitions in Sec. 2 that

$$\mathbf{L}^2 = L_-L_+ + L_3 + L_3^2, \quad L_\mp \equiv L_1 \mp iL_2, \tag{A1}$$

$$\mathbf{U}^2 = U_-U_+ + U_3 + U_3^2, \quad U_\mp \equiv U_1 \mp iU_2, \tag{A2}$$

$$L_+ = \bar{a}b + \bar{c}d, \quad L_- = \bar{b}a + \bar{d}c, \tag{A3}$$

$$U_+ = \bar{a}c + \bar{b}d, \quad U_- = \bar{c}a + \bar{d}b, \tag{A4}$$

$$L_3 = \tfrac{1}{2}(\bar{a}a - \bar{b}b + \bar{c}c - \bar{d}d), \tag{A5}$$

$$U_3 = \tfrac{1}{2}(\bar{a}a + \bar{b}b - \bar{c}c - \bar{d}d). \tag{A6}$$

Consider the state $\overline{\Lambda}\,|\,\rangle$, where

$$\overline{\Lambda} = \sum_k \frac{\bar{a}^k \bar{b}^{j+\mu-k} \bar{c}^{j+m-k} \bar{d}^{k-m-\mu}}{k!\,(j+\mu-k)!\,(j+m-k)!\,(k-m-\mu)!}. \tag{A7}$$

By explicit commutation, we have

$$L_-L_+\overline{\Lambda}\,|\,\rangle = [L_-, [L_+, \overline{\Lambda}]]\,|\,\rangle = (j+m+1)(j-m)\overline{\Lambda}\,|\,\rangle, \tag{A8}$$

$$U_-U_+\overline{\Lambda}\,|\,\rangle = (j+\mu+1)(j-\mu)\overline{\Lambda}\,|\,\rangle. \tag{A9}$$

Moreover, since each term in the sum in $\overline{\Lambda}$ is an eigenstate of L_3 to the eigenvalue m and of U_3 to the eigenvalue μ, it follows that

$$\mathbf{U}^2\overline{\Lambda}\,|\,\rangle = j(j+1)\overline{\Lambda}\,|\,\rangle, \quad \mathbf{L}^2\overline{\Lambda}\,|\,\rangle = j(j+1)\overline{\Lambda}\,|\,\rangle,$$
$$U_3\overline{\Lambda}\,|\,\rangle = \mu\overline{\Lambda}\,|\,\rangle, \quad L_3\overline{\Lambda}\,|\,\rangle = m\overline{\Lambda}\,|\,\rangle. \tag{A10}$$

Next, we note that the operator $\mathcal{N}$, whose eigenvalue is the degree of the homogeneous polynomial constructed out of $\bar{a}$, $\bar{b}$, $\bar{c}$, and $\bar{d}$, is obviously

$$\mathcal{N} = \bar{a}a + \bar{b}b + \bar{c}c + \bar{d}d. \tag{A11}$$

Clearly,

$$\mathcal{N}\overline{\Lambda}\,|\,\rangle = 2j\overline{\Lambda}\,|\,\rangle. \tag{A12}$$

Consider the object $(\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j}$. Since it commutes with $\mathbf{U}^2$, $\mathbf{L}^2$, U_3, and L_3, and since

$$[\mathcal{N}, (\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j}] = (N-2j)(\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j}, \tag{A13}$$

it follows that $\overline{\Lambda}(\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j}$ is proportional to $|N\mu jm\rangle$. This proves Eq. (38) to within a constant of proportionality.

To determine the constant of proportionality, we write

$$|N\mu jm\rangle = K^{-\frac{1}{2}}\overline{\Lambda}(\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j}\,|\,\rangle, \tag{A14}$$

so that the normalization condition $\langle N\mu jm \,|\, N\mu jm\rangle = 1$ becomes

$$K = \langle\,|\,(ad-bc)^{\frac{1}{2}N-j}\Lambda\overline{\Lambda}(\bar{a}\bar{d} - \bar{b}\bar{c})^{\frac{1}{2}N-j}\,|\,\rangle. \tag{A15}$$

We note that (as can be proved by induction on $\frac{1}{2}N - j$)

$$(-1)^{\frac{1}{2}N-j}(ad-bc)^{\frac{1}{2}N-j}\Lambda = \sum_k g^{\frac{1}{2}N}_{\mu jm}(k)a^k b^{\frac{1}{2}N+\mu-k} c^{\frac{1}{2}N+m-k} d^{k-m-\mu}, \tag{A16}$$

where

$$g^{\frac{1}{2}N}_{\mu jm}(k) = (\Delta/\Delta k)^{\frac{1}{2}N-j} \times [(k - \tfrac{1}{2}N + j)!\,(k - \tfrac{1}{2}N + j - m - \mu)! \times (\tfrac{1}{2}N + m - k)!\,(\tfrac{1}{2}N + \mu - k)!]^{-1}, \tag{A17}$$

and we remind the reader that

$$\left(\frac{\Delta}{\Delta k}\right)^n f(k) = \sum_p (-1)^p \binom{n}{p} f(k+n-p) = \sum_p (-1)^{n-p}\binom{n}{p} f(k+p). \tag{A18}$$

Using Eq. (A16) and

$$\langle\,|\,a^k\bar{a}^l\,|\,\rangle = k!\,\delta_{kl}, \tag{A19}$$

etc., we obtain

$$K = \sum_k [g^{\frac{1}{2}N}_{\mu jm}(k)]^2 / g^{\frac{1}{2}N}_{\mu N/2m}(k). \tag{A20}$$

If we replace one of the $g^{\frac{1}{2}N}_{\mu jm}(k)$ by Eq. (A17), we can manipulate Eq. (A20) into

$$K = \sum_{k,p} (-1)^p \binom{\frac{1}{2}N - j}{p} \frac{g^{\frac{1}{2}N}_{\mu jm}(k)/g^{\frac{1}{2}N}_{\mu N/2m}(k)}{(k-p)!\,(k-p-m-\mu)!\,(j+m-k+p)!\,(j+\mu-k+p)!} = \sum_r \frac{(\Delta/\Delta r)^{\frac{1}{2}N-j} h^{\frac{1}{2}N}_{\mu jm}(r)}{r!\,(r-m-\mu)!\,(j+m-r)!\,(j+\mu-r)!}, \tag{A21}$$

where we have used Eq. (A18), relabeled some dummy indices, and defined for convenience

$$h^{\frac{1}{2}N}_{\mu jm}(r) \equiv (-1)^{\frac{1}{2}N-j} g^{\frac{1}{2}N}_{\mu jm}(r)/g^{\frac{1}{2}N}_{\mu N/2m}(r). \tag{A22}$$

It is straightforward to show from all these definitions that we have the recursion relation

$$h^{\frac{1}{2}N}_{\mu jm}(r) = r(r-m-\mu)h^{\frac{1}{2}N-1}_{\mu jm}(r-1) - (\tfrac{1}{2}N + m - r)(\tfrac{1}{2}N + \mu - r)h^{\frac{1}{2}N-1}_{\mu jm}(r), \tag{A23}$$

and from Eq. (A23) one can show by induction on $\frac{1}{2}N-j$ that $h^{\frac{1}{2}N}_{\mu jm}(r)$ is a polynomial in r of degree $\frac{1}{2}N-j$ with the coefficient of $r^{\frac{1}{2}N-j}$ given by $(\frac{1}{2}N+j+1)^{[\frac{1}{2}N-j]}$. Hence,

$$(\Delta/\Delta r)^{\frac{1}{2}N-j}h^{\frac{1}{2}N}_{\mu jm}(r) = (\tfrac{1}{2}N-j)!\,(\tfrac{1}{2}N+j+1)^{[\frac{1}{2}N-j]} \tag{A24}$$

and, therefore,

$$\begin{aligned} K &= (\tfrac{1}{2}N-j)!\,(\tfrac{1}{2}N+j+1)^{[\frac{1}{2}N-j]} \\ &\quad\times[(j+m)!\,(j-m)!]^{-1} \\ &\quad\times\sum_r \binom{j+m}{r}\binom{j-m}{j+\mu-r} \\ &= \frac{(\frac{1}{2}N-j)!\,(\frac{1}{2}N+j+1)^{[\frac{1}{2}N-j]}}{(j+m)!\,(j-m)!}\binom{2j}{j+\mu}. \end{aligned} \tag{A25}$$

APPENDIX B

In this appendix, we prove Eq. (39). Since

$$[E(Fa+Gb+G^{-1}c+F^{-1}d)^2 + H(ad-bc)]^{\frac{1}{2}N} \equiv P(a,b,c,d) \tag{B1}$$

is a homogeneous polynomial in a, b, c, and d of degree N, we may express it as

$$P(a,b,c,d) = \sum X_{k_1k_2k_3k_4}a^{k_1}b^{k_2}c^{k_3}d^{k_4}, \tag{B2}$$

where $X_{k_1k_2k_3k_4}$ is a c number and the sum is over all k_1, k_2, k_3, k_4 subject to

$$k_1+k_2+k_3+k_4 = N. \tag{B3}$$

On the other hand, from the multinomial theorem we have

$$(Aa+Bb+Cc+Dd)^N = N!\sum\frac{(Aa)^{l_1}(Bb)^{l_2}(Cc)^{l_3}(Dd)^{l_4}}{l_1!\,l_2!\,l_3!\,l_4!}, \tag{B4}$$

where the sum is over all l_1, l_2, l_3, and l_4 subject to

$$l_1+l_2+l_3+l_4 = N. \tag{B5}$$

When these equations are combined with Eq. (A19) of Appendix A, we obtain

$$\langle\,|\,P(a,b,c,d)(A\bar{a}+B\bar{b}+C\bar{c}+D\bar{d})^N\,|\,\rangle = N!\,P(A,B,C,D), \tag{B6}$$

which proves Eq. (39).

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Properties of a Simplified Liquid ^{4}He Ground State*

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A many-body wavefunction is constructed by antisymmetrization, with respect to the electron variables, of a product of ^{4}He-atom wavefunctions, each in its individual ground state. This wavefunction is shown to have the following properties: (1) The pair distribution function $D(R_{ij})$ vanishes at zero separation $R_{ij} = 0$; part of the mutual repulsion of ^{4}He atoms is built into the wavefunction as a result of the exclusion principle acting between the electron shells on different atoms. (2) Neither the nuclei nor the whole atoms undergo Bose condensation, but there is a "Fermi condensation" similar to that shown by Yang to characterize superconductivity, arising from off-diagonal long-range order of the appropriate reduced density matrix.

1. INTRODUCTION

It is customary in microscopic theories of liquid ^{4}He to regard ^{4}He atoms as little Bose billiard balls. It is well known that the mutual impenetrability of pairs of atoms arises from the effects of the exclusion principle together with the filled-shell electronic configuration, and that the long-range attraction which makes the system a liquid arises from coupled virtual electromagnetic transitions of pairs of atoms. However, it has been thought that these effects could be adequately simulated by a suitable phenomenological potential acting between pairs of elementary bosons, without introducing electronic degrees of freedom into the model explicitly. The λ transition is then viewed as a Bose–Einstein condensation in a system of interacting bosons.

It has recently been pointed out[1] that exchange effects in a system of ^{4}He atoms are qualitatively different from those in a system of bosons, in spite of the tight binding of the ^{4}He atoms. One consequence is that Bose condensation, in the sense of macroscopic occupation of any single ^{4}He atom state, cannot in fact occur in liquid ^{4}He. On the other hand, a less extreme condensation which we call "Fermi condensation" can occur. It is characterized by off-diagonal long-range order (ODLRO) in the sense that

$$D_3(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}') \xrightarrow[\text{infinite separation}]{} \text{nonzero limit.} \tag{1}$$

Here, each $\mathbf{R}$ stands for the position of a nucleus (α particle); each x_j stands for both the position $\mathbf{r}_j$ and spin z-component of an electron. The reduced density matrix D_3 is defined by

$$\begin{aligned} D_3(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}') = \int & \psi(x_1 \cdots x_{2n}\mathbf{R}\mathbf{R}_2 \cdots \mathbf{R}_n) \\ & \times \psi^*(x_1'x_2'x_3 \cdots x_{2n}\mathbf{R}'\mathbf{R}_2 \cdots \mathbf{R}_n) \\ & \times dx_3 \cdots dx_{2n} d^3R_2 \cdots d^3R_n, \end{aligned} \tag{2}$$

where $\int dx_j$ stands for integration over $\mathbf{r}_j$ and summation over σ_j. And, finally, ψ is the normalized wavefunction of the system of n ^{4}He atoms, expressed in terms of both nuclear and electronic coordinates. The limit implied in (1) is one in which the group $(\mathbf{r}_1\mathbf{r}_2\mathbf{R})$ and the group $(\mathbf{r}_1'\mathbf{r}_2'\mathbf{R}')$ are allowed to separate infinitely keeping $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{R}$ all at a finite distance from each other, and similarly for $\mathbf{r}_1'$, $\mathbf{r}_2'$, and $\mathbf{R}'$; this ODLRO occurs only if both $\sigma_2 = -\sigma_1$ and $\sigma_2' = -\sigma_1'$. Since the ground state of a ^{4}He atom is a bound state and a spin singlet ($\sigma_2 = -\sigma_1$), one would expect ODLRO in the sense (1) to occur in a wavefunction ψ in which ground-state ^{4}He atoms move freely throughout the system. It has been proposed[1] that this is indeed the case, and that the λ transition and peculiar properties of liquid ^{4}He are to be understood on the basis of a Fermi condensation associated with ODLRO of the form (1). This is the closest possible analog, for real ^{4}He atoms, of the ODLRO of the 1-particle density matrix which is associated with Bose condensation in boson models of liquid ^{4}He. However, the fact that ODLRO of the form (1) does not imply macroscopic occupation of a single ^{4}He atom state means that a correct microscopic theory of liquid ^{4}He will differ qualitatively from theories based on boson models. Since Feynman's arguments[2,3] for the low phonon–roton spectrum are unchanged by the inclusion of electronic coordinates in the ground state $\psi_0(x_1 \cdots x_{2n}\mathbf{R}_1 \cdots \mathbf{R}_n)$, the picture of the nature of the low excitations and hence the low-temperature thermodynamics need not be changed by the distinction between Bose and Fermi condensations. On the other hand, the details of the λ transition are probably sensitive to this distinction, and the structure of ψ_0 certainly is.

Yang has shown[4] that superconductivity is characterized by ODLRO of the 2-particle density matrix $D_2(x_1x_2, x_1'x_2')$, analogous to (1). Thus, it appears that a correct microscopic theory of liquid ^{4}He would be much closer to theories of superconductivity than are the boson models. It is worth noticing that ODLRO [Eq. (1)] cannot occur in liquid ^{3}He due to the effects of Fermi statistics of the nuclei.[4]

Let $f_0(x_1x_2\mathbf{R})$ be the ground state of a single ^{4}He atom. The closest analog of the ideal Bose gas many-body ground state $f_0(\mathbf{R}_1)\cdots f_0(\mathbf{R}_n)$ which can be constructed from single ^{4}He-atom states is

$$\psi_0(x_1\cdots x_{2n}\mathbf{R}_1\cdots\mathbf{R}_n) = \mathcal{C}A_{2n}[f_0(x_1x_2\mathbf{R}_1)f_0(x_3x_4\mathbf{R}_2)\cdots f_0(x_{2n-1}x_{2n}\mathbf{R}_n)], \quad (3)$$

where $\mathcal{C}$ is a normalization constant and A_{2n} is the antisymmetrizer with respect to the electronic coordinates $x_1\cdots x_{2n}$. This wavefunction is automatically symmetric in the nuclear coordinates $\mathbf{R}_1\cdots\mathbf{R}_n$, since exchange of nuclei between atoms is equivalent to exchange of a pair of electrons between the same atoms. The purpose of this paper is to examine the properties of the wavefunction (3). We find that it does exhibit Fermi condensation and ODLRO in the sense of Eq. (1). We also find that, in contradistinction to the boson models, part of the mutual repulsion of ^{4}He atoms is already kinematically built into the wavefunction (3) as a result of the antisymmetrization (exclusion principle), together with the closed-shell structure of f_0. This antisymmetrization also implies that the physical interpretation of ψ_0 is not as simple as one might naively expect. After exchange of a pair of electrons between two atoms, the product f_0f_0 can be expanded in terms of unexchanged functions $f_\alpha f_\beta$, where $\{f_\alpha(x_1x_2\mathbf{R})\}$ is a complete set of ^{4}He atom wavefunctions:

$$f_0(x_3x_2\mathbf{R}_1)f_0(x_1x_4\mathbf{R}_2) = \sum_{\alpha\beta} c_{\alpha\beta}f_\alpha(x_1x_2\mathbf{R}_1)f_\beta(x_3x_4\mathbf{R}_2). \quad (4)$$

Note added in proof: Only that part of f_0f_0 which is antisymmetric both in the pair (x_1x_2) and in the pair (x_3x_4) can be so expanded. However, since this part is nonvanishing, our conclusion is the same.

On the other hand, in the Bose-gas model, $f_0(\mathbf{R}_1)f_0(\mathbf{R}_2)$ has no such nontrivial expansion. This distinction lies at the heart of the difference between Bose and Fermi condensations.[1] The wavefunction (3) cannot be interpreted as representing a situation where all the ^{4}He atoms are in their internal ground states and all have zero momentum; the antisymmetrization implies components with many of the atoms moving, and many virtually internally excited.

2. FORMULATION

The state (3) has the standard quantized-field representation

$$|\psi_0\rangle = [(2n)!\,n!]^{-\frac{1}{2}}\int dx_1\cdots dx_{2n}d^3R_1\cdots d^3R_n \times \psi_0(x_1\cdots x_{2n}\mathbf{R}_1\cdots\mathbf{R}_n) \times \psi^\dagger(x_1)\cdots\psi^\dagger(x_{2n})\psi^\dagger(\mathbf{R}_1)\cdots\psi^\dagger(\mathbf{R}_n), \quad (5)$$

where $\psi(x)$ and $\psi^\dagger(x)$ are electron annihilation and creation operators satisfying the Fermi anticommutation relations

$$\{\psi(x),\psi(x')\} = \{\psi^\dagger(x),\psi^\dagger(x')\} = 0,$$
$$\{\psi(x),\psi^\dagger(x')\} = \delta(x-x') \equiv \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'}; \quad (6)$$

and $\psi(\mathbf{R})$ and $\psi^\dagger(\mathbf{R})$ are α-particle annihilation and creation operators satisfying the Bose[5] commutation relations

$$[\psi(\mathbf{R}),\psi(\mathbf{R}')] = [\psi^\dagger(\mathbf{R}),\psi^\dagger(\mathbf{R}')] = 0,$$
$$[\psi(\mathbf{R}),\psi^\dagger(\mathbf{R}')] = \delta(\mathbf{R}-\mathbf{R}'). \quad (7)$$

Defining the creation operator $A_0^\dagger$ for a ground-state ^{4}He atom by

$$A_0^\dagger = 2^{-\frac{1}{2}}\int dx_1\,dx_2d^3Rf_0(x_1x_2\mathbf{R}) \times \psi^\dagger(x_1)\psi^\dagger(x_2)\psi^\dagger(\mathbf{R}), \quad (8)$$

one can write (5) together with (3) in the simple form

$$|\psi_0\rangle = [2^n/(2n)!\,(n!)]^{\frac{1}{2}}\mathcal{C}(A_0^\dagger)^n|0\rangle, \quad (9)$$

reminiscent of the ideal Bose-gas ground state. However, A_0 and $A_0^\dagger$ are not Bose annihilation and creation operators, since their commutator differs from the Bose value (the c-number unity) by operator terms involving $\psi^\dagger\psi^\dagger\psi\psi$ and $\psi^\dagger\psi$.

The properties of the state (9) are easier to evaluate if one uses an orbital approximation[6] for f_0:

$$f_0(x_1x_2\mathbf{R}) = (2\Omega)^{-\frac{1}{2}}u_0(|\mathbf{r}_1-\mathbf{R}|)u_0(|\mathbf{r}_2-\mathbf{R}|) \times (\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow} - \delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow}), \quad (10)$$

where u_0 is the normalized ground-state $1s$ orbital and Ω is the volume of the system. We assume periodic boundary conditions.[7] Then (8) becomes

$$A_0^\dagger = \Omega^{-\frac{1}{2}}\int d^3Ra_\uparrow^\dagger(\mathbf{R})a_\downarrow^\dagger(\mathbf{R})\psi^\dagger(\mathbf{R}). \quad (11)$$

Here $a_\sigma^\dagger(\mathbf{R})$ is the creation operator for an electron in the orbital u_0 centered on a nucleus at $\mathbf{R}$,

$$a_\sigma^\dagger(\mathbf{R}) = \int d^3ru_0(|\mathbf{r}-\mathbf{R}|)\psi^\dagger(\mathbf{r}\sigma), \quad (12)$$

which satisfies the anticommutation relations

$$\{a_\sigma(\mathbf{R}),a_{\sigma'}(\mathbf{R}')\} = \{a_\sigma^\dagger(\mathbf{R}),a_{\sigma'}^\dagger(\mathbf{R}')\} = 0,$$
$$\{a_\sigma(\mathbf{R}),a_{\sigma'}^\dagger(\mathbf{R}')\} = \delta_{\sigma\sigma'}w(|\mathbf{R}-\mathbf{R}'|), \quad (13)$$

where w is the overlap integral

$$w(R) = \int u_0^*(r)u_0(|\mathbf{r}+\mathbf{R}|)d^3r. \quad (14)$$

The atomic creation operator (11) and its Hermitian

conjugate A_0 satisfy the commutation relation

$$[A_0, A_0^\dagger] = 1 - \Omega^{-1}\int d^3R[a_\uparrow^\dagger(\mathbf{R})a_\uparrow(\mathbf{R}) + a_\downarrow^\dagger(\mathbf{R})a_\downarrow(\mathbf{R})] + \Omega^{-1}\int d^3Rd^3R'w^2(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R}')\psi(\mathbf{R}) + \Omega^{-1}\int d^3Ra_\uparrow^\dagger(\mathbf{R})a_\downarrow^\dagger(\mathbf{R})a_\downarrow(\mathbf{R})a_\uparrow(\mathbf{R}) - \Omega^{-1}\int d^3Rd^3R'w(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R}') \times [a_\uparrow^\dagger(\mathbf{R}')a_\uparrow(\mathbf{R}) + a_\downarrow^\dagger(\mathbf{R}')a_\downarrow(\mathbf{R})]\psi(\mathbf{R}). \tag{15}$$

It is convenient to slightly relax the strict conservation of the number of ^{4}He atoms, replacing (9) by

$$|\psi_0\rangle = U|0\rangle, \qquad U = e^F, \quad F = c(A_0^\dagger - A_0), \tag{16}$$

where c is a real c-number chosen so that

$$\langle\psi_0|N|\psi_0\rangle = n, \tag{17}$$

with N the number operator for α particles, hence for ^{4}He atoms

$$N = \int d^3R\psi^\dagger(\mathbf{R})\psi(\mathbf{R}). \tag{18}$$

We find that, for $n \to \infty$, the fractional fluctuation in N is only of order $n^{-\frac{1}{2}}$, hence negligible. The situation in this respect is the direct analog of that in the Bardeen–Cooper–Schrieffer (BCS) theory.[8]

The expectation value of any operator O in the state (16) is

$$\langle\psi_0|O|\psi_0\rangle = \langle 0|U^{-1}OU|0\rangle. \tag{19}$$

Thus, the evaluation of such expectation values can be carried out by first transforming the operators ψ and $\psi^\dagger$ by the unitary operator U and then evaluating the resultant vacuum expectation values by Wick's theorem. Owing to the complicated commutation relations of the ψ and $\psi^\dagger$ operators with A_0 and $A_0^\dagger$, these transformations cannot be carried out in closed form. Therefore, we carry out an approximate evaluation based on the multiple commutator expansion

$$U^{-1}OU = e^{-F}Oe^F = O + [O,F] + \tfrac{1}{2}[[O,F],F] + \tfrac{1}{6}[[[O,F],F],F] + \cdots. \tag{20}$$

We find that this yields an expansion in powers of the dimensionless density ρa_0^3 ($\rho = n/\Omega$, a_0 = Bohr radius), so that the first few terms are sufficient at low density. It then follows from (16), (11)–(13), and Wick's theorem that

$$\begin{aligned} U^{-1}\psi(\mathbf{R})U = {} & \psi(\mathbf{R}) + c\Omega^{-\frac{1}{2}}a_\uparrow^\dagger(\mathbf{R})a_\downarrow^\dagger(\mathbf{R}) \\ & + \tfrac{1}{2}c^2\Omega^{-1}\int d^3R'w^2(|\mathbf{R}-\mathbf{R}'|)\psi(\mathbf{R}') \\ & - \tfrac{1}{2}c^2\Omega^{-1}\int d^3R'w(|\mathbf{R}-\mathbf{R}'|)[a_\uparrow^\dagger(\mathbf{R})a_\uparrow(\mathbf{R}') \\ & + a_\downarrow^\dagger(\mathbf{R})a_\downarrow(\mathbf{R}')]\psi(\mathbf{R}') \\ & + \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}\int d^3R'w^2(|\mathbf{R}-\mathbf{R}'|)a_\uparrow^\dagger(\mathbf{R}') \\ & \times a_\downarrow^\dagger(\mathbf{R}') - \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}\int d^3R'w(|\mathbf{R}-\mathbf{R}'|) \\ & \times [a_\uparrow^\dagger(\mathbf{R})a_\downarrow^\dagger(\mathbf{R}') - a_\downarrow^\dagger(\mathbf{R})a_\uparrow^\dagger(\mathbf{R}')] \\ & - \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}\int d^3R'w(|\mathbf{R}-\mathbf{R}'|) \\ & \times [a_\uparrow^\dagger(\mathbf{R})a_\uparrow^\dagger(\mathbf{R}')a_\downarrow^\dagger(\mathbf{R}')a_\uparrow(\mathbf{R}') \\ & + a_\downarrow^\dagger(\mathbf{R})a_\uparrow^\dagger(\mathbf{R}')a_\downarrow^\dagger(\mathbf{R}')a_\downarrow(\mathbf{R}')] \\ & - \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}\int d^3R'd^3R''w(|\mathbf{R}-\mathbf{R}'|) \\ & \times w(|\mathbf{R}'-\mathbf{R}''|)[a_\uparrow^\dagger(\mathbf{R})a_\downarrow^\dagger(\mathbf{R}'') \\ & - a_\downarrow^\dagger(\mathbf{R})a_\uparrow^\dagger(\mathbf{R}'')]\psi^\dagger(\mathbf{R}'')\psi(\mathbf{R}') \\ & - \tfrac{1}{3}c^3\Omega^{-\frac{3}{2}}\int d^3R'd^3R''w(|\mathbf{R}-\mathbf{R}'|) \\ & \times w(|\mathbf{R}-\mathbf{R}''|)\psi(\mathbf{R}'')\psi(\mathbf{R}') \\ & \times a_\downarrow(\mathbf{R}'')a_\uparrow(\mathbf{R}') + O(c^4\Omega^{-2}) \end{aligned} \tag{21}$$

and

$$\begin{aligned} U^{-1}\psi(\mathbf{r}\sigma)U = {} & \psi(\mathbf{r}\sigma) + s_\sigma c\Omega^{-\frac{1}{2}} \\ & \times \int d^3Ru_0(|\mathbf{r}-\mathbf{R}|)a_{-\sigma}^\dagger(\mathbf{R}) \\ & \times \psi^\dagger(\mathbf{R}) + \tfrac{1}{2}c^2\Omega^{-1}\int d^3Ru_0(|\mathbf{r}-\mathbf{R}|) \\ & \times [a_{-\sigma}^\dagger(\mathbf{R})a_{-\sigma}(\mathbf{R})a_\sigma(\mathbf{R}) - a_\sigma(\mathbf{R})] \\ & - \tfrac{1}{2}c^2\Omega^{-1}\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|) \\ & \times w(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R})\psi(\mathbf{R}')a_\sigma(\mathbf{R}') \\ & + \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}s_\sigma\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|) \\ & \times w^2(|\mathbf{R}-\mathbf{R}'|)a_{-\sigma}^\dagger(\mathbf{R})\psi^\dagger(\mathbf{R}') \\ & - \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}s_\sigma\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|) \\ & \times w(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R}')a_{-\sigma}^\dagger(\mathbf{R}') \\ & - \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}s_\sigma\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|) \\ & \times w(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R}')a_{-\sigma}^\dagger(\mathbf{R}) \\ & \times [a_\uparrow^\dagger(\mathbf{R}')a_\uparrow(\mathbf{R}) + a_\downarrow^\dagger(\mathbf{R}')a_\downarrow(\mathbf{R})] \end{aligned}$$

$$
\begin{aligned}
&- \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|)\\
&\times w(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R})a_\uparrow^\dagger(\mathbf{R}')a_\downarrow^\dagger(\mathbf{R}')a_\sigma(\mathbf{R}')\\
&- \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}s_\sigma\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|)\\
&\times w(|\mathbf{R}-\mathbf{R}'|)\psi^\dagger(\mathbf{R})a_{-\sigma}^\dagger(\mathbf{R}')\\
&- \tfrac{1}{6}c^3\Omega^{-\frac{3}{2}}s_\sigma\int d^3Rd^3R'd^3R''u_0(|\mathbf{r}-\mathbf{R}|)\\
&\times w(|\mathbf{R}-\mathbf{R}'|)w(|\mathbf{R}'-\mathbf{R}''|)\\
&\times \psi^\dagger(\mathbf{R})\psi^\dagger(R'')\psi(\mathbf{R}')a_{-\sigma}^\dagger(\mathbf{R}'')\\
&- \tfrac{1}{3}c^3\Omega^{-\frac{3}{2}}\int d^3Rd^3R'u_0(|\mathbf{r}-\mathbf{R}|)\\
&\times w(|\mathbf{R}-\mathbf{R}'|)a_\downarrow(\mathbf{R})a_\uparrow(\mathbf{R})\\
&\times \psi(\mathbf{R}')a_\sigma(\mathbf{R}') + O(c^4\Omega^{-2}), \qquad (22)
\end{aligned}
$$

where

$$s_\uparrow = 1 \quad \text{and} \quad s_\downarrow = -1.$$

The expectation value needed in (17) is then

$$
\begin{aligned}
\langle\psi_0|\,\psi^\dagger(\mathbf{R})\psi(\mathbf{R})\,|\psi_0\rangle &= c^2\Omega^{-1} - \tfrac{2}{3}c^4\Omega^{-2}\\
&\times\int w^2(R')[1-\tfrac{1}{2}w^2(R')]d^3R' + O(c^6\Omega^{-3}), \qquad (23)
\end{aligned}
$$

so that (17) implies

$$c^2\Omega^{-1} = \rho[1 + \tfrac{2}{3}(x-\tfrac{1}{2}y)\rho a_0^3 + O((\rho a_0^3)^2)], \qquad (24)$$

where a_0 is the Bohr radius ($\sim$ the range of w), and x and y are numbers of order unity defined by

$$\int w^2(R)d^3R = xa_0^3 \quad \text{and} \quad \int w^4(R)d^3R = ya_0^3. \qquad (25)$$

3. α-PARTICLE MOMENTUM DISTRIBUTION

The α-particle momentum distribution function $n_\mathbf{k}$, the mean number of ^{4}He nuclei with momentum $\hbar\mathbf{k}$, is

$$n_\mathbf{k} = n(\varphi_\mathbf{k}, \rho_1\varphi_\mathbf{k}) = n\int\varphi_\mathbf{k}^*(\mathbf{R})D_1(\mathbf{R},\mathbf{R}')\varphi_\mathbf{k}(\mathbf{R}')d^3Rd^3R', \qquad (26)$$

where $\varphi_\mathbf{k}(\mathbf{R}) = \Omega^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{R}}$ and D_1 is the 1-particle density matrix[9]

$$D_1(\mathbf{R},\mathbf{R}') = n^{-1}\langle\psi_0|\,\psi^\dagger(\mathbf{R}')\psi(\mathbf{R})\,|\psi_0\rangle. \qquad (27)$$

One finds by (21), (24), and Wick's theorem that

$$
\begin{aligned}
n_\mathbf{k} = \rho a_0^3x_k + \tfrac{2}{3}(\rho a_0^3)^2\Big(&xx_k + \tfrac{1}{2}x_k^2\\
&- (2\pi)^{-3}a_0^3\int z_{|\mathbf{k}-\mathbf{k}'|}z_{k'}^2d^3k'\Big) + O((\rho a_0^3)^3), \qquad (28)
\end{aligned}
$$

where x_k and z_k are real, spherically symmetric functions of $\mathbf{k}$, of range $\sim a_0^{-1}$ and of order unity within this range, defined by

$$\int w^2(R)e^{-i\mathbf{k}\cdot\mathbf{R}}d^3R = x_ka_0^3,$$
$$\int w(R)e^{-i\mathbf{k}\cdot\mathbf{R}}d^3R = z_ka_0^3. \qquad (29)$$

In the term involving the z_k, the replacement $\Sigma_\mathbf{k}\to(2\pi)^{-3}\Omega\int d^3k$, valid asymptotically for $\Omega\to\infty$, has been made.

The first term in (28) is just n times the nuclear momentum distribution function for a single ^{4}He atom, whereas the remaining terms give modifications due to interaction of the ^{4}He atoms via the exclusion principle. $n_\mathbf{k}$ is a smooth function of k of range $\sim a_0^{-1}$, with no δ-function spike at $k=0$ (no Bose–Einstein condensation); correspondingly, D_1 does not exhibit ODLRO, but falls to zero as $|\mathbf{R}-\mathbf{R}'|\to\infty$. This behavior is to be expected, since even on the Bohr model the momentum of the nucleus fluctuates by an amount $\sim\hbar a_0^{-1}$ as the electrons go around. ODLRO of D_1 would imply that the many-body wavefunction, evaluated at a given position $\mathbf{R}$ of one α particle, has a sizeable overlap with the wavefunction differing through a *large* displacement of the α particle to the point $\mathbf{R}'$, keeping the positions of all the other α particles *and all the electrons* fixed; such a displacement without motion of the electrons would imply breakup of the helium atom, which does not in fact occur with appreciable probability in liquid ^{4}He. Equivalently, ODLRO of D_1 would imply macroscopic occupation (by α particles) of a spatially extended orbital, which is incompatible with localization of each α particle relative to two electrons so as to form a helium atom. The distribution of momenta of whole ^{4}He atoms is discussed in Sec. 6.

4. PAIR DISTRIBUTION FUNCTION

Next, we calculate the pair distribution function $D(R_{ij})$, the relative probability of finding two nuclei (hence two ^{4}He atoms) at a separation R_{ij}. Adopting the usual normalization $D(R_{ij})\to 1$ as $R_{ij}\to\infty$, one has

$$
\begin{aligned}
D(R_{ij}) &= \rho^{-2}\langle\psi_0|\,\psi^\dagger(\mathbf{R}_i)\psi^\dagger(\mathbf{R}_j)\psi(\mathbf{R}_j)\psi(\mathbf{R}_i)\,|\psi_0\rangle\\
&= \rho^{-2}\langle\psi_0|\,\psi^\dagger(\mathbf{R}_{ij})\psi^\dagger(0)\psi(0)\psi(\mathbf{R}_{ij})\,|\psi_0\rangle, \qquad (30)
\end{aligned}
$$

use having been made of translational invariance ($|\psi_0\rangle$ is an eigenstate of total linear momentum with eigenvalue zero). It follows from (21), (24), and

Wick's theorem that

$$D(R_{ij}) = [1 + \tfrac{4}{3}(x - \tfrac{1}{2}y)\rho a_0^3][1 - w^2(R_{ij})]^2 - \tfrac{4}{3}\rho[1 - w^2(R_{ij})]\int w(R) \times [w(R) - w(R_{ij})w(|\mathbf{R}_{ij} - \mathbf{R}|)]d^3R + \tfrac{2}{3}\rho\int w^2(R)[w(R) - w(R_{ij})w(|\mathbf{R}_{ij} - \mathbf{R}|)]^2 d^3R + \tfrac{2}{3}\rho\int w(R)w(|\mathbf{R}_{ij} - \mathbf{R}|) \times [w(|\mathbf{R}_{ij} - \mathbf{R}|) - w(R_{ij})w(R)] \times [w(R) - w(R_{ij})w(|\mathbf{R}_{ij} - \mathbf{R}|)]d^3R + O((\rho a_0^3)^2). \quad (31)$$

Since $w(0) = 1$, $D(R_{ij})$ vanishes at zero separation, $R_{ij} = 0$. This is a direct result of the exclusion principle acting between the electron shells on different ^{4}He atoms. Mathematically, it arises from the equation

$$[a_\sigma^\dagger(\mathbf{R})]^2 = 0, \quad (32)$$

which follows from (13) and expresses the fact that only a single electron of each spin can occupy the orbital $u_0(|\mathbf{r} - \mathbf{R}|)$ centered on the point $\mathbf{R}$. Furthermore, $D(R_{ij})$ remains small in a neighborhood of the origin, since

$$D(R_{ij}) = O((R_{ij}/a_0)^4) \quad \text{for} \quad R_{ij} \to 0. \quad (33)$$

Thus, part of the mutual repulsion of ^{4}He atoms is built into the state $|\psi_0\rangle$ as a result of the exclusion principle. In the opposite limit of large separation, one has

$$D(R_{ij}) \xrightarrow[R_{ij}\to\infty]{} 1 \quad (34)$$

by (31) and (25), since $w(R_{ij})$ vanishes in the same limit.

More explicit results can be obtained if u_0 is taken to be the best hydrogenic orbital[10]:

$$u_0(r) = (Z^3/\pi a_0^3)^{\frac{1}{2}}e^{-Zr/a_0}, \quad Z = \tfrac{27}{16} = 1.69. \quad (35)$$

Then

$$w(R) = (1 + S + \tfrac{1}{3}S^2)e^{-S}, \quad S = ZR/a_0. \quad (36)$$

In principle, all the integrals in (31) can then be evaluated in closed form with the aid of the convolution theorem, but the expressions resulting are so lengthy and unwieldy that they are best evaluated numerically. The method of evaluation is discussed in Appendix A. The resultant $D(R_{ij})$ is shown in Fig. 1 at liquid ^{4}He density ($\rho a_0^3 = 0.0033$) along with experimental values.[3] The rather large discrepancy is not surprising, in view of the extremely simplified

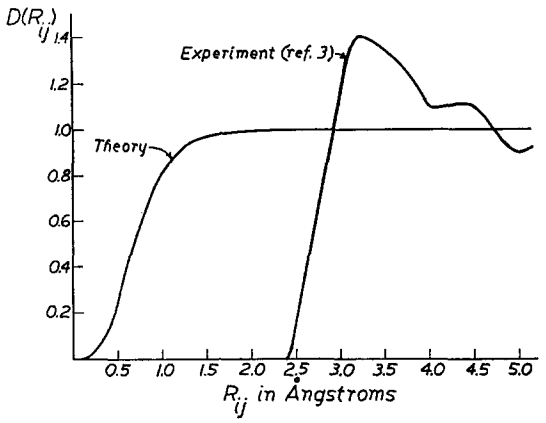

FIG. 1. Theoretical and experimental pair distribution functions.

nature of the state (16). It should be noted, however, that the pair distribution function of (16) is a considerable improvement over that of the ground state of the ideal Bose gas, which gives the trivial result $D(R_{ij}) = 1$. The state (16) can be regarded as the simplest possible approximation to the ground state of real ^{4}He atoms, whereas the ideal Bose gas ground state is the simplest possible ground state of structureless bosons. Possible improvements to the state (16) are discussed in Sec. 7.

5. NUMBER FLUCTUATIONS

It follows trivially from the commutation relations (7) that

$$\int d^3Rd^3R'\psi^\dagger(\mathbf{R})\psi^\dagger(\mathbf{R}')\psi(\mathbf{R}')\psi(\mathbf{R}) = N(N-1), \quad (37)$$

where N is the number operator (18). It then follows from (30) and (17) that the expectation value of N^2 is

$$\langle\psi_0|\, N^2\,|\psi_0\rangle = n + n\rho\int D(R)d^3R. \quad (38)$$

Since $D(R)$ approaches unity for $R \to \infty$, one has

$$\langle\psi_0|\, N^2\,|\psi_0\rangle = n^2 + O(n), \quad (39)$$

so that the fractional rms fluctuation in N is only of order $n^{-\frac{1}{2}}$:

$$n^{-1}[\langle\psi_0|\, N^2\,|\psi_0\rangle - n^2]^{\frac{1}{2}} = O(n^{-\frac{1}{2}}). \quad (40)$$

This verifies our previous remark to the effect that the fluctuations in the number of ^{4}He atoms in the state (16) are negligible for a macroscopic system ($n \to \infty$).

6. ODLRO AND FERMI CONDENSATION

The 2-electron, one α-particle density matrix D_3 [Eq. (2)] of the state (16) can be expressed in the form

$$D_3(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}') = [2n(2n-1)n]^{-1} \times \langle\psi_0|\, \psi^\dagger(x_1')\psi^\dagger(x_2')\psi^\dagger(\mathbf{R}')\psi(\mathbf{R})\psi(x_2)\psi(x_1)\,|\psi_0\rangle, \quad (41)$$

in analogy with (27). Making use of (21), (24), and Wick's theorem, one can find the first few terms in the density expansion of D_3. The result is

$$D_3(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}') = \chi(x_1x_2\mathbf{R})\chi^*(x_1'x_2'\mathbf{R}') + D_3'(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}'), \quad (42)$$

where

$$\begin{aligned}\chi(x_1x_2\mathbf{R}) = [2n(2n-1)\Omega]^{-\frac{1}{2}}a_0^{-3}&(\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow} - \delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow})\\ &\times [u_0(|\mathbf{r}_1 - \mathbf{R}|)u_0(|\mathbf{r}_2 - \mathbf{R}|)a_0^3\\ &- \tfrac{1}{2}\rho a_0^3 u_0(|\mathbf{r}_1 - \mathbf{R}|)v_0(|\mathbf{r}_2 - \mathbf{R}|)\\ &- \tfrac{1}{2}\rho a_0^3 u_0(|\mathbf{r}_2 - \mathbf{R}|)v_0(|\mathbf{r}_1 - \mathbf{R}|)\\ &+ \tfrac{1}{2}\rho a_0^3 w_0(\mathbf{r}_1 - \mathbf{R}, \mathbf{r}_2 - \mathbf{R}) + O((\rho a_0^3)^2)]\end{aligned} \quad (43)$$

and D_3' is a very complicated expression given in Appendix B. The functions v_0 and w_0 in (43) are given by the following integrals:

$$v_0(r) = \int u_0(|\mathbf{r} - \mathbf{R}|)w(R)d^3R,$$

$$w_0(\mathbf{r}_1, \mathbf{r}_2) = \int u_0(|\mathbf{r}_1 - \mathbf{R}|)u_0(|\mathbf{r}_2 - \mathbf{R}|)w^2(R)d^3R. \quad (44)$$

With the substitutions (35) and (36), v_0 is easily evaluated by the convolution technique discussed in Appendix A, with the result

$$v_0(r) = (\tfrac{7}{2})\pi^{\frac{1}{2}}(a_0/z)^{\frac{3}{2}}e^{-s}[1 + s + \tfrac{3}{7}s^2 + \tfrac{2}{21}s^3 + \tfrac{1}{105}s^4], \quad (45)$$

where $s = zr/a_0$. On the other hand, w_0 is a 3-center integral and cannot be evaluated in closed form.

It is easily seen from (B1) that D_3' falls to zero as the set of positions $(\mathbf{r}_1\mathbf{r}_2\mathbf{R})$ is taken far from the set $(\mathbf{r}_1'\mathbf{r}_2'\mathbf{R}')$, keeping the relative distances within each set microscopic ($\sim a_0$). Thus, the ODLRO in D_3 arises entirely from the separable term $\chi\chi^*$, which is independent of the separation of these two groups. Physically, this ODLRO implies that the state $|\psi_0\rangle$ is such that, when one ^{4}He atom is displaced an arbitrary distance from its original position, keeping all other atoms fixed, the new wavefunction generated by this displacement has nonzero overlap with the original wavefunction, no matter how large the displacement. Thus, $|\psi_0\rangle$ exhibits long-range configurational order of a type analogous to that in a many-boson system with Bose–Einstein condensation.

The mean occupation number n_α of any normalized single-^{4}He-atom state $\varphi_\alpha(x_1x_2\mathbf{R})$ is[1]

$$\begin{aligned}n_\alpha &= (\varphi_\alpha, \rho_3\varphi_\alpha)\\ &= \int \varphi_\alpha^*(x_1x_2\mathbf{R})\rho_3(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}')\\ &\quad\times \varphi_\alpha(x_1'x_2'\mathbf{R}')\, dx_1\, dx_2 d^3R\, dx_1'\, dx_2' d^3R'.\end{aligned} \quad (46)$$

The separation (42) of D_3 into the part $\chi\chi^*$ exhibiting ODLRO and the residue D_3' implies that

$$n_\alpha = n\,|(\varphi_\alpha, \chi)|^2 + n_\alpha', \quad (47)$$

where

$$(\varphi_\alpha, \chi) = \int \varphi_\alpha^*(x_1x_2\mathbf{R})\chi(x_1x_2\mathbf{R})\, dx_1\, dx_2 d^3R \quad (48)$$

and n_α' differs from (46) only in the replacement of D_3 by D_3'. It follows from (B1) and the normalization of φ_α that n_α' is of order n^{-2} or smaller in the thermodynamic limit ($n \to \infty$, $\Omega \to \infty$, $n/\Omega \to \rho$, $0 < \rho < \infty$). Thus, taking

$$\varphi_0(x_1x_2\mathbf{R}) = (\chi, \chi)^{-\frac{1}{2}}\chi(x_1x_2\mathbf{R}) \quad (49)$$

and φ_α orthogonal to φ_0 for $\alpha \neq 0$, one has

$$n_\alpha = n(\chi, \chi)\delta_{\alpha 0} + O(n^{-2}). \quad (50)$$

It follows from (43) and (10) that

$$\chi(x_1x_2\mathbf{R}) \xrightarrow[\rho a_0^3 \to 0]{} [n(2n-1)]^{-\frac{1}{2}}f_0(x_1x_2\mathbf{R}), \quad (51)$$

and hence, since f_0 is normalized,

$$\begin{aligned}n_0 &\xrightarrow[\rho a_0^3 \to 0]{} \tfrac{1}{2}n^{-1},\\ n_\alpha &= O(n^{-2}), \quad \alpha \neq 0.\end{aligned} \quad (52)$$

This δ-function behavior of n_α is similar to the behavior of electron-pair occupation numbers in a superconductor.[1] It is quite different from Bose condensation, since Bose condensation would require macroscopic occupation in the sense $n_0 = O(n)$, which has been shown to be impossible for ^{4}He atoms,[1] and since an n_0 of order n^{-1} makes a negligible contribution to the sum rule[11]

$$\sum_\alpha n_\alpha = n, \quad (53)$$

in contrast to the situation in the case of Bose condensation. Thus, we shall call the behavior typified by (52) "Fermi condensation."[12] Although the extreme value (52) of n_0 is only attained in the limit of zero density, one expects that, for the state (16), the value of n_0 at liquid ^{4}He density is only slightly less than $\frac{1}{2}n^{-1}$. This is due to the fact that ρa_0^3 is very small, so that χ differs from the right-hand side of (51) only by a very small amount except at large distances, where both f_0 and χ are very small, but v_0 falls off less rapidly than u_0.

The true liquid ^{4}He ground state $\psi_0^{(\text{true})}$ is, of course, much more complicated than (16). Nevertheless, it seems likely that it shares with (16) the property that there is an "effective single-atom wavefunction" $\varphi_0(x_1x_2\mathbf{R})$, such that the occupation

number n_0 of φ_0 in the state $\psi_0^{(\text{true})}$ is of order n^{-1}, whereas n_α is of order n^{-2} for all φ_α orthogonal to φ_0. This would be associated with ODLRO of D_3 due to a separable term $\chi\chi^*$, where χ differs from φ_0 only in normalization. This ODLRO would be present not only in the ground state, but also at sufficiently low temperatures $T > 0$. The λ transition would then arise because of the existence of a temperature T_λ such that for $T < T_\lambda$, $n_0 = O(n^{-1})$ due to ODLRO in D_3, whereas, for $T > T_\lambda$, D_3 would not exhibit ODLRO and n_α would be of order n^{-2} or smaller for all α.

The quantum number α in (52) includes both the translational wave vector $\mathbf{k}$ and all the internal quantum numbers of a single ^{4}He atom. One can therefore define an over-all momentum distribution function of ^{4}He atoms by summing n_α over all internal states for fixed $\mathbf{k}$. One can then ask whether this momentum distribution function might exhibit Bose–Einstein condensation in the usual sense, i.e., might contain a term $nf\delta_{\mathbf{k}0}$ with $f > 0$ and independent of n. We have not thus far been able to answer this question. The difficulty is that the approximation of identifying the center of mass of the atoms with the nuclear position $\mathbf{R}$ cannot be validly made in such a calculation, since even for a single ^{4}He atom at rest ($\mathbf{k} = 0$) the nucleus orbits in reaction to the motion of the electrons, with a momentum fluctuation of order $\hbar a_0^{-1}$. Thus, the usual m/M expansion breaks down for a calculation of the atomic (as opposed to nuclear) momentum distribution. The question is to a certain extent academic, since the characterization of the condensation of ^{4}He atoms by ODLRO of D_3 and the related behavior of the occupation numbers (52) is simple and unambiguous.

7. IMPROVED WAVEFUNCTIONS

The most obvious physical oversimplification of the state (16) is that the state f_0 is not only the internal ground state of a ^{4}He atom, but also the translational ground state: i.e., it corresponds to zero translational momentum of the atom. In the actual liquid ^{4}He ground state, the atoms certainly do not all have zero momentum. It is true that this is also the case for the state (16), due to the virtual transitions associated with (4), but in the state (16) the translational motions and internal excitations do not correspond to the correct dynamics (in fact, we have not even written down the Hamiltonian). This suggests an improved approximate ground state of the form

$$|\psi_0\rangle = U|0\rangle,$$
$$U = e^F, \quad F = \tfrac{1}{2}\sum_{\mathbf{k}} c_{\mathbf{k}}(A_{\mathbf{k}}^\dagger A_{-\mathbf{k}}^\dagger - A_{-\mathbf{k}}A_{\mathbf{k}}), \quad (54)$$

where [cf. (11)]

$$A_{\mathbf{k}}^\dagger = \Omega^{-\frac{1}{2}}\int d^3R e^{i\mathbf{k}\cdot\mathbf{R}} a_\uparrow^\dagger(\mathbf{R})a_\downarrow^\dagger(\mathbf{R})\psi^\dagger(\mathbf{R}). \quad (55)$$

This is the simplest state allowing explicit translational motions of the atoms, yet with total linear momentum zero. The function $c_{\mathbf{k}}$ would be chosen to eliminate or reduce the discrepancy between the calculated and experimental $D(R_{ij})$ (Fig. 1) or, more fundamentally, by minimization of the expectation value of the full many-electron, many-α Hamiltonian. An even more realistic trial state would also allow explicit internal excitation of the atoms, allowing the coupling between translation and virtual internal excitation to correspond as closely as possible to the actual dynamics.

APPENDIX A: PAIR DISTRIBUTION FUNCTION

The expression (31) can be rewritten in the form

$$D(R_{ij}) = D_0(R_{ij}) + \rho a_0^3 D_1(R_{ij}), \quad (A1)$$

where

$$\begin{aligned} D_0(R_{ij}) &= [1 - w^2(R_{ij})]^2, \\ D_1(R_{ij}) &= \tfrac{4}{3}(x - \tfrac{1}{2}y)[1 - w^2(R_{ij})]^2 \\ &\quad - \tfrac{4}{3}[1 - w^2(R_{ij})][x - w(R_{ij})I_{11}(R_{ij})] \\ &\quad + \tfrac{2}{3}y - \tfrac{8}{3}w(R_{ij})I_{31}(R_{ij}) \\ &\quad + \tfrac{2}{3}[1 + 2w^2(R_{ij})]I_{22}(R_{ij}) \end{aligned} \quad (A2)$$

and

$$I_{\mu\nu}(R_{ij}) = a_0^{-3}\int [w(R)]^\mu [w(|\mathbf{R}_{ij} - \mathbf{R}|)]^\nu d^3R. \quad (A3)$$

By (25), (35), and (36), we have

$$x = \frac{33\pi}{2Z^3} = 10.7, \quad y = \frac{57637\pi}{12288Z^3} = 4.32, \quad (A4)$$

so that at ^{4}He density ($\rho a_0^3 = 0.0033$) one has

$$\tfrac{4}{3}(x - \tfrac{1}{2}y)\rho a_0^3 = 0.028. \quad (A5)$$

It follows that the first line in the expression for D_1 makes only a 3% contribution to $D(R_{ij})$. It turns out that the contributions of the remaining terms in D_1 are also small. However, since this is not certain *a priori*, we discuss the evaluation of these terms here.

The integrals (A3) can be reduced to 1-dimensional integrals by use of the convolution theorem. Define

$$q = ka_0/z, \quad S = zR/a_0 \quad (A6)$$

and

$$\begin{aligned} \tilde{w}_\mu(q) &= \int [w(R)]^\mu e^{-i\mathbf{k}\cdot\mathbf{R}} d^3R \\ &= \left(\frac{a_0}{z}\right)^3 \int [w(R)]^\mu e^{-i\mathbf{q}\cdot\mathbf{S}} d^3S. \end{aligned} \quad (A7)$$

Then

$$I_{\mu\nu}(R) = \frac{z^3}{2\pi^2 S a_0^6}\int_0^\infty q\tilde{w}_\mu(q)\tilde{w}_\nu(q)\sin(qS)\,dq. \quad \text{(A8)}$$

One has,[13] by (35) and (36),

$$\tilde{w}_1(q) = 64\pi\left(\frac{a_0}{z}\right)^3(1+q^2)^{-4},$$

$$\tilde{w}_2(q) = \pi\left(\frac{a_0}{z}\right)^3\left(1+\frac{1}{4}q^2\right)^{-6}\left(\frac{33}{2}+\frac{11}{12}q^2+\frac{1}{32}q^4\right),$$

$$\tilde{w}_3(q) = \frac{8\pi}{27}\left(\frac{a_0}{z}\right)^3\left(1+\frac{1}{9}q^2\right)^{-8}$$
$$\times\left(\frac{57752}{2187}+\frac{21472}{19683}q^2+\frac{10064}{177147}q^4\right.$$
$$\left.+\frac{2080}{1594323}q^6+\frac{8}{531441}q^8\right). \quad \text{(A9)}$$

The integral I_{11} then has a simple closed form[14]:

$$I_{11}(R) = \frac{33\pi}{2z^3}e^{-S}\left(1+S+\frac{5}{11}S^2+\frac{4}{33}S^3\right.$$
$$\left.+\frac{2}{99}S^4+\frac{1}{495}S^5+\frac{1}{10395}S^6\right). \quad \text{(A10)}$$

In principle, I_{31} and I_{22} can also be expressed in closed form, but the algebraic reductions are so involved that it is easier to evaluate them numerically. This was done by Filon's formula,[15] which avoids difficulty due to rapid oscillations of the factor $\sin(qS)$ in the integrands. The corrections due to D_1 were found to be less than 5% at all R_{ij} for which the calculation was carried out. The resultant $D(R_{ij})$ is plotted in Fig. 1.

APPENDIX B: EXPLICIT EXPRESSION FOR D_3'

The evaluation of D_3 [Eq. (41)] is straightforward, though very tedious. We exhibit here the terms in D_3' [Eq. (42)] of lowest order in the density:

$$D_3'(x_1x_2\mathbf{R}, x_1'x_2'\mathbf{R}') = [2n(2n-1)\Omega]^{-1}$$
$$\times\rho[(\delta_{\sigma_1\uparrow}\delta_{\sigma_2\downarrow}-\delta_{\sigma_1\downarrow}\delta_{\sigma_2\uparrow})(\delta_{\sigma_1'\uparrow}\delta_{\sigma_2'\downarrow}-\delta_{\sigma_1'\downarrow}\delta_{\sigma_2'\uparrow})D_3^{(1)}$$
$$+\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}D_3^{(2)}+\delta_{\sigma_1\sigma_2'}\delta_{\sigma_2\sigma_1'}D_3^{(3)}], \quad \text{(B1)}$$

where

$$D_3^{(1)} = -2w(|\mathbf{R}-\mathbf{R}'|)\int u_0^*(|\mathbf{r}_1'-\mathbf{R}''|)u_0^*(|\mathbf{r}_2'-\mathbf{R}''|)$$
$$\times[u_0(|\mathbf{r}_1-\mathbf{R}|)u_0(|\mathbf{r}_2-\mathbf{R}''|)$$
$$+u_0(|\mathbf{r}_2-\mathbf{R}|)u_0(|\mathbf{r}_1-\mathbf{R}''|)]w(|\mathbf{R}'-\mathbf{R}''|)d^3R''$$
$$-2w(|\mathbf{R}-\mathbf{R}'|)\int[u_0^*(|\mathbf{r}_1'-\mathbf{R}'|)u_0^*(|\mathbf{r}_2'-\mathbf{R}''|)$$
$$+u_0^*(|\mathbf{r}_2'-\mathbf{R}'|)u_0^*(|\mathbf{r}_1'-\mathbf{R}''|)]$$
$$\times u_0(|\mathbf{r}_1-\mathbf{R}''|)u_0(|\mathbf{r}_2-\mathbf{R}''|)w(|\mathbf{R}-\mathbf{R}''|)d^3R''$$
$$+w^2(|\mathbf{R}-\mathbf{R}'|)\int u_0^*(|\mathbf{r}_1'-\mathbf{R}''|)u_0^*(|\mathbf{r}_2'-\mathbf{R}''|)$$
$$\times u_0(|\mathbf{r}_1-\mathbf{R}''|)u_0(|\mathbf{r}_2-\mathbf{R}''|)d^3R'', \quad \text{(B2)}$$

$$D_3^{(2)} = w(|\mathbf{R}-\mathbf{R}'|)[u_0^*(|\mathbf{r}_1'-\mathbf{R}'|)u_0(|\mathbf{r}_1-\mathbf{R}|)$$
$$\times w(|\mathbf{r}_2-\mathbf{r}_2'|)+u_0^*(|\mathbf{r}_2'-\mathbf{R}'|)$$
$$\times u_0(|\mathbf{r}_2-\mathbf{R}|)w(|\mathbf{r}_1-\mathbf{r}_1'|)]$$
$$+u_0^*(|\mathbf{r}_1'-\mathbf{R}'|)u_0(|\mathbf{r}_2-\mathbf{R}|)\int u_0^*(|\mathbf{r}_2'-\mathbf{R}''|)$$
$$\times u_0(|\mathbf{r}_1-\mathbf{R}''|)w(|\mathbf{R}-\mathbf{R}''|)w(|\mathbf{R}'-\mathbf{R}''|)d^3R''$$
$$+u_0^*(|\mathbf{r}_2'-\mathbf{R}'|)u_0(|\mathbf{r}_1-\mathbf{R}|)\int u_0^*(|\mathbf{r}_1'-\mathbf{R}''|)$$
$$\times u_0(|\mathbf{r}_2-\mathbf{R}''|)w(|\mathbf{R}-\mathbf{R}''|)w(|\mathbf{R}'-\mathbf{R}''|)d^3R'' \quad \text{(B3)}$$

and

$$D_3^{(3)} = -w(|\mathbf{R}-\mathbf{R}'|)[u_0^*(|\mathbf{r}_1'-\mathbf{R}'|)u_0(|\mathbf{r}_2-\mathbf{R}|)$$
$$\times w(|\mathbf{r}_1-\mathbf{r}_2'|)+u_0^*(|\mathbf{r}_2'-\mathbf{R}'|)$$
$$\times u_0(|\mathbf{r}_1-\mathbf{R}|)w(|\mathbf{r}_2-\mathbf{r}_1'|)]$$
$$-u_0^*(|\mathbf{r}_1'-\mathbf{R}'|)u_0(|\mathbf{r}_1-\mathbf{R}|)\int u_0^*(|\mathbf{r}_2'-\mathbf{R}''|)$$
$$\times u_0(|\mathbf{r}_2-\mathbf{R}''|)w(|\mathbf{R}-\mathbf{R}''|)w(|\mathbf{R}'-\mathbf{R}''|)d^3R''$$
$$-u_0^*(|\mathbf{r}_2'-\mathbf{R}'|)u_0(|\mathbf{r}_2-\mathbf{R}|)\int u_0^*(|\mathbf{r}_1'-\mathbf{R}''|)$$
$$\times u_0(|\mathbf{r}_1-\mathbf{R}''|)w(|\mathbf{R}-\mathbf{R}''|)w(|\mathbf{R}'-\mathbf{R}''|)d^3R''. \quad \text{(B4)}$$

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[5] There is nothing to be gained at this point by descending to the next level of the hierarchy, at which one would have to take account of the composite nature of the α particle.

[6] We also make the excellent approximation of identifying the center of mass of the atom with the position of the α particle.

[7] Strictly speaking, u_0 must then differ from a spherically symmetric function due to the presence of periodic images outside the periodicity cell (volume Ω). However, since this cell is macroscopic whereas the range of u_0 is microscopic, these images are entirely negligible.

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[9] In terms of the normalized Schrödinger wavefunction

$$\psi_0(x_1\cdots x_{2n}\mathbf{R}_1\cdots\mathbf{R}_n),$$

one has

$$D_1(\mathbf{R},\mathbf{R}') = \int\psi_0(x_1\cdots x_{2n}\mathbf{R}\mathbf{R}_2\cdots\mathbf{R}_n)\psi_0^*$$
$$\times(x_1\cdots x_{2n}\mathbf{R}'\mathbf{R}_2\cdots\mathbf{R}_n)\,dx_1\cdots dx_{2n}d^3R_2\cdots d^3R_n.$$

[10] See, e.g., L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Co., Inc., New York, 1949), pp. 172–174.

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Spin Representations of the Orthogonal Groups

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The spin representations of the algebras B_n and D_n are constructed from the spin representations of the canonical subalgebras B_{n-1} and D_{n-1}, respectively.

I. INTRODUCTION

The operator techniques[1] for constructing the weight space diagrams for the classical simple groups are extended to the spin "representations" of the orthogonal groups.

II. RESULTS AND EXAMPLES

Irreducible representations of the algebras D_n and B_n are described uniquely[2] by their highest weights $\bar{M}^h$. They can also be described uniquely by means of extended partitions defined by $\bar{\lambda} = \bar{M}^h$. These extended partitions have the usual[3-5] properties

$$B_n: \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0,$$
$$D_n: \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq |\lambda_n| \geq 0.$$

All λ_i are either integral or half-integral.

Branching rules under the canonical embeddings $SO(2n+1) \downarrow SO(2n) \downarrow SO(2n-1)$ are given by

$$[\lambda]_{2n+1} \xrightarrow{B_n \downarrow D_n} \sum [\lambda']_{2n}:$$
$$\lambda_1 \geq \lambda_1' \geq \lambda_2 \geq \lambda_2' \geq \cdots \geq \lambda_n \geq |\lambda_n'| \geq 0, \quad (1)$$

$$[\lambda']_{2n} \xrightarrow{D_n \downarrow B_{n-1}} \sum [\lambda'']_{2n-1}:$$
$$\lambda_1' \geq \lambda_1'' \geq \lambda_2' \geq \lambda_2'' \geq \cdots \geq \lambda_{n-1}' \geq \lambda_{n-1}'' \geq |\lambda_n'|. \quad (2)$$

Equations (1) and (2) are conveniently summarized using the box annihilation operator[1]

$$P_n = \frac{1}{1-\epsilon_n}\frac{1}{1-\epsilon_{n-1}}\cdots\frac{1}{1-\epsilon_2}\frac{1}{1-\epsilon_1}, \quad (3)$$

$$[\lambda]_{2n+1} \xrightarrow{B_n \downarrow D_n} \sum P_n[\lambda]_{2n}, \quad (1')$$

$$[\lambda']_{2n} \xrightarrow{D_n \downarrow B_{n-1}} \sum P_n[\lambda']_{2n-1}. \quad (2')$$

The modification rules are

$B_n \downarrow D_n$: none

$D_n \downarrow B_{n-1}$: $[\lambda_1' \cdots \lambda_{n-1}', \lambda_n']_{2n-1}$
$= [\lambda_1, \cdots \lambda_{n-1}']_{2n-1}, \quad \lambda_n' = 0, \pm\frac{1}{2}, \pm 1,$
$= 0, \quad$ otherwise.

In order to construct the weight spaces for the spin representations of D_n from those of D_{n-1} (and of B_n from B_{n-1}), it is necessary to apply these operators successively:

$$D_n \downarrow B_{n-1} \downarrow D_{n-1}: [\bar{\lambda}]_{2n} \xrightarrow{D_n \downarrow D_{n-1}} P_{n-1}P_n[\bar{\lambda}]_{2n-2},$$
$$B_n \downarrow D_n \downarrow B_{n-1}: [\bar{\lambda}]_{2n+1} \xrightarrow{B_n \downarrow B_{n-1}} P_nP_n[\bar{\lambda}]_{2n-1}. \quad (4)$$

The weight space diagram for $[\bar{\lambda}]_{2n}$ of D_n is constructed by the following algorithm:

(1) P_{n+} operates on λ, annihilating boxes and adding $+1$ for each box annihilated.

(2) The modification rules for $D_n \downarrow B_{n-1}$ are applied. At the same time, λ_n' is added to the positive integer above the partition $\bar{\lambda}$.

(3) $P_{(n-1)-}$ operates on all nonvanishing partitions describing representations of B_{n-1}, adding -1 for each box annihilated ($\lambda_n'' > 0$). For $\lambda_n'' < 0$, $m' = -m$, the latter defined by

$$[\lambda_1'', \lambda_2'', \cdots \overset{m'}{-} |\lambda_{n-1}''|]_{2n-2} = [\lambda_1'', \lambda_2'', \cdots |\lambda_{n-1}''|]_{2n-2}.$$
$$-m$$

(4) The half-integral number m above the partition $[\lambda'']_{2n-2}$ indicates the plane $Z_n = m$ in which the weight space of $[\lambda'']_{2n-2}$ lies in the synthesis of $[\bar{\lambda}]_{2n}$.

Example 1: Construct the weight space for $\begin{smallmatrix}\square\diagdown\\ \diagdown_4\end{smallmatrix}$ of D_2:

(1) $P_{2+}\begin{smallmatrix}\square\diagdown\\ \diagdown_4\end{smallmatrix} = \overset{0}{\begin{smallmatrix}\square\diagdown\\ \diagdown_3\end{smallmatrix}} + \overset{1}{\begin{smallmatrix}\diagdown\\ \diagdown_3\end{smallmatrix}}.$

(2) $\equiv \overset{\frac{1}{2}}{\square\diagdown_3} + \overset{\frac{3}{2}}{\diagdown_3}.$

(3) $P_{1-}\overset{\frac{1}{2}}{\square\diagdown_3} = 2\overset{-\frac{1}{2}}{\diagdown\square} + 2\overset{\frac{1}{2}}{\diagdown} + \overset{-\frac{1}{2}}{\diagdown_2} + \overset{\frac{1}{2}}{\square\diagdown_2}$

$P_{1-}\overset{\frac{3}{2}}{\diagdown_3} = \qquad\qquad 2\overset{-\frac{3}{2}}{\diagdown} + 2\overset{\frac{3}{2}}{\diagdown}.$

(4) Results of this construction are plotted in Fig. 1.

The construction of the irreducible spin representations of B_n from those of B_{n-1} follows an analogous procedure:

(1) P_{n+} operates on $\bar{\lambda}$, annihilating boxes and adding $+1$ for each box annihilated ($\lambda'_n > 0$). Once again,

$$[\lambda'_1, \cdots - \lambda'_n]_{2n} \equiv [\lambda'_1, \cdots + \lambda'_n]_{2n}.$$

(2) $P_n^{\mp}$ operates on the remaining partitions, annihilating boxes and adding -1 if $\lambda'_n > 0$ and $+1$ if $\lambda'_n < 0$.

(3) The modification rules for $D_n \downarrow B_{n-1}$ are applied, and λ''_n is added to each integer above the associated partition.

Example 2: Construct the weight space for $\square\!\!\square_5$ of B_2:

(1) $P_2^+ \square\!\!\square_5 \to \square\!\!\square_4 + \square_4$

$$+ \square_4 + \square\!\square_4.$$

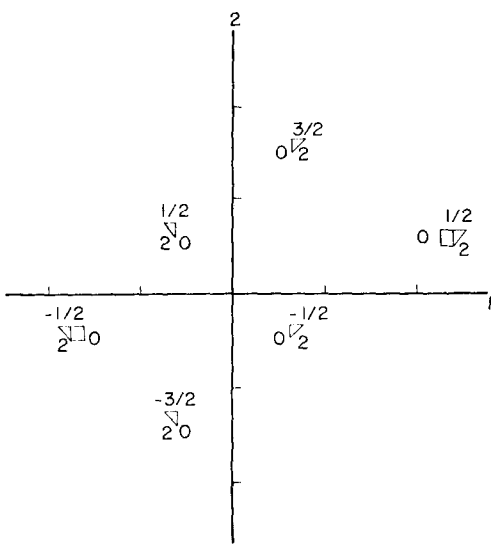

FIG. 1. The weight space of $\square_4$ as constructed in Example 1. The weight space for $\square_4$ may be computed as in Example 1 or obtained from $\square_4$ by reflection in the $Z_2 = 0$ hyperplane.

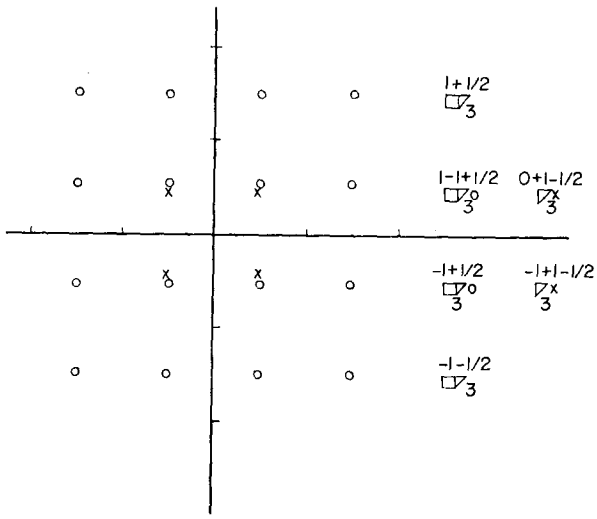

FIG. 2. The weight space of $\square\!\!\square_5$ as constructed in Example 2.

(2) $P_2^{\mp} \square\!\!\square_4 \to \square\!\!\square_3 + \square_3 \equiv - + \square_3$,

$$P_2^{\mp} \square_4 \to \square_3 + \square_3 \equiv \square_3 + \square_3,$$

$$P_2^{\mp} \square_4 \to \square_3 + \square_3 \equiv \square_3 + \square_3,$$

$$P_2^{\mp} \square\!\square_4 \to \square\!\square_3 + \square_3$$

$$\equiv - + \square_3.$$

(3) The results of this calculation are shown in Fig. 2.

III. CONCLUSION

With these algorithms and those presented in Ref. 1, it is possible to construct weight spaces for all the finite-dimensional irreducible representations of the simple classical rank-n Lie algebras from the weight spaces of the canonically embedded subalgebra of rank $n - 1$.

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Spectrum of Casimir Invariants for the Simple Classical Lie Groups

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The spectra of the Casimir invariants for the classical compact simple Lie groups are presented. It is proved that these invariants are irreducible and functionally independent. The highest weight of a representation is determined in terms of its invariant spectrum.

I. INTRODUCTION

The Casimir invariants[1] of Lie groups, and their spectra, are of interest to both physicists and mathematicians. Invariants of the unitary groups have been used in discussions on nuclear[2] and elementary particle[3] physics. Invariants of the symplectic groups have been used in the discussion of elementary particle[4] physics. Invariants of the orthogonal and related groups have been used in the description of the hydrogen atom[5] and of free-particle[6,7] states. A knowledge of the invariants and their spectra is also necessary for a complete description of the unitary irreducible representations of the noncompact real forms associated with the algebras A_n, B_n, C_n, and D_n.[8,9] The invariants of the unitary series A_n have been determined, together with a partial eigenvalue spectrum.[10,11]

We present here the spectrum of the irreducible invariants of the UIR's associated with the compact forms of A_n, B_n, C_n, and D_n.

II. PROPERTIES OF THE INVARIANTS

The UIR's of the compact simple Lie groups may be uniquely classified according to

(i) highest[1] weight $\mathbf{M}^h$,
(ii) extended[12] partition $\boldsymbol{\lambda}$,
(iii) Casimir-invariant spectrum $\mathbf{C}$.

The relation between (i) and (ii) is

$$(M^h)_i = \lambda_i - \frac{1}{n+1}\sum_{j=1}^{n+1}\lambda_j, \quad \text{for } A_n,$$
$$\mathbf{M} = \quad , \quad \text{for } C_n, B_n, \text{ and } D_n. \tag{1}$$

Representations have not generally been characterized by their Casimir-invariant spectrum, since this has not generally been available.

Some useful properties[1] of the invariants of a simple group are as follows:

(a) They are symmetric homogeneous polynomial functions of the group generators which commute with all elements of the Lie algebra.

(b) They are invariant under the automorphisms induced by the Weyl group of reflections.

(c) The product of the orders of the n functionally independent irreducible invariants associated with a simple algebra of rank n is equal to the order of the Weyl group of reflections for the algebra.

(d) The spectrum of the invariant operators $C(\mathbf{M}^h)$ on an irreducible representation with highest weight $\mathbf{M}^h$ is given by

$$C(\mathbf{M}^h) = f(\mathbf{M}^h + \mathbf{R}) - f(\mathbf{R}). \tag{2}$$

Here, $f(x)$ are those terms in the irreducible polynomial invariant which depend on the diagonal group generators H_i *only*, and $\mathbf{R}$ is half the sum of all positive roots of the algebra

$$\mathbf{R} = \tfrac{1}{2}\sum_{\vec{\alpha}>0}\vec{\alpha}. \tag{3}$$

We shall call $f(H_i)$ the associated invariant.

(e) The Jacobian $J(H) = \|\partial C_i/\partial H_j\|$ of the irreducible invariants is a basis for the alternating representation of the Weyl group.[13]

III. ASSOCIATED INVARIANTS

The associated invariants are

$$f_j^{A_n}(\mathbf{H}) = \sum_{i_r \neq i_s}\prod_{r=1}^{j} H_{i_r}, \quad \text{for } A_n,$$
$$f_j(\mathbf{H}) = \sum_{i_r \neq i_s}\prod_{r=1}^{j} H_{i_r}^2, \quad \text{for } C_n, B_n, \text{ and } D_n, \tag{4}$$

except the nth associated invariant for D_n is

$$f_n^{D_n}(H) = \prod_{r=1}^{n} H_i. \tag{4'}$$

The vector $\mathbf{R}$ is given by

$$\begin{aligned} R_i &= \tfrac{1}{2}n + 1 - i, && \text{for } A_n,\\ R_i &= \tfrac{1}{2}(2n+2) - i, && \text{for } C_n,\\ R_i &= \tfrac{1}{2}(2n+1) - i, && \text{for } B_n,\\ R_i &= \tfrac{1}{2}(2n) - i, && \text{for } D_n. \end{aligned} \tag{3'}$$

IV. IRREDUCIBILITY OF INVARIANTS

From (4) it is seen that the product of the orders of the invariants is equal to the order of the Weyl group, for each algebra [cf. Sec. II, observation (c)]. They are therefore irreducible.

V. FUNCTIONAL INDEPENDENCE OF INVARIANTS

The order of the Jacobian is equal to the number of positive roots in the algebra. From observation (e) of Sec. II we conclude that

$$J(\mathbf{M}^h + \mathbf{R})/J(\mathbf{O} + \mathbf{R}) = \dim(\mathbf{M}^h). \tag{5}$$

Since the Jacobian is nonvanishing, the invariants are functionally independent.

VI. HIGHEST WEIGHTS FROM INVARIANTS

It is easily verified that the ordered roots $x_1 \geq x_2 \geq \cdots \geq x_{n+1}$ of the equation

$$\sum_{i=0}^{n+1}(-1)^i x^{n+1-i} f_i^{A_n}(\mathbf{M} + \mathbf{R}) = 0 \tag{6}$$

are related to the highest weights of the representation whose associated invariants are $\mathbf{f}_n^{A_n}(\mathbf{M} + \mathbf{R})$ by

$$x_i = M_i^h + R_i. \tag{7}$$

Similarly, the ordered roots x_i^2 of

$$\sum_{i=0}^{n}(-1)^i (x^2)^{n-i} f_i(\mathbf{M}^h + \mathbf{R}) = 0 \tag{6}$$

are related to the highest weights of C_n, B_n, and D_n by

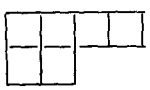
$$x_i^2 = (M_i^h + R_i)^2. \tag{7}$$

For D_n, $f_n^{D_n}$ must be replaced by its square. Then

$$M_n + R_n = M_n = \pm |x_n| \tag{8}$$

depending on whether $f_n^{D_n} \gtrless 0$.

VII. EXAMPLE

The representation (4, 2)  of $SU(3)$ has highest weight (2, 0, −2) [cf. Eq. (1)]. From (3′), $\mathbf{R} = (1, 0, -1)$. From Eq. (4) the associated invariants are

$$\begin{aligned} f_1^{A_2} &= \textstyle\sum H_i &&= 0, \\ f_2^{A_2} &= (3)(0) + (0)(-3) + (-3)(3) &&= -9, \\ f_3^{A_2} &= (3)(0)(-3) &&= 0. \end{aligned}$$

The Casimir invariants are $C_2 = -8$ and $C_3 = 0$. For the unitary groups, C_1 is always zero. From Eq. (5), this representation has dimension 27. The highest weight may be found by solving Eq. (6),

$$x^3 - 0x^2 + (-9)x - 0 = 0.$$

Then $\mathbf{x}_i = (3, 0, -3)$ and

$$\mathbf{M}^h = \mathbf{x} - \mathbf{R} = (3, 0, -3) - (1, 0, -1) = (2, 0, -2).$$

VIII. CONCLUSION

The spectra of the Casimir invariants of the classical compact simple Lie groups has been presented. They may be used to label representations *conveniently*. The relationship between the labelling schemes using $\mathbf{M}^h$, $\boldsymbol{\lambda}$, and $\mathbf{C}$ is contained in Eqs. (1), (6), and (7).

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Transmission Properties of an Isotopically Disordered One-Dimensional Harmonic Crystal. II. Solution of a Functional Equation

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The amplitude of a wave of frequency ω which is transmitted by a disordered array of N isotopic defects in a 1-dimensional harmonic crystal is investigated in the limit $N \to \infty$. In particular, the ratio $\hat{T}_N(\omega)$ of the amplitude of the Nth defect to the amplitude of the first defect is represented as $\exp[-N\hat{\alpha}_N(\omega, Q, \{a_n\})]$, where $\{a_n\}$, $n = 2, \cdots, N$, is the sequence of nearest-neighbor spacings and $Q = (M - m)/m$. It is known from earlier work that $\hat{\alpha}_N(\omega, Q, \{a_n\})$ is the logarithm of the Nth root of the magnitude of a continuant determinant of order N. The value of the continuant is expressed formally as a product of N factors $\hat{g}_n$ which are recursively related. In the present case, the $\hat{g}_n$ happen to lie on a circle K_0 in the complex $\hat{g}$ plane. Assuming that the spacings between defects are independent identically distributed random variables with the mean value c^{-1} and going to the limit $N \to \infty$, a functional equation for the limiting distribution function of the $\hat{g}_n$ on K_0 is derived. The limiting value $\alpha(\omega, Q, c) = \lim \hat{\alpha}_N(\omega, Q, \{a_n\})$, as $N \to \infty$, can be determined from the limiting distribution function of the $\hat{g}_n$. We determine the solution of the functional equation in three different ways for three different cases: (a) In the case of the special frequency of Matsuda, $\omega = 2^{-\frac{1}{2}}$ and $Q = 1$, we obtain exact values of the integral of the $\hat{g}$ distribution function which are in excellent agreement with Monte Carlo estimates; (b) in the physically interesting case where the mean spacing between defects is small compared to the incident wavelength, i.e., $c^{-1}\omega \ll 1$, we obtain the solution of the functional equation correct to first order in $c^{-1}\omega$ and we calculate the lowest-order nonzero value of $\alpha(\omega, Q, c)$; (c) for the general case of moderate values of ω, Q, and c, we develop a numerical method for solving the functional equation and present the results of the numerical calculations in several representative cases. These numerical results are in good agreement with Monte Carlo estimates. One of the principal results, obtained by solving the functional equation, is that $\alpha(\omega, Q, c) > 0$ for $\omega \ll c < 1$ and $\omega(|Q| + c^{-1}) \ll 1$ with $Q \neq 0$.

1. INTRODUCTION

This paper is a continuation of a study of the transmission properties of a disordered array of isotopic defects of mass M substituted in an otherwise perfect 1-dimensional harmonic crystal composed of particles of mass m.[1] In R1 the transmitted amplitude of a wave of frequency ω incident on a section of crystal containing N defects was shown to be the reciprocal of the magnitude of an Nth-order determinant whose elements depend explicitly on $(M - m)/m$, ω, and the spacings between adjacent pairs of defects. The principal problem treated in R1 dealt with the case in which the spacings between successive pairs of defects were assumed to be independent random variables with a common probability distribution and a common mean value c^{-1}. (The parameter c plays the role of concentration.) Based on the assumption of statistical independence of spacings, the dependence of the transmitted amplitude on N in the limit $N \to \infty$ was investigated. The transmitted amplitude can be expressed in the form $T_N = \exp[-N\alpha_N(\omega, Q, \{a_j\})]$, where $Q = (M - m)/m$ and $\{a_j\}$, $j = 2, \cdots, N$, denotes the particular set of spacings between adjacent pairs of defects. It was shown in R1 that there is a range of concentration $0 < c < \bar{c}(\omega, Q)$ such that

$$\lim_{N\to\infty} \alpha_N(\omega, Q, \{a_j\}) = \alpha(\omega, Q, c) > 0. \qquad (1)$$

Conservation of energy insures that $\alpha_N(\omega, Q, \{a_j\}) \geq 0$. Therefore, the most significant aspect of Eq. (1) is that the limiting value of $\alpha_N(\omega, Q, \{a_j\})$ is independent of N and strictly positive. In Eq. (1), $\alpha_N(\omega, Q, \{a_j\})$ is the average contribution of a defect to the attenuation of the incident wave. On physical grounds it is expected that, if the mean spacing c^{-1} between defects is sufficiently large compared to the wavelength of the incident wave, then $\alpha_N(\omega, Q\{a_j\})$ approaches $a_1(\omega, Q)$, the attenuation of a single isolated defect. This physical argument forms the basis of the derivation of Eq. (1) and of the determination of $\bar{c}(\omega, Q)$. The method of derivation is limited to low concentrations. However, it was emphasized in R1 that the limitation on the range of concentration $0 < c < \bar{c}(\omega, Q)$ in Eq. (1) is not a necessary condition for the inequality in Eq. (1). One of the principal results of this paper is that $\alpha(\omega, Q, c) > 0$ in a range of frequency and concentration where the mean spacing between defects is *small* compared to the incident wavelength, i.e., $\omega \ll c < 1$.

In the remainder of this section, we first summarize those results in R1 which will be required in the present analysis, and then we outline the order of the calculations in the present paper. The model system which is considered is an infinite 1-dimensional harmonic crystal with nearest-neighbor force constants only. All particles have the mass m except for N isotopic

defect particles at lattice sites $A_j, j = 1, \cdots, N$. The mass of each of the defect particles is M. It is assumed that $A_1 = 0$ and that the subscript j on A_j specifies the order of the defects, i.e., $0 = A_1 < \cdots < A_N$. If a wave of unit amplitude and frequency ω is incident from the left on the array of defects, then the steady-state amplitude of lattice site $r \leq 0$ is

$$x(r) = e^{-ikr} + R_N e^{ikr+i\Lambda_N}, \tag{2}$$

where $\omega = \sin \frac{1}{2}k$ and R_N is the amplitude of the reflected wave. The steady-state amplitude of the transmitted wave is obtained from Eqs. (21), (22), and (26) of R1:

$$x(s) = e^{-iks}/D_N = T_N e^{-iks+i\Psi_N}, \tag{3}$$

where $s \geq A_N$ and D_N is the determinant of an $N \times N$ matrix and has the tridiagonal or continuant form

$$D_N = \begin{vmatrix} 1 + i\Delta & -e^{-ka_2 i} & & & & \\ -e^{-ka_2 i} & 1 + i\Delta + (1 - i\Delta)e^{-2ka_2 i} & -e^{-ka_3 i} & & & \\ & -e^{-ka_3 i} & 1 + i\Delta + (1 - i\Delta)e^{-2ka_3 i} & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & -e^{-ka_N i} & \\ & & & & -e^{-ka_N i} & 1 + i\Delta + (1 - i\Delta)e^{-2ka_N i} \end{vmatrix}, \tag{4}$$

where $\Delta = Q\omega(1 - \omega^2)^{-\frac{1}{2}}$, $Q = (M - m)/m$, and $a_n = A_n - A_{n-1}$ and where

$$D_N^{-1} = T_N e^{i\Psi_N}, \tag{5}$$

with $T_N = |D_N|^{-1}$. The determinant D_N satisfies the recurrence relation

$$D_N = [1 + i\Delta + (1 - i\Delta)e^{-2ka_N i}]D_{N-1} - e^{-2ka_N i}D_{N-2} \tag{6}$$

with $D_0 = 1$ and $D_1 = 1 + i\Delta$. The steady-state amplitude of the right-most defect has the same form as Eq. (3),

$$x(A_N) = e^{-ikA_N}/D_N, \tag{7}$$

and the steady-state amplitude of the left-most defect at $A_1 = 0$ is given in R1 as

$$x(0) = t_{N-1}/D_N = \hat{D}_N/D_N, \tag{8}$$

where t_{N-1} is an $(N - 1) \times (N - 1)$ tridiagonal determinant which satisfies the same recurrence relation (6) as D_N. It is possible, and convenient, to express t_{N-1} as an $N \times N$ determinant $\hat{D}_N$. The elements of the augmented determinant are identical with those of D_N given in Eq. (4) except that the upper left-hand-corner element of $\hat{D}_N$ is 1 instead of $1 + i\Delta$. Therefore, the determinant $\hat{D}_N$ satisfies the same recurrence relation (6) as D_N but with the starting values $\hat{D}_0 = 1$ and $\hat{D}_1 = 1$. Equation (3) is an explicit expression for the amplitude and phase shift of the transmitted wave in terms of the determinant D_N. Similarly, by combining Eq. (2) for $r = 0$ with Eq. (8), the amplitude and phase shift of the reflected wave can be expressed as

$$R_N e^{i\Lambda_N} = -1 + (\hat{D}_N/D_N). \tag{9}$$

Since $\hat{D}_N$ and D_N satisfy the same recurrence relation, it can be shown that

$$\hat{D}_N/D_N = (i/\Delta)[-1 + (D_{N-1}/D_N)],$$

and

$$R_N e^{i\Lambda_N} = (i/\Delta)[-1 + i\Delta + (D_{N-1}/D_N)]. \tag{9'}$$

In studying the transmission properties of the array of defects in the limit $N \to \infty$, two alternatives present themselves. First, one can investigate the asymptotic properties of the transmitted amplitude $T_N = |D_N|^{-1}$; or second, as noted in R1, one can investigate the asymptotic properties of the ratio $\hat{T}_N = |\hat{D}_N|^{-1}$ of the amplitude of the Nth defect to the first defect. In the former alternative, it is convenient to express D_N^{-1} as a product of N factors

$$D_N^{-1} = \left(\prod_{n=1}^{N} g_n\right) e^{-N\phi i}, \tag{10}$$

where $g_n = e^{\phi i}D_{n-1}/D_n$, $1 + i\Delta = \delta e^{\phi i}$, and where g_n satisfies the recurrence relation

$$g_n = [\delta + (\delta - g_{n-1})e^{-2ka_n i - 2\phi i}]^{-1} \tag{11}$$

with $g_1 = \delta^{-1}$. If the transmitted amplitude is expressed in the form

$$T_N = \exp[-N\alpha_N(\omega, Q, \{a_j\})], \tag{12}$$

then

$$\alpha_N(\omega, Q, \{a_j\}) = -N^{-1}\sum_{n=1}^{N} \ln(|g_n|). \tag{13}$$

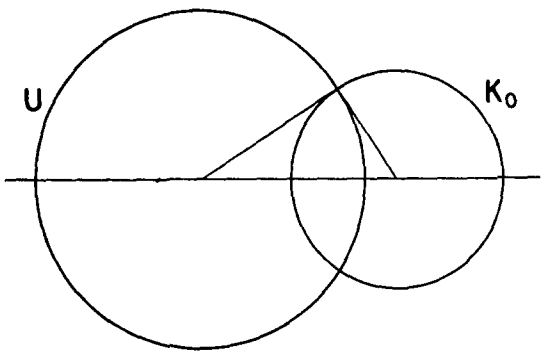

FIG. 1. The complex g plane showing the unit circle U with its center at the origin and the circle K_0 whose radius is Δ and whose center is at $\delta = (1 + \Delta^2)^{\frac{1}{2}}$.

The g_n in Eq. (13) have the property that they are confined to the interior of the circle K_0 in Fig. 1. Successive values of g_n are determined by the sequence of spacings $\{a_n\}$ through the recurrence relation (11). In obtaining the result in R1 that

$$\lim_{N\to\infty} \alpha_N(\omega, Q, \{a_j\}) = \alpha(\omega, Q, c) > 0$$

for a sequence of random, independent spacings $\{a_j\}$ with $\langle a_j \rangle = c^{-1}$ and for $0 < c < \bar{c}(\omega, Q)$, the question of the precise form of the distribution of the values of g_n inside K_0 was ignored. We examine this question in more detail in the present paper; consequently, we are able to obtain stronger results regarding the limiting value $\alpha(\omega, Q, c)$ (see Sec. 3B).

The second starting point, and the one used in this paper, for the investigation of the transmission properties of a random array of defects is the relation

$$\hat{T}_N = |\hat{D}_N|^{-1} = \exp\,[-N\hat{\alpha}_N(\omega, Q, \{a_j\})]. \quad (14)$$

Because $\hat{D}_N$ satisfies the same recurrence relation as D_N, analogous ratios $\hat{g}_n = e^{\phi i}\hat{D}_{n-1}/\hat{D}_n$ can be defined which satisfy the recurrence relation (11) for g_n but with $\hat{g}_1 = e^{\phi i}$. Then, the expression for $\hat{\alpha}_N(\omega, Q, \{a_j\})$ is formally the same as for $\alpha(\omega, Q, \{a_j\})$ in Eq. (13):

$$\hat{\alpha}_N(\omega, Q, \{a_j\}) = -N^{-1}\sum_{n=1}^{N} \ln\,(|\hat{g}_n|). \quad (15)$$

The advantage in working with the $\hat{g}_n$, as noted in R1, is that the $\hat{g}_n$ are confined to the circumference of the circle K_0 in Fig. 1 and, thus, have a 1-dimensional distribution. Assuming that the spacings a_j are statistically independent with the mean value c^{-1}, we have a limiting distribution function of the $\hat{g}_n$ on K_0 which we denote by $f_c[\chi]$. The determination of this limiting distribution function is our primary concern because the limiting value of $\hat{\alpha}_N(\omega, Q, \{a_j\})$ can be calculated from it.

In Sec. 2, we derive a functional equation for $f_c[\chi]$ and for $F_c[\chi] = \int_0^\chi f_c[\chi]\,d\chi$. In Sec. 3, we determine the solution of the functional equation in three different ways for three different cases: (a) In the case of the special frequency of Matsuda,[2] $\omega = 2^{-\frac{1}{2}}$ and $Q = 1$, we obtain exact values of $F_c[\chi]$ which are in excellent agreement with Monte Carlo estimates; (b) in the physically interesting case where the mean spacing between defects is small compared to the incident wavelength, i.e., $c^{-1}\omega \ll 1$, we determine $f_c[\chi]$ correct to the first order in $c^{-1}\omega$ and we calculate the lowest-order nonzero limiting value of $\hat{\alpha}_N(\omega, Q, \{a_j\})$ (this limiting value, which is positive, and $f_c[\chi]$ are in excellent agreement with Monte Carlo estimates); (c) for the general case of moderate values of ω, Q, and c, we have developed a numerical method for solving the functional equation for $F_c[\chi]$. The numerical results for $F_c[\chi]$ and the associated limiting value of $\hat{\alpha}_N(\omega, Q, \{a_j\})$ are presented and compared with Monte Carlo estimates for several cases.

We expect on physical grounds that the limiting values of $\alpha_N(\omega, Q, \{a_j\})$ and $\hat{\alpha}_N(\omega, Q, \{a_j\})$ are identical, i.e.,

$$\lim_{N\to\infty} \alpha_N(\omega, Q, \{a_j\}) = \lim_{N\to\infty} \hat{\alpha}_N(\omega, Q, \{a_j\}). \quad (16)$$

We assume that the a_j are statistically independent and that $\langle a_j \rangle = c^{-1}$; we denote the limiting value of $\hat{\alpha}_N(\omega, Q, \{a_j\})$ by

$$\alpha(\omega, Q, c) = \lim_{N\to\infty} \hat{\alpha}_N(\omega, Q, \{a_j\}). \quad (16')$$

If $\alpha(\omega, Q, c) > 0$, we can prove that $\alpha_N(\omega, Q, \{a_j\})$ approaches $\hat{\alpha}_N(\omega, Q, \{a_j\})$. The basic reason is that, if $\alpha(\omega, Q, c) > 0$, then g_n approaches $\hat{g}_n$. To show that $|g_n - \hat{g}_n| \to 0$ if $\alpha(\omega, Q, c) > 0$, we multiply the recurrence relation (6) for D_N by $\hat{D}_{N-1}$, multiply the corresponding relation for $\hat{D}_N$ by D_{N-1}, and form the difference

$$D_N\hat{D}_{N-1} - \hat{D}_N D_{N-1} = e^{-2ka_n i}(D_{N-1}\hat{D}_{N-1} - \hat{D}_{N-1}D_{N-2}). \quad (17)$$

We use Eq. (17) repeatedly to reduce its right-hand side and rewrite the left-hand side to give

$$e^{-\phi i}D_N\hat{D}_N(e^{\phi i}\hat{D}_{N-1}\hat{D}_N^{-1} - e^{\phi i}D_{N-1}D_N^{-1}) = e^{-2kA_N i}(D_1\hat{D}_0 - \hat{D}_0 D_1)$$

or

$$|\hat{g}_N - g_N| = |\Delta|\,T_N\hat{T}_N. \quad (18)$$

If $\alpha(\omega, Q, c) > 0$, Eq. (18) can be used to prove Eq. (16).

2. DERIVATION OF FUNCTIONAL EQUATION FOR THE DISTRIBUTION OF THE $\hat{g}_n$

In this section, we derive a functional equation for the distribution of the $\hat{g}_n$ on the circle K_0 in Fig. 1. The recurrence equation relating $\hat{g}_n$ to $\hat{g}_{n-1}$ is the same as Eq. (11),

$$\hat{g}_n = [\delta + (\delta - \hat{g}_{n-1})e^{-2ka_ni-2\phi i}]^{-1}, \tag{19}$$

but with $\hat{g}_1 = e^{\phi i}$. If $\hat{g}_n$ is expressed as

$$\hat{g}_n = \delta + |\Delta|\, e^{i\chi_n}, \tag{20}$$

then Eq. (19) provides a relation between χ_n and χ_{n-1},

$$e^{i\chi_n} = \left(\frac{\delta - |\Delta|\, e^{-i(\chi_{n-1}-2a_nk-2\phi)}}{\delta - |\Delta|\, e^{i(\chi_{n-1}-2a_nk-2\phi)}}\right) e^{i(\chi_{n-1}-2a_nk-2\phi)}. \tag{21}$$

We assume that N is large compared to unity and that the set of spacings $\{a_j\}$ are independent random variables with the same probability distribution

$$P(a) = c(1 - c)^{a-1}. \tag{22}$$

Consider an interval $(\chi, \chi + d\chi)$ on the circle K_0 and denote the fraction of the $\hat{g}_n$ which are located in this interval by $f_c(\chi)\, d\chi$. We assume that, for sufficiently large N, $f_c(\chi)$ is independent of N. We invert Eq. (21) and obtain an expression for the angle $\chi_{n-1} \equiv \chi'$, in terms of $a_n \equiv a$ and $\chi_n \equiv \chi$,

$$\chi' = \chi - 2\Psi(\chi) + 2ak + 2\phi, \tag{23}$$

where

$$\begin{aligned}\Psi(\chi) &= \tan^{-1}\,[|\Delta| \sin \chi/(\delta + |\Delta| \cos \chi)] \\ &= \tan^{-1}\,[\sin|\phi| \sin \chi/(1 + \sin|\phi| \cos \chi)].\end{aligned} \tag{24}$$

A functional equation for $f_c(\chi)$ can be obtained by identifying the intervals from which the $\hat{g}$ in $(\chi, \chi + d\chi)$ originate; that is,

$$f_c(\chi)\, d\chi = \sum_{a=1}^{\infty} c(1 - c)^{a-1} f_c(\chi')\, d\chi'. \tag{25}$$

In Eq. (25) $d\chi$ and $d\chi'$ are related by (23)

$$d\chi' = d\chi/(\delta^2 + \Delta^2 + 2\delta\,|\Delta| \cos \chi). \tag{26}$$

Thus, the functional equation for $f_c(\chi)$, the fraction of the $\hat{g}_n$ in the interval $(\chi, \chi + d\chi)$, is

$$f_c(\chi) = \sum_{a=1}^{\infty} c(1 - c)^{a-1} \frac{f_c(\chi - 2\Psi(\chi) + 2ak + 2\phi)}{\delta^2 + 2\,|\Delta|\,\delta \cos \chi + \Delta^2}, \tag{27}$$

where $\int_0^{2\pi} f_c(\chi)\, d\chi = 1$. The limiting form for

$$\alpha(\omega, Q, c) = \lim_{N\to\infty} -N^{-1} \sum_{n=1}^{N} \ln(|\hat{g}_n|),$$

when expressed in terms of $f_c(\chi)$, is

$$\begin{aligned}&\alpha(\omega, Q, c) \\ &\quad = -\int_0^{2\pi} f_c(\chi) \ln(\delta + |\Delta|\, e^{i\chi})\, d\chi \\ &\quad = -\tfrac{1}{2}\int_0^{2\pi} f_c(\chi) \ln(\delta^2 + 2\,|\Delta|\,\delta \cos \chi + \Delta^2)\, d\chi.\end{aligned} \tag{28}$$

Before considering various solutions of the functional equation (27) in the next section, we note that in the limit $c \to 0$ the sum over a in Eq. (27) is proportional[3] to the integral of $f_0(\chi - 2\Psi(\chi) + \beta + 2\phi)$ over the interval $0 \le \beta \le 2\pi$ (provided that k is not a rational fraction of π). In particular,

$$\begin{aligned}\lim_{c\to 0} \sum_{a=1}^{\infty} c(1 - c)^{a-1} f_c(\chi - 2\Psi(\chi) + 2ak + 2\phi) \\ = \frac{1}{2\pi}\int_0^{2\pi} f_0(\chi - 2\Psi(\chi) + \beta + 2\phi)\, d\beta.\end{aligned} \tag{29}$$

The range of integration in Eq. (29) covers a complete period of the argument and so the right-hand side of Eq. (29) is simply $(2\pi)^{-1}$. Therefore, in the limit $c \to 0$, the functional equation reduces to the simple form

$$f_0(\chi) = (2\pi)^{-1}(\delta^2 + 2\,|\Delta|\,\delta \cos \chi + \Delta^2)^{-1}, \tag{30}$$

provided that k is not a rational fraction of π. The foregoing restriction on the values of k is obviously necessary in the case where the condition for the existence of Matsuda's special frequencies is satisfied.[1,2]

It can be verified readily by substitution of (30) in Eq. (28) that[4]

$$\begin{aligned}\lim_{c\to 0} \alpha(\omega, Q, c) \\ = -\frac{1}{4\pi}\int_0^{2\pi} \frac{\ln(\delta^2 + 2\,|\Delta|\,\delta \cos \chi + \Delta^2)}{\delta^2 + 2\,|\Delta|\,\delta \cos \chi + \Delta^2}\, d\chi \\ = \ln \delta.\end{aligned} \tag{31}$$

This result for $\alpha(\omega, Q, 0^+)$, which was obtained in a slightly different way in R1, expresses the physical fact that when the average nearest-neighbor spacing in a random array of defects is large compared to the incident wavelength, the defects each scatter independently.

The form of the functional equation which is most convenient for analysis in the next section is a functional equation for

$$F_c(\chi) = \int_0^{\chi} f_c(\chi)\, d\chi.$$

This new functional equation is obtained directly by integrating both sides of Eq. (25) from 0 to χ:

$$F_c(\chi) = \sum_{a=1}^{\infty} c(1-c)^{a-1} \int_{2ak+2\phi}^{\chi-2\Psi(\chi)+2ak+2\phi} f_c(\chi)\, d\chi$$
$$= \sum_{a=1}^{\infty} c(1-c)^{a-1} \times \{F_c[\chi - 2\Psi(\chi) + 2ak + 2\phi] - F_c[2ak + 2\phi]\}. \quad (32)$$

An expression for $\alpha(\omega, Q, c)$ in terms of $F_c(\chi)$ can be obtained by integrating Eq. (28) by parts to obtain

$$\alpha(\omega, Q, c) = -\ln(\delta + |\Delta|) - \Delta\delta \int_0^{2\pi} F_c(\chi) \left(\frac{\sin\chi}{\delta^2 + 2|\Delta|\,\delta\cos\chi + \Delta^2} \right) d\chi. \quad (33)$$

In the limit $c \to 0$,

$$F_0(\chi) = (2\pi)^{-1}[\chi - 2\Psi(\chi)]. \quad (34)$$

3. SOLUTION OF FUNCTIONAL EQUATION

In this section we first treat a special case in which it is possible to obtain exact values of the solution of the functional equation (33) for $F_c(\chi)$. Next, an approximate solution of Eq. (33) is obtained which is an expansion in the parameter $c^{-1}\omega$, the mean spacing between defects divided by the wavelength of the incident wave. Satisfactory agreement between the first-order solution in $c^{-1}\omega$ and Monte Carlo estimates are obtained. Finally, a numerical procedure for solving Eq. (33) is outlined and a comparison is made between the numerical solution in several representative cases and Monte Carlo estimates.

A. Exact Values of $F_c(\chi)$ in Case $k = \frac{1}{2}\pi$, $Q = 1$

We consider the case $k = \frac{1}{2}\pi$, $Q = 1$. It was shown in R1 that in this case the $\hat{g}_n$ generated by the transformation (19) are limited to segments of the circumference of the circle K_0 (Fig. 1) which lie inside the unit circle U. This fact is used to derive values of $F_c(\chi)$ from the functional equation (33). The same arguments apply if $Q > 1$; however, the details become more involved. For this reason, we treat only the case $Q = 1$.

The transformation (19) can be regarded as a product of two transformations. First, the denominator in (19) is formed by rotating the difference vector $\delta - \hat{g}_{n-1}$ through the angle $-(a_n\pi + 2\phi) = -(a_n + \frac{1}{2})\pi$ and then adding the resulting vector to δ. Note that the angle of rotation assumes only two values, modulo 2π, depending upon whether a_n is odd or even. Second, the reciprocal of the vector $\delta + (\delta - \hat{g}_{n-1})e^{-(a_n+\frac{1}{2})\pi i}$ is formed. Figure 2(a) shows the circles U and K_0 and the result of the first transformation. Points on the arc ABC are shifted to corresponding points on the arc $A_oB_oC_o$ if a_n is odd and to points on $A_eB_eC_e$ if a_n is even. Figure 2(b) shows several stages in the second transformation. The reciprocal of a point such as B_e in Fig. 2(a) is located geometrically by first forming its mirror image B_e' in the line OX. The reciprocal of B_e is then located at B_e'', the intersection of OB_e' with circle K_0.[5] The two images of the arc ABC, $A_o''B_o''C_o''$ and $A_e''B_e''C_e''$, are contained in the arc ABC. Since the starting value $\hat{g}$ corresponds to the point A, all subsequent values of $\hat{g}_n$ must be located either in the arc $A_o''B_o''C_o''$ or $A_e''B_e''C_e''$. No $\hat{g}_n$ appear in the arc $A_o''BC_e''$. Clearly, there will be images of this gap $A_o''BC_e''$ in the $\hat{g}$ distribution around the points B_o'' and B_e''. Images of these images also coincide with gaps in the $\hat{g}$ distribution and so on.

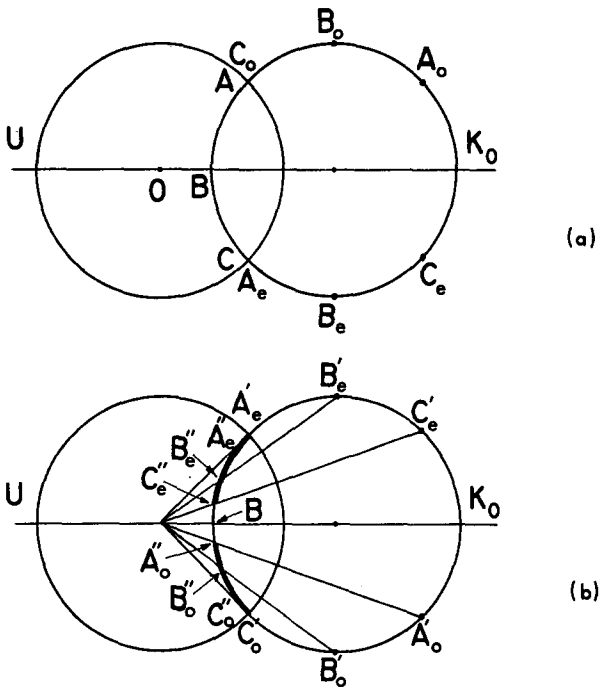

FIG. 2. Two stages of the transformation in Eq. (19) in case $k = \frac{1}{2}\pi$ and $Q = 1$.

We now consider the functional equation (33) in the present case. There is a considerable simplification because the difference $F_c[\chi - 2\Psi(\chi) + (2 + \frac{1}{2})\pi] - F_c[(a + \frac{1}{2})\pi]$, which is a periodic function of χ with period 2π, assumes one of two values depending upon whether a is odd or even. The functional equation reduces to

$$F_c[\chi] = (2-c)^{-1}\{F_c[\chi - 2\Psi(\chi) + \tfrac{3}{2}\pi] - F_c[\tfrac{3}{2}\pi]\} + (1-c)(2-c)^{-1} \times \{F_c[\chi - 2\Psi(\chi) + \tfrac{1}{2}\pi] - F_c[\tfrac{1}{2}\pi]\}, \quad (35)$$

for $0 < \chi < 2\pi$, where

$$\Psi(\chi) = \tan^{-1}[\sin\chi/(2^{\frac{1}{2}} + \cos\chi)] \leq \tfrac{1}{4}\pi.$$

Since the $\hat{g}_n$ are confined to portions of the arc ABC, the integral distribution function $F_c[\chi]$ has the values

$$F_c[\chi] = 0, \quad 0 < \chi \leq \tfrac{3}{4}\pi,$$
$$= 1, \quad \tfrac{5}{4}\pi < \chi \leq 2\pi + \tfrac{3}{4}\pi.$$

As a result, Eq. (35) can be rewritten as

$$F_c[\chi] = (2-c)^{-1}\{F_c[\chi - 2\Psi(\chi) + \tfrac{3}{2}\pi] - 1\} + (1-c)(2-c)^{-1}F_c[\chi - 2\Psi(\chi) + \tfrac{1}{2}\pi], \quad 0 < \chi < 2\pi. \quad (36)$$

As χ increases from $\frac{3}{4}\pi$ to π to $\frac{5}{4}\pi$, the two arguments of $F_c[\ ]$ on the right-hand side of Eq. (36), $\chi - 2\Psi(\chi) + \frac{3}{2}\pi$ for odd a and $\chi - 2\Psi(\chi) + \frac{1}{2}\pi$ for even a, increase from $\frac{7}{4}\pi$ to $2\pi + \frac{1}{2}\pi$ to $2\pi + \frac{5}{4}\pi$ and from $\frac{3}{4}\pi$ to $\frac{3}{2}\pi$ to $2\pi + \frac{1}{4}\pi$, respectively. Thus, it can be seen that Eq. (36) is equivalent to the following set of relations:

$$F_c(\chi) = 0, \quad 0 < \chi < \tfrac{3}{4}\pi, \quad (37a)$$
$$= (1-c)(2-c)^{-1}F_c[\chi - 2\Psi(\chi) + \tfrac{1}{2}\pi], \quad \tfrac{3}{4}\pi < \chi < \chi_1, \quad (37b)$$
$$= (1-c)(2-c)^{-1}, \quad \chi_1 < \chi < \chi_2, \quad (37c)$$
$$= (2-c)^{-1}\{F_c[\chi - 2\Psi(\chi) + \tfrac{3}{2}\pi] + 1\} + (1-c)(2-c)^{-1}, \quad \chi_2 < \chi < \tfrac{5}{4}\pi, \quad (37d)$$
$$= 1, \quad \tfrac{5}{4}\pi < \chi < 2\pi. \quad (37e)$$

In Eqs. (37) the angle χ_1 is defined by the condition $\chi_1 - 2\Psi(\chi_1) + \frac{1}{2}\pi = \frac{5}{4}\pi$ and χ_2 by the condition $\chi_2 - 2\Psi(\chi_2) + \frac{3}{2}\pi = 2\pi + \frac{3}{4}\pi$. The angles χ_1 and χ_2 correspond to the limits of the principal gap in the $\hat{g}$ distribution, arc $A_0''BC_e''$ in Fig. 2(b).

We next determine the limits of the subinterval of the interval $(\frac{3}{4}\pi, \pi)$ for which the argument $\chi - 2\Psi(\chi) + \frac{1}{2}\pi$ lies in the range χ_1 to χ_2. The limits of this subinterval are determined by the conditions

$$\chi_3 - 2\Psi(\chi_3) + \tfrac{1}{2}\pi = \chi_1,$$

and

$$\chi_4 - 2\Psi(\chi_4) + \tfrac{1}{2}\pi = \chi_2.$$

Thus, for $\frac{3}{4}\pi < \chi_3 < \chi < \chi_4 < \pi$,

$$F_c(\chi) = [(1-c)(2-c)^{-1}]^2, \quad (38)$$

and the interval (χ_3, χ_4) corresponds to the image of the gap interval $A_0''BC_e''$ around the point B_e''. Similarly, for $\pi < \chi < \frac{5}{4}\pi$ there is a subinterval $\pi < \chi_5 < \chi < \chi_6 < \frac{5}{4}\pi$ corresponding to the image of the gap $A_0''BC_e''$ around B_0'', where

$$\chi_5 - 2\Psi(\chi_5) + \tfrac{3}{2}\pi = 2\pi + \chi_1$$

and

$$\chi_6 - 2\Psi(\chi_6) + \tfrac{3}{2}\pi = 2\pi + \chi_2.$$

In the interval (χ_5, χ_6),

$$F_c[\chi] = \frac{1}{2-c}\left(1 + \frac{1-c}{2-c} - 1\right) + \frac{1-c}{2-c} = \frac{(1-c)(3-c)}{(2-c)^2}. \quad (39)$$

The intervals (χ_3, χ_4) and (χ_5, χ_6) are symmetrically located with respect to the angle π. The above procedure can be continued indefinitely to give additional, exact values of $F_c[\chi]$.

There is, in addition, a pair of angles $\chi = \pi - \lambda_1$ and $\chi = \pi + \lambda_2$ which satisfy the conditions

$$\pi - \lambda_1 - 2\Psi(\pi - \lambda_1) + \tfrac{1}{2}\pi = \pi + \lambda_2 \quad (40)$$

and

$$\pi + \lambda_2 - 2\Psi(\pi + \lambda_2) + \tfrac{3}{2}\pi = 2\pi + \pi - \lambda_1. \quad (41)$$

In the present case where $Q = 1$, there is a symmetry with respect to the angle π so that $\lambda_1 = \lambda_2 = \lambda$ in (40) and (41). The value of λ obtained from (40) or (41) is $\frac{1}{12}\pi$. Thus, from Eqs. (37b) and (37d), we obtain

$$F_c[\pi - \tfrac{1}{12}\pi] = [(1-c)(2-c)^{-1}]F_c[\pi + \tfrac{1}{12}\pi] \quad (42)$$

and

$$F_c[\pi + \tfrac{1}{12}\pi] = (2-c)^{-1}\{1 + F_c[\pi - \tfrac{1}{12}\pi] - 1\} + (1-c)(2-c)^{-1}. \quad (43)$$

Equations (42) and (43) constitute a pair of simultaneous equations whose solution is

$$F_c[\pi - \tfrac{1}{12}\pi] = (1-c)^2(3 - 3c + c^2)^{-1}, \quad (44)$$

$$F_c[\pi + \tfrac{1}{12}\pi] = (1-c)(2-c)(3 - 3c + c^2)^{-1}. \quad (45)$$

Once these exact values have been determined from Eqs. (37b) and (37d), additional exact values of $F_c[\chi]$ can be generated with the aid of the same relations.

In this section, we have determined some exact values of $F_c[\chi]$ from the functional equation (32). For purposes of comparison, we present some numerical results of the calculation of $F_c[\chi]$ for a particular random configuration of 10^5 defects in the case $c = 0.375$, $Q = 1$, $\omega = 2^{-\frac{1}{2}}$. The χ_n are formed recursively using Eq. (21), which in the present case reduces to

$$e^{i\chi_n} = \left(\frac{2^{\frac{1}{2}} - e^{-i\chi_{n-1}+i(a_n+\frac{1}{2})\pi}}{2^{\frac{1}{2}} - e^{i\chi_{n-1}-i(a_n+\frac{1}{2})\pi}}\right)e^{i\chi_{n-1}-i(a_n+\frac{1}{2})\pi}, \quad (21')$$

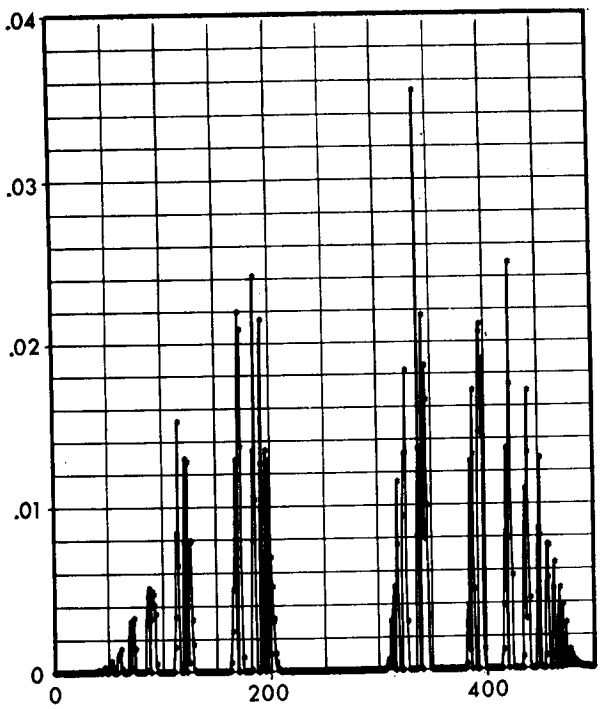

FIG. 3. Distribution of values of the χ_n for a particular disordered array of 10^5 defects in the case $c = 0.375$, $Q = 1$, $\omega = 2^{-\frac{1}{2}}$. The range of values of the χ_n is $\frac{3}{4}\pi$ to $\frac{5}{4}\pi$. This range is divided into 500 equal intervals and the fraction of χ_n contained in each interval is plotted as a function of the interval number.

with $\chi_1 = \frac{3}{4}\pi$. All of the calculations described here and in succeeding sections were performed on a CDC 6600 at the Los Alamos Scientific Laboratory. A sequence of random integer values of the spacings is generated in which each spacing a_n has the frequency distribution $c(1-c)^{a_n}$. As each value of a_n, $n = 2, \cdots, N$, is generated, a value of χ_n is determined from Eq. (21′). The values of χ_n are limited to the range $\frac{3}{4}\pi \leq \chi \leq \frac{5}{4}\pi$. This range has been divided into 500 equal intervals, and a count is made of the fraction of all values of χ_n which either lie in a given interval or to the left of that interval. The results of this count are presented in Figs. 3 and 4. In Fig. 3 the fraction of the values of χ_n in each interval is plotted as a function of the interval number from 1 to 500. In Fig. 4, the Monte Carlo estimate of $F_c[\chi]$, the fraction of values lying in or to the left of a given interval is plotted as a function of the interval number. The principal gap region and a number of its images can be clearly seen in these figures. The differences between the exact values of $F_c[\chi]$ in the principal gap regions, Eqs. (37c), (38), and (39), and their Monte Carlo estimates in the case shown in Figs. 3 and 4 are of the order of the relative root-mean-square fluctuation $\{1 - F_c[\chi]\}^{\frac{1}{2}}N^{-\frac{1}{2}}$.

B. An Approximate Solution of the Functional Equation for $F_c[\chi]$

An approximate solution of the functional equation (32) can be obtained if the average of the argument appearing on the right-hand side is close to χ, i.e., if

$$|\Psi(\chi)| + c^{-1}k + |\phi| \ll \pi. \tag{46}$$

Since $k = 2\sin^{-1}\omega$, $\phi = \tan^{-1}[Q\tan(\frac{1}{2}k)]$, and $|\phi^{-1}\Psi(\chi)| \ll 1$, Eq. (46) is essentially a condition that the frequency is small. Although frequency is a natural expansion parameter, it is convenient in our calculation to take ϕ as the expansion parameter and rewrite (46) as

$$2|\phi|(1 + c^{-1}|Q|^{-1}) \ll \pi. \tag{47}$$

When condition (47) is satisfied, the integral distribution functions on the right-hand side of (32) can be expanded in a Taylor series (assuming that the derivatives exist). The result is

$$\begin{aligned} F_c[\chi] = \sum_{a=1}^{\infty} & c(1-c)^{a-1} \\ & \times \{F_c[\chi] + 2[ak + \phi - \Psi(\chi)]f_c[\chi] \\ & + 2[ak + \phi - \Psi(\chi)]^2 f_c'[\chi] + \cdots \\ & - 2[ak + \phi]f_c[0] - 2[ak + \phi]^2 f_c'[0] - \cdots\}. \end{aligned} \tag{48}$$

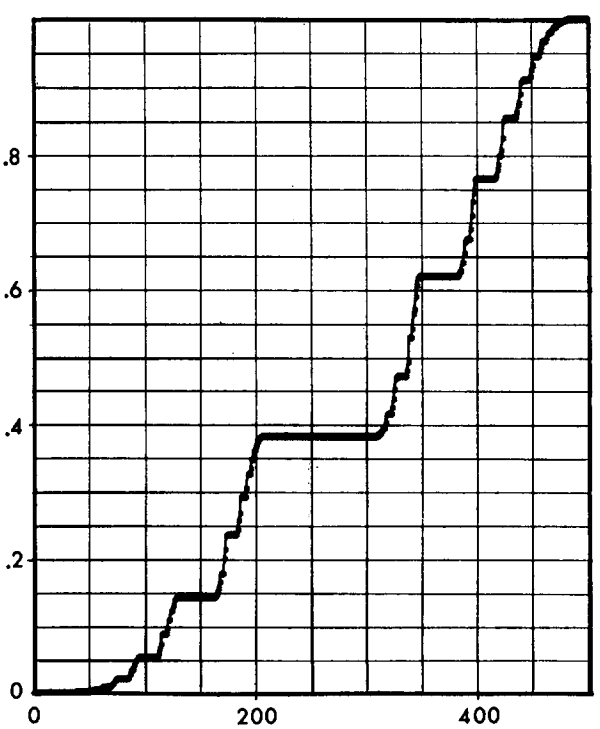

FIG. 4. Plot of the Monte Carlo estimate of the distribution of values of the χ_n for the case shown in Fig. 3: $c = 0.375$, $Q = 1$, $\omega = 2^{-\frac{1}{2}}$, and $N = 10^5$. The fraction of values of the χ_n lying in or to the left of each interval is plotted as a function of the interval number from 1 to 500.

The terms containing $F_c[\chi]$ in Eq. (48) cancel, and the coefficient of the mth derivative of $f_c[\chi]$ is of the order ϕ^m. If Eq. (48) is rearranged so that $f_c[\chi]$ is expressed in terms of $f_c[0]$ and derivatives of $f_c[\chi]$, we obtain

$$f_c[\chi] = \frac{1+b}{1+b-\phi^{-1}\Psi(\chi)} f_c[0] - \phi\left[\left(\frac{[1+b-\phi^{-1}\Psi(\chi)]^2 + b^2(1-c)}{1+b-\phi^{-1}\Psi(\chi)}\right) f_c'[\chi] - \left(\frac{(1+b)^2 + b^2(1-c)}{1+b-\phi^{-1}\Psi(\chi)}\right) f_c'[0]\right] - \cdots, \quad (49)$$

where $b = kc^{-1}\phi^{-1}$. The first two terms in the expansion of the parameter b in powers of ϕ are

$$b = 2c^{-1}\phi^{-1}\tan^{-1}(Q^{-1}\tan\phi) \cong b_0 + \tfrac{1}{3}b_0(1-Q^{-2})\phi^2 + \cdots, \quad (50)$$

where $b_0 = 2c^{-1}Q^{-1}$. The coefficient of $f_c[0]$ in Eq. (49) is expressible as a power series in ϕ [see Eq. (24)]. The first two terms in the expansion are

$$\frac{1+b}{1+b-\phi^{-1}\Psi(\chi)} = \frac{1+b_0}{1+b_0-\epsilon(Q)\sin\chi} - \frac{(1+b_0)\sin\chi\cos\chi}{[1+b_0-\epsilon(Q)\sin\chi]^2}\phi + \cdots, \quad (51)$$

where

$$\epsilon(Q) = \begin{cases} 1, & Q > 0, \\ -1, & Q < 0. \end{cases}$$

A zeroth-order approximation for $f_c[\chi]$ can be obtained by substituting the ϕ independent term in Eq. (51) for the coefficient of the first term in Eq. (49). An expression for $f_c[\chi]$ correct through the first order in ϕ can be obtained by substituting the first two terms in Eq. (51) for the coefficient of $f_c[0]$ in Eq. (49) and by replacing the derivatives, $f_c'[\chi]$ and $f_c'[0]$, by their zeroth-order approximations. The result is

$$f_c[\chi] = (1+b_0)f_c[0]\left[\frac{1}{1+b_0-\epsilon(Q)\sin\chi} - \frac{\sin\chi\cos\chi}{[1+b_0\epsilon(Q)\sin\chi]^2}\phi - \phi\left(\frac{\epsilon(Q)\cos\chi}{1+b_0-\epsilon(Q)\sin\chi} + \frac{b_0^2(1-c)\epsilon(Q)\cos\chi}{[1+b_0-\epsilon(Q)\sin\chi]^3} - \frac{\epsilon(Q)}{1+b_0-\epsilon(Q)\sin\chi} - \frac{b_0^2(1-c)\epsilon(Q)/(1+b_0)^2}{1+b_0-\epsilon(Q)\sin\chi}\right)\right]. \quad (52)$$

The expression (52) for $f_c[\chi]$ contains the constant $f_c[0]$ which can be determined from the normalization condition $\int_0^{2\pi} f_c[\chi]\,d\chi = 1$. The terms containing the single factor $\cos\chi$ in the numerator in Eq. (52) give a zero contribution to the normalization condition. The value obtained for $f_c(0]$ is then

$$f_c[0] = \tfrac{1}{2}\pi\frac{[b_0(2+b_0)]^{\frac{1}{2}}}{|1+b_0|}\left[1 - |\phi|\left(1 + \frac{b_0^2(1-c)}{(1+b_0)^2}\right)\right]. \quad (53)$$

The expression for $f_c[\chi]$ can be substituted in Eq. (28) to calculate the value of $\alpha(\omega, Q, c)$, the average contribution of a defect to the attenuation of the incident wave. In the limit being considered, the logarithmic term in Eq. (28) can be expanded in powers of ϕ:

$$\alpha(\omega, Q, c) = -\tfrac{1}{2}\int_0^{2\pi} f_c(\chi) \times \ln(\sec^2\phi + 2\tan|\phi|\sec\phi\cos\chi + \tan^2\phi)\,d\chi \cong -\int_0^{2\pi} f_c(\chi)(|\phi|\cos\chi + \phi^2\sin^2\chi)\,d\chi. \quad (54)$$

When the expression for $f_c[\chi]$ in Eqs. (52) and (53), correct to the first order in ϕ, is substituted in Eq. (54), the resulting value of $\alpha(\omega, Q, c)$ will be correct through the second order in ϕ. The result is

$$\alpha(\omega, Q, c) \cong \tfrac{1}{2}\phi^2 b_0(1-c)(2+b_0)^{-1}$$

or

$$\alpha(\omega, Q, c) \cong \tfrac{1}{2}(1-c)(1+cQ)^{-1}Q^2\omega^2, \quad (55)$$

where $\phi^2 \cong Q^2\omega^2$.

It should be recalled that the value of $\alpha(\omega, Q, c)$ in Eq. (55) is an approximate one based on the condition that

$$2|\phi|(1 + c^{-1}|Q|^{-1}) \ll \pi. \quad (47)$$

When this condition is satisfied for a particular set of values of ω', Q', and c', it is clearly satisfied for all values of the concentration $c' \leq c < 1$. It should be expected on physical grounds that in the limit $c \to 1$, the roles of the host and defect atoms are interchanged. That is, it should be expected that the inhomogeneities which contribute to the reflection of the incident wave are isolated host atoms (mass m) in a background of defect atoms (mass M). To verify this expectation, we consider the average attenuation coefficient for N defects

$$N\alpha(\omega, Q, c) = \tfrac{1}{2}(1-c)A_N(1+cQ)^{-1}Q^2\omega^2(NA_N^{-1}). \quad (56)$$

In Eq. (56), $NA_N^{-1} = c$ and $(1-c)A_N = N_h$, the number of host particles (mass m) between 0 and A_N.

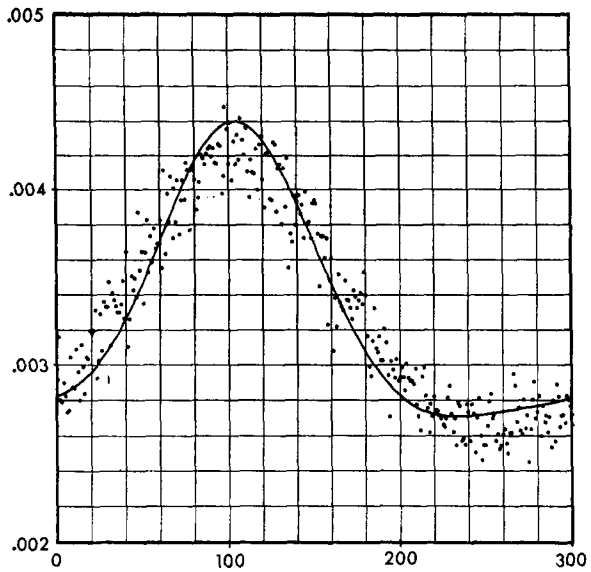

FIG. 5. Distribution of values of the χ_n for a particular disordered array of $N = 2 \times 10^5$ defects in the case $c = 0.5$, $Q = 1$, $\omega = 0.1$. The range of the χ_n, which is 0 to 2π, is divided into 301 equal intervals and the fraction of the χ_n contained in each interval is plotted with an asterisk as a function of the interval number. The solid curve is a plot of the expression for $f_c[\chi]$ in Eq. (52).

[The concentration of host atoms is $c_h = N_h A_N^{-1} = 1 - c$.] So, in the limit $c \to 1$,

$$N\alpha(\omega, Q, 1^-) = N_h \tfrac{1}{2} Q^2 \omega^2 (1 + Q)^{-1}, \qquad (57)$$

and $\frac{1}{2}Q^2\omega^2(1 + Q)^{-1}$ is the average contribution per host atom to the attentuation of the incident wave. In the limit $c \to 1$, the concentration of host atoms c_h in the disordered section of crystal approaches zero, and the mean spacing between host atoms is large compared to the incident wavelength. We have shown in R1 and in Eq. (31) that if the host particles have mass M and the defect particles have mass m and their concentration is c_h, then

$$\lim_{c_h \to 0} \alpha(\tilde{\omega}, Q, c_h) = \ln \delta \cong \tfrac{1}{2} Q^2 \tilde{\omega}^2, \quad |\phi| \ll 1, \qquad (58)$$

where $\tilde{\omega}$ is the frequency of the incident wave measured in units of the maximum frequency in a perfect crystal composed of atoms of mass M. If, instead, frequency is measured in units of the maximum frequency of a perfect crystal composed of atoms of mass m, Eq. (58) can be written as

$$\lim_{c_h \to 0} \alpha(\omega, Q, c_h) \cong \tfrac{1}{2} Q^2 \omega^2 (mM^{-1}) \cong \tfrac{1}{2} Q^2 \omega^2 (1 + Q)^{-1}, \quad Q\omega \ll 1. \qquad (59)$$

Combining Eqs. (57) and (59), we have the expected result

$$N\alpha(\omega, Q, c = 1^-) = N_h \alpha(\omega, Q, c_h = 0^+), \quad Q\omega \ll 1. \qquad (60)$$

This result ought to hold over the entire frequency range instead of being limited by the condition $Q\omega \ll 1$. A proof of this result for arbitrary values of ω will most likely have to start with the determinantal expression (14) for $\hat{T}_N$.

The normalized expression for $f_c[\chi]$ in Eqs. (52) and (53) should be compared with the expansion obtained for $\lim_{c \to 0} f_c[\chi]$ from Eq. (30)

$$\lim_{c \to 0} f_c[\chi] \cong (2\pi)^{-1}[1 - 2|\phi| \cos \chi]. \qquad (61)$$

The zeroth-order terms in ϕ are, respectively,

$$(2\pi)^{-1}[b_0(2 + b_0)]^{\frac{1}{2}}(|1 + b_0| - \sin \chi)^{-1} \quad \text{and} \quad (2\pi)^{-1}.$$

In view of the foregoing difference, it must be regarded as fortuitous that if the condition (47) is ignored and c is set equal to zero in Eq. (55), the correct value is obtained for $\lim \alpha(\omega, Q, c) \cong \frac{1}{2}Q^2\omega^2$, as $c \to 0$.

Finally, for two sets of values of ω, Q, and c, we compare the numerical value of the expression (52) for $f_c[\chi]$ with a Monte Carlo estimate of the same distribution. The procedure for generating a sequence of values of χ_n has already been outlined in Sec. 3A. In the present cases, the range of χ_n, which is 0 to 2π, is divided into 301 intervals. For arrays of 2×10^5 defects, the fraction of the χ_n which fall in each interval is determined. In Fig. 5 for the case $c = 0.5$, $Q = 1$, $\omega = 0.1$, the fraction of the χ_n in each interval are plotted as a function of the interval number 0 to 300 where interval number 0 is the

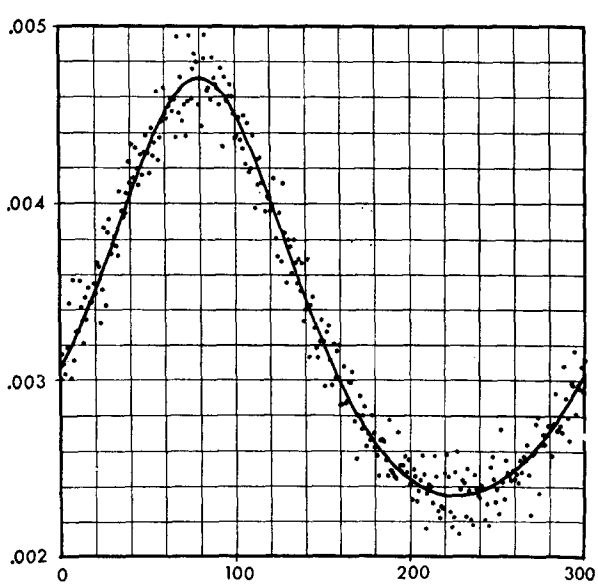

FIG. 6. Distribution of values of the χ_n for a particular disordered array of $N = 2 \times 10^5$ defects in the case $c = 0.5$, $Q = 2$, $\omega = 0.01$. The range of the χ_n, which is 0 to 2π, is divided into 301 equal intervals and the fraction of the χ_n contained in each interval is plotted with an asterisk as a function of the interval number. The solid curve is a plot of the expression for $f_c[\chi]$ in Eq. (52).

interval near $\chi = 0$. Each value is plotted with an asterisk. The solid curve is a plot of the expression for $f_c[\chi]$ in Eq. (52), the distribution function of values of χ_n on the circle K_0 derived from the functional equation (32). The first-order correction to $f_c^{(0)}[\chi]$ is relatively large in this case: $f_c^{(1)}[0] \cong -0.12 f_c^{(0)}[0]$, $f_c^{(1)}[\pi] \cong +0.12 f_c^{(0)}[\pi]$, and $f_c^{(1)}[\frac{1}{2}\pi] = f_c^{(1)}[\frac{3}{2}\pi] = 0$. Nevertheless, the correspondence between the curve and the distribution of Monte Carlo points is close. The order of magnitude of the scatter in the Monte Carlo points is roughly that expected for a sample size of 2×10^5. A similar comparison is presented in Fig. 6 for the case $c = 0.5$, $Q = 2$, $\omega = 0.01$ and $N = 2 \times 10^5$. In this case, the first-order correction to $f_c^{(0)}[\chi]$ is one-fifth as large as in the previous case; and, the correspondence between the curve representing $f_c[\chi]$ and the Monte Carlo points is closer.

C. An Iterative Method for Obtaining Numerical Solutions of the Functional Equation for $F_c[\chi]$

We now describe an iterative method for obtaining numerical solutions of the functional equation

$$F_c[\chi] = \sum_{a=1}^{\infty} c(1-c)^{a-1}\{F_c[\chi - 2\Psi(\chi) + 2ak + 2\phi] - F_c[2ak + 2\phi]\}. \quad (32)$$

The method is based on the assumption that we have an approximate solution $F_c^{(n)}[\chi]$ of Eq. (32) and that we can construct a more accurate solution $F_c^{(n+1)}[\chi]$ with the aid of Eq. (32)

$$F_c^{(n+1)}[\chi] = \sum_{a=1}^{\infty} c(1-c)^{a-1}\{F_c^{(n)}[\chi - 2\Psi(\chi) + 2ak + 2\phi] - F_c^{(n)}[2ak + 2\phi]\}. \quad (62)$$

Then, repeated use of Eq. (62) will result in the convergence of $F_c^{(n+1)}[\chi]$ to the exact solution $F_c[\chi]$ of Eq. (32). In our numerical calculations we have found that $F_0[\chi]$ in Eq. (34), the solution of Eq. (32) in the limit $c = 0$, is a suitable starting choice for the iteration process, i.e.,

$$F_c^{(0)}[\chi] = (2\pi)^{-1}[\chi - 2\Psi(\chi)]. \quad (63)$$

In practice, divide the fundamental interval $0 \leq \chi \leq 2\pi$ into M equal subintervals

$$[2\pi(m-1)M^{-1}, 2\pi m M^{-1}], \quad m = 1, \cdots, M. \quad (64)$$

We evaluate the starting function $F_c^{(0)}[\chi]$ at the points

$$\chi_m = 2\pi(m - \tfrac{1}{2})M^{-1}, \quad m = 1, \cdots, M.$$

Then, for a given set of parameters ω, Q, c, we evaluate the two arguments on the right-hand side of Eq. (62) at the points

$$\chi_m = 2\pi(m - \tfrac{1}{2})M^{-1}, \quad m = 1, \cdots, M,$$

for all values of a such that

$$c(1-c)^{a-1} < 10^{-11}. \quad (65)$$

Each value of the two arguments is reduced, modulo 2π, to the fundamental interval, and the subinterval in which the reduced value lies is determined. If the subinterval is $[2\pi(s-1)M^{-1}, 2\pi s M^{-1}]$, then the reduced argument is identified with subintervals. If the reduced value of $\chi_m - 2\Psi(\chi_m) + 2a_1k + 2\phi$ corresponds to subinterval s and the reduced value of $2a_1k + 2\phi$ to subinterval t with $s > t$, then the difference

$$F_c^{(0)}[\chi_m - 2\Psi(\chi_m) + 2a_1k + 2\phi] - F_c^{(0)}[2a_1k + 2\phi]$$

is assigned the value

$$F_c^{(0)}[\chi_s(m, a_1)] - F_c^{(0)}[\chi_t(a_1)].$$

However, if $s < t$, the difference $F_c^{(0)}[\chi_m - 2\Psi(\chi_m) + 2a_1k + 2\phi] - F_c^{(0)}[2a_1k + 2\phi]$ is assigned the value

$$1 + F_c^{(0)}[\chi_s(m, a_1)] - F_c^{(0)}[\chi_t(a_1)].$$

With the above assignments, a new set of values $F_c^{(1)}[\chi_m]$ is determined by using Eq. (62) and summing over all a satisfying condition (65). This procedure is repeated until the set of values $F_c^{(n+1)}[\chi_m]$ is sufficiently close to the set $F_c^{(n)}[\chi_m]$.

Finally, for two cases we present a comparison of the solution of the functional equation with Monte Carlo estimates of the distribution of values of χ_n. In Fig. 7, for the case $c = 0.5$, $Q = 1$, $\omega = 0.3$, and

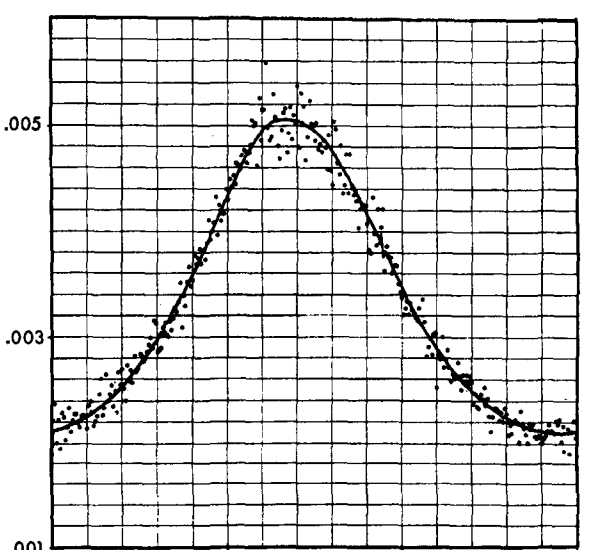

FIG. 7. Distribution of values of the χ_n for a particular disordered array of $N = 2 \times 10^5$ defects in the case $c = 0.5$, $Q = 1$, $\omega = 0.3$. The range of the χ_n, which is 0 to 2π, is divided into 301 equal intervals and the fraction of the χ_n contained in each interval is plotted with an asterisk as a function of the interval number. The solid curve is a plot of values of $F_c[\chi_m] - F_c[\chi_{m-1}]$ obtained from the iterative solution of functional equation (32), where m is the interval number.

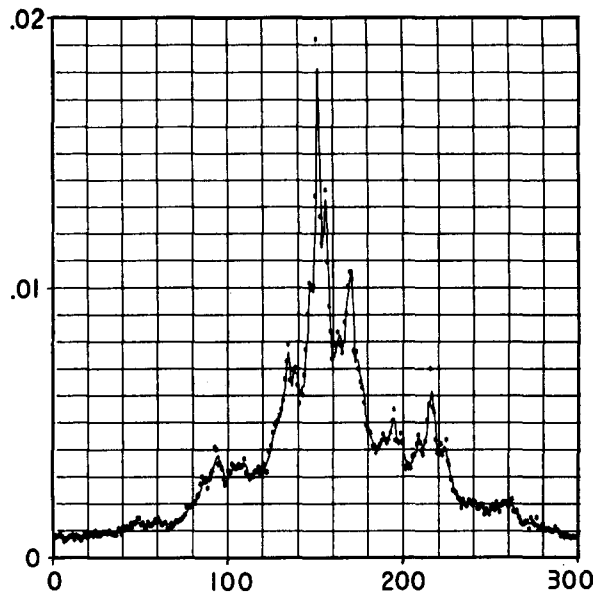

FIG. 8. Distribution of values of the χ_n for a particular disordered array of $N = 2 \times 10^5$ defects in the case $c = 0.5$, $Q = 1$, $\omega = \sin \frac{1}{5}\pi$. The range of the χ_n, which is 0 to 2π, is divided into 301 equal intervals and the fraction of the χ_n contained in each interval is plotted with an asterisk as a function of the interval number. The solid curve is a plot of values of $F_c[\chi_m] - F_c[\chi_{m-1}]$ obtained from the iterative solution of functional equation (32), where m is the interval number.

$N = 2 \times 10^5$ and a division of the 0 to 2π range of χ_n into 301 intervals, the fraction of the χ_n in each interval is indicated by an asterisk and is plotted as a function of interval number. The solution obtained from the functional equation for a division of the range of χ into $M = 301$ intervals results in a set of values for $F_c[\chi_m]$. The curve shown in Fig. 7 is a plot of the values of $F_c[\chi_m] - F_c[\chi_{m-1}]$ as a function of the interval number m. The agreement between this curve and the distribution of Monte Carlo points is good. In Fig. 8, we show a similar comparison between the Monte Carlo distribution of values of χ_n and the corresponding distribution obtained from the iterative solution of Eq. (32) in the case $c = 0.5$, $Q = 1$, $\omega = \sin(\frac{1}{5}\pi)$, and $N = 2 \times 10^5$. Even in this case, where the distribution contains several sharp peaks, the agreement is good.[6]

4. REMARK

The principal problem which has motivated the work in R1 and in the present paper is the determination of the limiting value of the Nth root of the transmitted amplitude

$$\lim_{N\to\infty} [T_N^{1/N}(\omega)] = \lim_{N\to\infty} |D_N|^{-1/N} = \exp[-\alpha(\omega, Q, c)].$$

In R1 it was shown that (i) $\alpha(\omega, Q, c) > 0$ for sufficiently small values of c at any given ω for $|Q| > 0$ and (ii) $\alpha[\sin(\pi r/2s), Q, c] > 0$ for all values of c, $0 < c < 1$, and for $Q \geq \cot(\pi/2s)\cot(\pi r/2s)$, where r and s are relatively prime integers. In Sec. 3B of this paper, we show that

$$\alpha(\omega, Q, c) \cong \tfrac{1}{2}(1 - c)(1 + cQ)^{-1}Q^2\omega^2 > 0$$

to the lowest order in $Q\omega$ for $\omega \ll c < 1$, $Q \neq 0$, and $\omega(|Q| + c^{-1}) \ll 1$. We conjectured in R1 that $\alpha(\omega, Q, c) > 0$ for *all* values of the parameters: $0 < \omega < 1$, $Q \neq 0$, and $0 < c < 1$. It may be possible to prove the foregoing conjecture by showing that the solution $F_c[\chi]$ of the functional equation (32) has the property that the value of $\alpha(\omega, Q, c)$ is positive for all the above values of the parameters. Thus far, with the exception of the restricted case treated in Sec. 3B, we have not succeeded in carrying out this program. Moreover, the result for $\alpha(\omega, Q, c)$ in Sec. 3B was derived by first obtaining an explicit expression for the solution of the functional equation.

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Unbounded Local Observables in Quantum Statistical Mechanics

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The algebraic formulation of quantum statistical mechanics is extended so as to include local unbounded observables. We start, in a usual way, with a C^*-algebra $\mathfrak{U}$ of quasilocal bounded observables in Fock space $\mathfrak{H}_F$, an arbitrary, locally normal state ϕ on $\mathfrak{U}$, and a corresponding Gel'fand–Naimark–Segal (GNS) representation R_ϕ of $\mathfrak{U}$ in a Hilbert space $\mathfrak{H}_\phi$. We then construct a set $\mathfrak{Q}_L$ of local, closed operators whose domains are dense in $\mathfrak{H}_F$, such that $\mathfrak{Q}_L$ includes all the local observables of the system. The representation R_ϕ is then extended so as to provide a $*$-homomorphism of $\mathfrak{Q}_L$ into the closed, densely defined operators in $\mathfrak{H}_\phi$. Correspondingly, a number of results previously established for the local bounded observables are extended to the unbounded ones. For appropriate classes of locally normal states, these extended results include the Kubo–Martin–Schwinger boundary conditions, the spatially asymptotic and ergodic properties of space-correlation functions, and the temporally ergodic properties of time-correlation functions. It is also shown that, for locally normal Gibbs states, the time correlations between elements of a specified subset of $\mathfrak{Q}_L$ are thermodynamical limits of the corresponding correlations for finite systems.

1. INTRODUCTION

The algebraic formulation of quantum statistical mechanics has been constructed according to the following scheme[1,2]:

(i) Let Γ be the Euclidean space of a physical system and let L be the set $\{\Lambda\}$ of all bounded subsets of Γ. One assigns to each $\Lambda \in L$ a von Neumann algebra $\mathfrak{U}_\Lambda$ of bounded operators in a Fock space $\mathfrak{H}_F$: this is the algebra generated by the bounded observables for the region Λ. One then defines $\mathfrak{U}$, the C^*-algebra of quasilocal bounded observables, to be the norm closure in $\bigcup_{\Lambda\in L} \mathfrak{U}_\Lambda$.

(ii) The states of the system are represented by positive linear functionals, of unit norm, on $\mathfrak{U}$.

(iii) The Gel'fand–Naimark–Segal (GNS) construction, corresponding to the state ϕ, yields a representation R_ϕ of $\mathfrak{U}$ in a Hilbert space $\mathfrak{H}_\phi$.

The object of the present article is to extend this scheme to local unbounded observables,[3] for cases where the states concerned are locally normal.[4] The restriction to locally normal states is equivalent to the assumption that the probability that any Λ $(\in L)$ contains an infinite number of particles is zero.[4]

The local unbounded observables may be defined as follows: Let $\mathfrak{Q}_\Lambda$ be the set of all closed, densely defined operators affiliated (in Dixmier's sense[5]) to $\mathfrak{U}_\Lambda$ in $\mathfrak{H}_F$ and let $\mathfrak{Q}_L = \bigcup_{\Lambda\in L} \mathfrak{Q}_\Lambda$. The unbounded local observables correspond to the self-adjoint elements of $\bigcup_{\Lambda\in L} (\mathfrak{Q}_\Lambda/\mathfrak{U}_\Lambda)$.

We incorporate $\mathfrak{Q}_L$ into the above algebraic scheme by constructing an extension of R_ϕ so that it provides a $*$-homomorphism of $\mathfrak{Q}_L$ into the closed, densely defined operators in $\mathfrak{H}_\phi$. This construction may be summarily described as follows. For $\Lambda \in L$, the space $\mathfrak{H}_F$ may be expressed[2] as a completed tensor product $\tilde{\mathfrak{H}} \,\overline{\otimes}\, \hat{\mathfrak{H}}_\Lambda$, of Hilbert spaces $\tilde{\mathfrak{H}}_\Lambda$ and $\hat{\mathfrak{H}}_\Lambda$, the former being the Fock space for the region Λ. Correspondingly, $\mathfrak{U}_\Lambda = \tilde{\mathfrak{U}}_\Lambda \otimes \hat{I}_\Lambda$, where $\tilde{\mathfrak{U}}_\Lambda$ is an algebra of bounded operators in $\tilde{\mathfrak{H}}_\Lambda$ and $\hat{I}_\Lambda$ is the unit operator in $\hat{\mathfrak{H}}_\Lambda$. Likewise, we show in Sec. 2 (Theorem 2.3) that $\mathfrak{Q}_\Lambda$ can be expressed as a tensor product $\tilde{\mathfrak{Q}}_\Lambda \otimes \hat{I}_\Lambda$, where $\tilde{\mathfrak{Q}}_\Lambda$ is the set of all closed, densely defined operators affiliated to $\tilde{\mathfrak{U}}_\Lambda$ in $\tilde{\mathfrak{H}}_\Lambda$ (of course, our definition of this latter tensor product will require an extension of that generally employed for bounded operators). Assuming ϕ to be locally normal, we may express[4] $\mathfrak{H}_\phi$ as a completed tensor product $\tilde{\mathfrak{H}}_\Lambda \,\overline{\otimes}\, \hat{\mathfrak{H}}_\Lambda$ between two Hilbert spaces $\tilde{\mathfrak{H}}_\Lambda$ and $\hat{\mathfrak{H}}_\Lambda$, in such a way that, if $\tilde{A}_\Lambda \in \tilde{\mathfrak{U}}_\Lambda$ and $A = \tilde{A}_\Lambda \otimes \hat{I}_\Lambda$, then $R_\phi(A) = W_\Lambda \tilde{A}_\Lambda W^{-1} \otimes \hat{\mathfrak{I}}_\Lambda$, where W_Λ is an isometry of $\tilde{\mathfrak{H}}_\Lambda$ onto $\tilde{\mathfrak{H}}_\Lambda$ and $\hat{\mathfrak{I}}_\Lambda$ is the unit operator in $\hat{\mathfrak{H}}_\Lambda$. Correspondingly, if $Q = \tilde{Q}_\Lambda \otimes \hat{I}_\Lambda$, with $\tilde{Q}_\Lambda \in \tilde{\mathfrak{Q}}_\Lambda$, we define

$$R_\phi(Q) = W_\Lambda \tilde{Q}_\Lambda W^{-1} \otimes \hat{\mathfrak{I}}_\Lambda.$$

Thus (Theorem 4.1) we obtain a consistently defined $*$-homomorphism R_ϕ of $\mathfrak{Q}_L$ into the closed, densely defined operators in $\mathfrak{H}_\phi$. Once this homomorphism is constructed, we are able to extend to $\mathfrak{Q}_L$ a number of results previously obtained for $\mathfrak{U}$.

The article is set out as follows. In Sec. 2, we derive a number of properties of closed operators in abstract Hilbert space that will be needed subsequently. In Sec. 3, we define our notation and summarize certain established properties of various classes of states on $\mathfrak{U}$. In Sec. 4, we employ the formalism of Secs. 2 and 3 to extend R_ϕ from $\mathfrak{U}$ to $\mathfrak{U} \cup \mathfrak{Q}_L$.

We then derive corresponding extensions, for appropriate classes of locally normal states, of (i) the Kubo–Martin–Schwinger boundary conditions (Theorem 4.2), (ii) the spatially asymptotic and ergodic properties of space-correlation functions (Theorem 4.3), and (iii) the temporally ergodic properties of time-correlation functions (Theorem 4.4). In Sec. 5 we show that, in the case of locally normal Gibbs states, the time correlations between elements of a certain specified subset of $\mathfrak{A}_L$ are thermodynamical limits of corresponding correlations for finite systems (Theorem 5.1). We also show that equations of motion for elements of this subset may be represented in the GNS space $\mathfrak{H}_\phi$.

2. CLOSED OPERATORS IN HILBERT SPACE

Let $\mathcal{H}$ be a Hilbert space. We denote the domain of an arbitrary operator L in $\mathcal{H}$ by D_L. Also, we denote the set of all bounded operators in $\mathfrak{H}$ by $\mathfrak{B}(\mathcal{H})$.

Let $\mathfrak{Q}^0$ be the set of all closed operators[6] $\{Q\}$ for which D_Q is dense in $\mathcal{H}$. Thus, if $Q \in \mathfrak{Q}^0$, then Q^* and $Q^*Q\ [= (Q^*Q)^*] \in \mathfrak{Q}^0$. We denote the family of spectral projectors for Q^*Q by $\{E_\lambda\}$, i.e., $Q^*Q = \int \lambda\, dE_\lambda$. Also, we denote QE_λ by Q_λ.

Theorem 2.1: Let $Q \in \mathfrak{Q}^0$ and let $\lambda < \infty$. Then:

(i) $E_\lambda \mathcal{H} \subseteq D_Q$.

(ii) $Q_\lambda \in \mathfrak{B}(\mathcal{H})$.

(iii) For fixed $f \in \mathcal{H}$, $\|Q_\lambda f\|$ is a non-decreasing function of λ.

(iv) For fixed $f \in \mathcal{H}$, the following statements are equivalent:

(a) $\|Q_\lambda f\|$ is a bounded function of λ and thus, by (iii), converges to a finite limit as $\lambda \to \infty$,

(b) $Q_\lambda f$ converges strongly as $\lambda \to \infty$,

(c) $f \in D_Q$.

Further, in cases where these conditions are satisfied, $\|Q_\lambda f\| \leq \|Qf\|$, $\forall\, \lambda < \infty$.

(v) $\text{s-lim}_{\lambda\to\infty} Q_\lambda = Q$.

(vi) $\text{s-lim}_{\lambda\to\infty} (Q_\lambda)^* = Q^*$ on D_{Q^*}.

Proof:

(i) It follows from the definition of E_λ that, for $\lambda < \infty$,

$$E_\lambda \mathcal{H} \subseteq D_{Q^*Q} \subseteq D_Q.$$

(ii) Since Q is closed, it follows that $QE_\lambda\ (= Q_\lambda)$ is closed. Further, since $E_\lambda \mathcal{H} \subseteq D_Q$, it follows that $D_{Q_\lambda} = \mathcal{H}$. Hence, Q_λ is a closed operator whose domain is $\mathcal{H}$ and, therefore, $Q_\lambda \in \mathfrak{B}(\mathcal{H})$.

(iii) Let $f \in \mathcal{H}$. Then $\|Q_\lambda f\|^2 = (QE_\lambda f, QE_\lambda f) = (E_\lambda f, Q^*QE_\lambda f) = (E_\lambda f, Q^*QE_\lambda f)$. Hence, since E_λ is a projection operator that commutes with Q^*Q, it follows that

$$\|Q_\lambda f\|^2 = (f, Q^*QE_\lambda f). \tag{2.1}$$

Likewise, if $\lambda < \lambda' < \infty$, then

$$\|(Q_{\lambda'} - Q_\lambda)f\|^2 = (f, Q^*Q(E_{\lambda'} - E_\lambda)f).$$

Therefore,

$$\|Q_{\lambda'}f\|^2 - \|Q_\lambda f\|^2 = \|(Q_{\lambda'} - Q_\lambda)f\|^2\ (\geq 0) \quad \text{if} \quad \lambda < \lambda' < \infty, \tag{2.2}$$

from which it follows that $\|Q_\lambda f\|$ is a nondecreasing function of λ.

(iv) It follows easily from Eq. (2.2) that (a) $\Leftrightarrow$ (b).

Assume (b). Then $QE_\lambda f$ converges strongly as $\lambda \to \infty$. Hence, since $E_\lambda f$ converges strongly to f and since Q is closed, it follows that $f \in D_Q$ and that $Q_\lambda f \to Qf$, strongly. Thus (a) $\Leftrightarrow$ (b) $\to$ (c).

Assume (c). Then $(Q - Q_\lambda)f \in \mathcal{H}$ and

$$\|(Q - Q_\lambda)f\|^2 = \|Qf\|^2 + \|Q_\lambda f\|^2 - (Qf, Q_\lambda f) - (Q_\lambda f, Qf). \tag{2.3}$$

Since $E_\lambda f \in D_{Q^*Q}$, it follows that $Q_\lambda f (\equiv QE_\lambda f) \in D_{Q^*}$ and, therefore, $(Qf, Q_\lambda f) = (f, Q^*QE_\lambda f) = \|Q_\lambda f\|^2$, by Eq. (2.1). Likewise, $(Q_\lambda f, Qf) = \|Q_\lambda f\|^2$ and, consequently, by Eq. (2.3),

$$\|(Q - Q_\lambda)f\|^2 = \|Qf\|^2 - \|Q_\lambda f\|^2. \tag{2.4}$$

It follows immediately that $\|Q_\lambda f\|$ is bounded above by $\|Qf\|$. Hence (c) $\to$ (b), which completes our proof that (a) $\Leftrightarrow$ (b) $\Leftrightarrow$ (c). Further, it follows from Eq. (2.4) that $\|Q_\lambda f\| \leq \|Qf\|$ when these conditions are fulfilled.

(v) This follows from (iv) and the above derivation of (ivc) from (ivb).

(vi) Since $Q_\lambda = QE_\lambda$, it follows that $(Q_\lambda)^* \supseteq E_\lambda Q^*$. Thus, if $f \in D_{Q^*}$, then $(Q_\lambda)^* f = E_\lambda Q^* f$. Hence $(Q_\lambda)^* f \to Q^* f$, strongly, as $\lambda \to \infty$, $\forall f \in D_{Q^*}$. QED

Let $\mathfrak{L}$ be the Hilbert–Schmidt class of operators in $\mathcal{H}$, i.e., $\mathfrak{L} = \{A \mid A \in \mathfrak{B}(\mathcal{H}); \text{Tr}\,(A^*A) < \infty\}$. Then $\mathfrak{L}$ is a Hilbert space, with $(A, B)_{\mathfrak{L}} = \text{Tr}\,(A^*B)$, and strong convergence in $\mathfrak{L}$ corresponds to ultrastrong convergence in $\mathcal{H}$.

Let ρ be a density matrix in $\mathcal{H}$, i.e.,

$$\rho = \sum c_n E_n, \tag{2.5}$$

where the c_n are real positive numbers such that $\sum c_n = 1$ and $\{E_n\}$ is the set of 1-dimensional projectors corresponding to an orthonormal set of vectors

$\{f_n\}$. Let Δ_ρ be the subset of $\mathfrak{Q}^0$ defined by

$$\Delta_\rho = \left\{ Q \mid Q \in \mathfrak{Q}^0, \{f_n\} \in D_Q, \sum_n c_n \|Qf_n\|^2 < \infty \right\}$$

or, equivalently, by $\Delta_\rho = \{Q \mid Q \in \mathfrak{Q}^0, Q\rho^{\frac{1}{2}} \in \mathfrak{L}\}$. We define

$$\mathrm{Tr}\,(Q'\rho Q^*) = (Q\rho^{\frac{1}{2}}, Q'\rho^{\frac{1}{2}})_{\mathfrak{L}} = \sum_n c_n (Qf_n, Q'f_n), \quad \forall\, Q, Q' \in \Delta_\rho. \tag{2.6}$$

It is evident that this reduces to the usual definition of $\mathrm{Tr}\,(Q'\rho Q^*)$ in cases where $Q, Q' \in \mathfrak{B}(\mathfrak{H})$. It may be noted that the sum in Eq. (2.6) is absolutely convergent, by virtue of our definition of Δ_ρ.

Theorem 2.2: Let $Q, Q' \in \mathfrak{Q}^0$. Then:

(i) $Q \in \Delta_\rho$ if and only if $\mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*)$ is a bounded function of λ;

(ii) if $Q \in \Delta_\rho$, then $\mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*) \to \mathrm{Tr}\,(Q\rho Q^*)$ as $\lambda \to \infty$;

(iii) if $Q, Q' \in \Delta_\rho$, then

$$\mathrm{Tr}\,(Q'_{\lambda'} \rho (Q_\lambda)^*) \to \mathrm{Tr}\,(Q'\rho Q^*)$$

as λ, λ' tend independently to ∞.

Proof:

(i) Let $Q \in \Delta_\rho$. Then it follows from Theorem 2.1(iv) and Eq. (2.6) that

$$\mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*) \leq \mathrm{Tr}\,(Q\rho Q^*) < \infty,$$

and thus $\mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*)$ is a bounded function of λ.

In order to prove the converse, we note that, by Eqs. (2.2) and (2.6) and our definition of $\mathfrak{L}$,

$$\|Q_{\lambda'}\rho^{\frac{1}{2}} - Q_\lambda \rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2 = \|Q_{\lambda'}\rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2 - \|Q_\lambda \rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2 \quad \text{for} \quad \lambda < \lambda' < \infty. \tag{2.7}$$

Proceeding as in Theorem 2.1(iv), we find from this equation that, if $\|Q_\lambda \rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2 [\equiv \mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*)]$ is a bounded function of λ, then $Q_\lambda \rho^{\frac{1}{2}}$ converges strongly in $\mathfrak{L}$ to A, say, as $\lambda \to \infty$. Thus $Q_\lambda \rho^{\frac{1}{2}}$ converges ultrastrongly and, hence, strongly to A in $\mathfrak{H}$, as $\lambda \to \infty$. Let $\{g_m\}$ be an orthonormal set of vectors, complementary and orthogonal to $\{f_n\}$ in $\mathfrak{H}$. Then

$$Af_n = \text{s-}\lim_{\lambda \to \infty} Q_\lambda \rho^{\frac{1}{2}} f_n$$

and

$$Ag_m = \text{s-}\lim_{\lambda \to \infty} Q_\lambda \rho^{\frac{1}{2}} g_m.$$

Hence, by Eq. (2.5) and our definition of $\{g_m\}$,

$$Af_n = \text{s-}\lim_{\lambda \to \infty} c_n^{\frac{1}{2}} Q_\lambda f_n \quad \text{and} \quad Ag_m = 0.$$

In view of Theorem 2.1(v) and Eq. (2.5), it follows that $A = Q\rho^{\frac{1}{2}}$. Therefore, since $A \in \mathfrak{L}$, it follows that $Q \in \Delta_\rho$, as required.

(ii) Let $Q \in \Delta_\rho$. Then $Q\rho^{\frac{1}{2}} \in \mathfrak{L}$ and thus, by Eqs. (2.4) and (2.6),

$$\|(Q - Q_\lambda)\rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2 = \|Q\rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2 - \|Q_\lambda \rho^{\frac{1}{2}}\|_{\mathfrak{L}}^2. \tag{2.8}$$

As proved in the course of the above derivation of (i), it follows that, if $Q \in \Delta_\rho$, then $Q_\lambda \rho^{\frac{1}{2}} \to Q\rho^{\frac{1}{2}}$, strongly in $\mathfrak{L}$, as $\lambda \to \infty$. Consequently, by Eqs. (2.6) and (2.8), $\mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*) \to \mathrm{Tr}\,(Q\rho Q^*)$ as $\lambda \to \infty$.

(iii) Let $Q, Q' \in \Delta_\rho$. Then $Q\rho^{\frac{1}{2}}, Q'\rho^{\frac{1}{2}} \in \mathfrak{L}$, and

$$\begin{aligned} &|(Q\rho^{\frac{1}{2}}, Q'\rho^{\frac{1}{2}})_{\mathfrak{L}} - (Q_\lambda \rho^{\frac{1}{2}}, Q'_{\lambda'}\rho^{\frac{1}{2}})_{\mathfrak{L}}| \\ &\quad = |(Q_\lambda \rho^{\frac{1}{2}}, (Q' - Q'_{\lambda'})\rho^{\frac{1}{2}})_{\mathfrak{L}} + ((Q - Q_\lambda)\rho^{\frac{1}{2}}, Q'\rho^{\frac{1}{2}})_{\mathfrak{L}}| \\ &\quad \leq \|Q_\lambda \rho^{\frac{1}{2}}\|_{\mathfrak{L}} \|(Q' - Q'_{\lambda'})\rho^{\frac{1}{2}}\|_{\mathfrak{L}} \\ &\qquad + \|Q'\rho^{\frac{1}{2}}\|_{\mathfrak{L}} \|(Q - Q_\lambda)\rho^{\frac{1}{2}}\|_{\mathfrak{L}}. \end{aligned}$$

By Eq. (2.8), $\|Q_\lambda \rho^{\frac{1}{2}}\|_{\mathfrak{L}} \leq \|Q\rho^{\frac{1}{2}}\|_{\mathfrak{L}}$. Hence, the above equality implies that

$$\begin{aligned} &|(Q\rho^{\frac{1}{2}}, Q'\rho^{\frac{1}{2}})_{\mathfrak{L}} - (Q_\lambda \rho^{\frac{1}{2}} Q'_{\lambda'}\rho^{\frac{1}{2}})_{\mathfrak{L}}| \\ &\qquad \leq \|Q\rho^{\frac{1}{2}}\|_{\mathfrak{L}} \|(Q' - Q'_{\lambda'})\rho^{\frac{1}{2}}\|_{\mathfrak{L}} \\ &\qquad\quad + \|Q'\rho^{\frac{1}{2}}\|_{\mathfrak{L}} \|(Q - Q_\lambda)\rho^{\frac{1}{2}}\|_{\mathfrak{L}}. \end{aligned}$$

Hence, by Eqs. (2.6) and (2.8),

$$\begin{aligned} &|\mathrm{Tr}\,(Q'\rho Q^*) - \mathrm{Tr}\,(Q'_{\lambda'}\rho (Q_\lambda)^*)| \\ &\quad \leq [\mathrm{Tr}\,(Q\rho Q^*)]^{\frac{1}{2}} [\mathrm{Tr}\,(Q'\rho Q'^*) - \mathrm{Tr}\,(Q'_{\lambda'}\rho (Q'_{\lambda'})^*)]^{\frac{1}{2}} \\ &\qquad + [\mathrm{Tr}\,(Q'\rho Q'^*)]^{\frac{1}{2}} [\mathrm{Tr}\,(Q\rho Q^*) - \mathrm{Tr}\,(Q_\lambda \rho (Q_\lambda)^*)]^{\frac{1}{2}}. \end{aligned} \tag{2.9}$$

It follows from this equation and (ii) that

$$\mathrm{Tr}\,(Q'_{\lambda'}\rho (Q_\lambda)^*) \to \mathrm{Tr}\,(Q'\rho Q^*)$$

as λ, λ' tend independently to ∞. QED

In the remainder of this section, it is assumed that $\mathfrak{H}$ is the completed tensor product of Hilbert spaces $\tilde{\mathfrak{H}}$ and $\hat{\mathfrak{H}}$, i.e., $\mathfrak{H} = \tilde{\mathfrak{H}} \bar{\otimes} \hat{\mathfrak{H}}$. Denoting the unit operators in $\tilde{\mathfrak{H}}$, $\hat{\mathfrak{H}}$ by $\tilde{I}$, $\hat{I}$, respectively, we define $\mathfrak{Q}$ to be the set of all closed, densely defined operators in $\mathfrak{H}$ that are affiliated to the algebra $\mathfrak{B}(\tilde{\mathfrak{H}}) \otimes \hat{I}$. Thus $\mathfrak{Q}$ is the subset of $\mathfrak{Q}^0$ that commutes with $\tilde{I} \otimes \mathfrak{B}(\hat{\mathfrak{H}})$; i.e., $\mathfrak{Q} = \{Q \mid Q \in \mathfrak{Q}^0,\ AQ \subseteq QA,\ \forall A \in \tilde{I} \otimes \mathfrak{B}(\hat{\mathfrak{H}})\}$. The set of all closed, densely defined operators in $\mathfrak{H}$ will be denoted by $\mathfrak{A}$.

Theorem 2.3:

(i) If $Q \in \mathfrak{Q}$, $f \in \tilde{\mathfrak{H}}$, $\chi_0 (\neq 0) \in \hat{\mathfrak{H}}$, and $f \otimes \chi_0 \in D_{Q'}$, then $f \otimes \chi \in D_Q$, $\forall\, \chi \in \hat{\mathfrak{H}}$.

(ii) If $Q \in \mathfrak{Q}$, then Q induces an operator $\tilde{Q}$ in $\tilde{\mathfrak{H}}$, such that $\tilde{Q} \in \tilde{\mathfrak{Q}}$, $D_{\tilde{Q}} = \{f \mid f \in \mathfrak{H}, f \otimes \chi \in D_Q, \forall\, \chi \in \hat{\mathfrak{H}}\}$, and $Q(f \otimes \chi) = (\tilde{Q}f) \otimes \chi$.

(iii) If $\tilde{Q} \in \tilde{\mathfrak{Q}}$, then $\exists$ a unique element Q of $\mathfrak{Q}$ that induces $\tilde{Q}$ in $\tilde{\mathfrak{K}}$, as in (ii).

Thus, there is a bijective mapping of $\mathfrak{Q}$ onto $\tilde{\mathfrak{Q}}$ such that each $Q\,(\in \mathfrak{Q})$ induces a unique operator $\tilde{Q}\,(\in \tilde{\mathfrak{Q}})$ in $\tilde{\mathfrak{K}}$. We denote this mapping by $\mathfrak{Q} = \tilde{\mathfrak{Q}} \otimes \hat{I}$, thereby extending the definition of tensor product generally employed for bounded operators.

Proof:

(i) Let $\hat{A}$ be the element of $\mathfrak{B}(\hat{\mathfrak{K}})$ defined by

$$\hat{A}\chi_0 = \chi, \quad \hat{A}\chi_0^{\perp} = 0,$$

where $\chi_0^{\perp}$ is the orthogonal complement of χ_0 in $\hat{\mathfrak{K}}$; and let $A = \tilde{I} \otimes \hat{A}$. Thus

$$A(f \otimes \chi_0) = f \otimes \chi, \quad \forall f \in \mathfrak{K}. \tag{2.10}$$

It follows from the definition of $\mathfrak{Q}$ that, if $Q \in \mathfrak{Q}$ and $f \otimes \chi_0 \in D_{Q'}$, then $A(f \otimes \chi_0) \in D_Q$. Thus, by Eq. (2.10), $f \otimes \chi \in D_Q$.

(ii) It also follows from the same assumption that, in view of Eq. (2.10),

$$Q(f \otimes \chi) = QA(f \otimes \chi_0) = AQ(f \otimes \chi_0). \tag{2.11}$$

Further, Eq. (2.10) implies that $A\mathfrak{K} \subseteq \tilde{\mathfrak{K}} \otimes \chi$. Hence $AQ(f \otimes \chi_0)$ is of the form $g \otimes \chi$ where $g \in \tilde{\mathfrak{K}}$. Thus, by Eq. (2.11),

$$Q(f \otimes \chi) = g \otimes \chi. \tag{2.12}$$

Applying this result to the case where $\chi = \chi_0$, we find that $\exists\, g_0 \in \tilde{\mathfrak{K}}$ such that

$$Q(f \otimes \chi_0) = g_0 \otimes \chi_0. \tag{2.13}$$

Hence, by Eq. (2.11), $A(g_0 \otimes \chi_0) = g \otimes \chi$, and thus, by Eq. (2.10), $g \otimes \chi = g_0 \otimes \chi$, i.e., $g = g_0$. This implies that g is independent of χ. Consequently, it follows from Eq. (2.12) that Q induces an operator $\tilde{Q}$ in $\tilde{\mathfrak{K}}$, where $\tilde{Q}$ is defined by

$$D_{\tilde{Q}} = \{f \mid f \in \tilde{\mathfrak{K}}, f \otimes \psi \in D_Q, \forall\, \chi \in \hat{\mathfrak{K}}\},$$
$$Q(f \otimes \chi) = (\tilde{Q}f) \otimes \chi.$$

It follows easily from this definition that, since $Q \in \mathfrak{Q}$, then $\tilde{Q}$ is closed and densely defined in $\tilde{\mathfrak{K}}$, i.e., $\tilde{Q} \in \tilde{\mathfrak{Q}}$.

(iii) Let $\tilde{Q} \in \tilde{\mathfrak{Q}}$, and let Q' be the associated operator in $\mathfrak{K}$, defined by

$$D_{Q'} = \left\{ \sum_{n=1}^{N} f_n \otimes \chi_n \,\middle|\, f_n \in D_{\tilde{Q}}, \chi_n \in \hat{\mathfrak{K}}, N < \infty \right\}$$

and

$$Q' \sum_{1}^{N} f_n \otimes \chi_n = \sum_{1}^{N} (\tilde{Q}f_n) \otimes \chi_n.$$

Since $\tilde{Q}$ is closed and densely defined in $\tilde{\mathfrak{K}}$, it follows from this definition that both Q' and its adjoint are densely defined in $\mathfrak{K}$. Therefore, the minimal closed extension[7] of Q' is $(Q')^{**} = Q$, say. Since $\tilde{I} \otimes \mathfrak{B}(\hat{\mathfrak{K}})$ commutes with Q', it follows that it also commutes with Q and, hence, $Q \in \mathfrak{Q}$. Thus, Q is an element of $\mathfrak{Q}$ that induces $\tilde{Q}$ in $\tilde{\mathfrak{K}}$.

Suppose that there is another element of $\mathfrak{Q}$, namely Q'', that induces $\tilde{Q}$ in $\tilde{\mathfrak{K}}$. Then it follows from our definitions of Q' and Q that $Q' \subseteq Q \subseteq Q''$, which implies that $D_{Q''} \setminus D_Q$ is nonvoid, since $Q'' \neq Q$.

Let ψ be a nonnull element of $D_{Q''} \setminus D_Q$, and let $\hat{\mathfrak{U}}$ be a complete orthonormal set of basis vectors in $\hat{\mathfrak{K}}$. Then we may express ψ in the form

$$\psi = \sum_{n=1}^{\infty} f_n \otimes \theta_n, \quad \text{with} \quad \{\theta_n\} \in \hat{\mathfrak{U}}. \tag{2.14}$$

Let $\hat{P}_n$ be the projection operator for θ_n in $\hat{\mathfrak{K}}$, and let $P_n = \tilde{I} \otimes \hat{P}_n$. Then, since $Q'' \in \mathfrak{Q}$ and $\psi \in D_{Q''}$, it follows that $P_n\psi = f_n \otimes \theta_n \in D_{Q''}$. Hence, since Q'' induces $\tilde{Q}$ in $\tilde{\mathfrak{K}}$ (by definition), it follows that

$$Q''(f_n \otimes \theta_n) = Q(f_n \otimes \theta_n) = Q'(f_n \otimes \theta_n)$$
$$= (\tilde{Q}f_n) \otimes \theta_n. \tag{2.15}$$

Let $M_N = \sum_1^N P_n$. Then it follows from Eq. (2.14) that

$$M_N\psi = \sum_{1}^{N} f_n \otimes \theta_n \tag{2.16}$$

and, therefore, by Eq. (2.15), that

$$Q''M_N\psi = QM_N\psi = Q'M_N\psi = \sum_{1}^{N} (\tilde{Q}f_n) \otimes \theta_n. \tag{2.17}$$

Further, since $\psi \in D_{Q''}$, $Q'' \in \mathfrak{Q}$, and $M_N \in \tilde{I} \otimes \mathfrak{B}(\hat{\mathfrak{K}})$, it follows that $M_NQ''\psi = Q''M_N\psi$. Hence, by Eq. (2.17),

$$\|QM_N\psi\| = \|M_NQ''\psi\| \leq \|Q''\psi\|$$
(since M_N is a projector), (2.18)

and

$$\|QM_{N'}\psi\|^2 - \|QM_N\psi\|^2 = \|QM_{N'}\psi - QM_N\psi\|^2 (\geq 0),$$
for $N < N' < \infty$. (2.19)

It follows from these last two equations that $\|QM_N\psi\|$ is a bounded nondecreasing function of N. Thus $\|QM_N\psi\|$ converges to a finite limit as $N \to \infty$ and, consequently, by Eq. (2.19), $QM_N\psi$ converges strongly as $N \to \infty$. Further, it follows from Eqs. (2.14) and (2.16) that $M_N\psi \to \psi$, strongly, as $N \to \infty$. Hence, since Q is a closed operator, $\psi \in D_Q$. This contradicts the assumption that $\psi \in D_{Q''} \setminus D_Q$ and thus refutes the supposition that $\mathfrak{Q}$ contains an element other than Q that induces $\tilde{Q}$ in $\tilde{\mathfrak{K}}$.

Corollary: Let $Q (\in \mathfrak{Q})$ induce $\tilde{Q} (\in \tilde{\mathfrak{Q}})$ in $\tilde{\mathcal{H}}$; i.e., $Q = \tilde{Q} \otimes \hat{I}$. Let

$$\xi (\in \mathcal{H}) = \sum_{n=1}^{\infty} g_n \otimes \theta_n,$$

where $\{\theta_n\}$ belongs to the complete orthonormal basis $\hat{\mathfrak{U}}$ of $\hat{\mathcal{H}}$. Then $\xi \in D_Q$ if and only if

$$\{g_n\} \in D \quad \text{and} \quad \sum_{1}^{N} \tilde{Q} g_n \otimes \theta_n$$

converges strongly as $N \to \infty$, in which case

$$Q\xi = \sum_{n=1}^{\infty} \tilde{Q} g_n \otimes \theta_n.$$

Proof: Let P_n and M_N be defined as above. Then

$$P_n \xi = g_n \otimes \theta_n, \tag{2.20}$$

$$M_N \xi = \sum_{1}^{N} g_n \otimes \theta_n, \quad N < \infty, \tag{2.21}$$

$$(\mathrm{s}, \mathcal{H})\text{-}\lim_{N \to \infty} M_N \xi = \xi. \tag{2.22}$$

We assume first that $\xi \in D_Q$. Then, since $Q \in \mathfrak{Q}$, it follows that $\{P_n \xi\} \in D_Q$ and hence, by Theorem 2.3 and Eq. (2.20), that $\{g_n\} \in D_Q$ and $Q(g_n \otimes \theta_n) = \tilde{Q} g_n \otimes \theta_n$. It also follows that $M_N \xi \in D_Q$ and that $Q M_N \xi = M_N Q \xi$. Hence, by Eq. (2.21),

$$M_N Q \xi = \sum_{1}^{N} \tilde{Q} g_n \otimes \theta_n. \tag{2.23}$$

Since M_N is a projection operator and since $\{\theta_n\}$ is an orthonormal set, it follows from this equation that

$$\sum_{1}^{N} \|\tilde{Q} g_n\|^2 = \|M_N Q \xi\|^2 \leq \|Q \xi\|^2 \tag{2.24}$$

and

$$\sum_{N}^{N'} \|\tilde{Q} g_n\|^2 = \|M_{N'} Q \xi - M_N Q \xi\|^2, \quad \text{for} \quad N' > N. \tag{2.25}$$

It follows from Eq. (2.24) that the sum $\sum_1^N \|\tilde{Q} g_n\|^2$ is bounded above and, therefore, converges to a finite limit as $N \to \infty$. Consequently, by Eq. (2.25), $M_N Q \xi$ converges strongly as $N \to \infty$ and, hence, by Eq. (2.23), $\sum_1^N \tilde{Q} g_n \otimes \theta_n$ converges strongly as $N \to \infty$.

Conversely, we assume that $\{g_n\} \in D_Q$ and that $\sum_1^N \tilde{Q} g_n \otimes \theta_n$ is strongly convergent as $N \to \infty$. Then it follows from this assumption and Eq. (2.21) that $M_N \xi \in D_Q$ and that $Q M_N \xi \, (= \sum_1^N \tilde{Q} g_n \otimes \theta_n)$ converges strongly as $N \to \infty$. Therefore, since Q is a closed operator, it follows from Eq. (2.22) that $\xi \in D_Q$ and that

$$Q\xi = \operatorname*{s-lim}_{N \to \infty} Q M_N \xi = \sum_{0}^{\infty} \tilde{Q} g_n \otimes \theta_n.$$

QED

Theorem 2.4: Let $Q = \tilde{Q} \otimes \hat{I}$ and $Q' = \tilde{Q}' \otimes \hat{I}$ be two elements of $\mathfrak{Q}$. Then:

(i) $Q^* = \tilde{Q}^* \otimes \hat{I} \, (\in \mathfrak{Q})$;

(ii) if $Q + Q' \in \mathfrak{Q}$, then $\tilde{Q} + \tilde{Q}' \in \tilde{\mathfrak{Q}}$ and

$$Q + Q' = (\tilde{Q} + \tilde{Q}') \otimes \hat{I};$$

(iii) if $QQ' \in \mathfrak{Q}$, then $\tilde{Q}\tilde{Q}' \in \tilde{\mathfrak{Q}}$ and $QQ' = \tilde{Q}\tilde{Q}' \otimes \hat{I}$;

(iv) if $\tilde{Q} + \tilde{Q}' \in \tilde{\mathfrak{Q}}$, then $Q + Q' \subseteq (\tilde{Q} + \tilde{Q}') \otimes \hat{I}$;

(v) if $\tilde{Q}\tilde{Q}' \in \tilde{\mathfrak{Q}}$, then $QQ' \subseteq \tilde{Q}\tilde{Q}' \otimes \hat{I}$.

Proof:

(i) It follows from the definition of $\mathfrak{Q}$ that, since $Q \in \mathfrak{Q}$, then $Q^* \in \mathfrak{Q}$. Hence, by Theorem 2.3, Q^* induces an operator $\tilde{S}$, say, in $\tilde{\mathcal{H}}$, where $\tilde{S} \in \tilde{\mathfrak{Q}}$; i.e., $Q^* = \tilde{S} \otimes \hat{I}$. Let $f \in D_{\tilde{Q}}$ and $g \in D_{\tilde{S}}$. Then $Q(f \otimes \chi) = (\tilde{Q} f) \otimes \chi$, and $Q^*(g \otimes \chi) = (\tilde{S} g) \otimes \chi$. Thus, since $(f \otimes \chi, Q^*(g \otimes \chi)) = (Q(f \otimes \chi), g \otimes \chi)$, it follows that $(f, \tilde{S} g) = (\tilde{Q} f, g)$. Hence, $\tilde{S} = \tilde{Q}^*$ and, therefore, $Q^* = \tilde{Q}^* \otimes \hat{I}$.

(ii) Let $Q'' = Q + Q' \in \mathfrak{Q}$. Then it follows from Theorem 2.3 that $Q'' = \tilde{Q}'' \otimes \hat{I}$ (with $\tilde{Q}'' \in \tilde{\mathfrak{Q}}$) and that, if χ is a nonnull element of $\hat{\mathcal{H}}$,

$$\begin{aligned}(f \in D_{Q''}) &\Leftrightarrow (f \otimes \chi \in D_{Q''}) \Leftrightarrow (f \otimes \chi \in D_Q \cap D_{Q'}) \\ &\Leftrightarrow (f \in D_{\tilde{Q}} \cap D_{\tilde{Q}'}) \Leftrightarrow (f \in D_{\tilde{Q}+\tilde{Q}'}).\end{aligned}$$

Thus $D_{\tilde{Q}''} = D_{\tilde{Q}+\tilde{Q}'}$. Further, if f lies in this domain, then

$$\begin{aligned}(\tilde{Q}'' f) \otimes \chi &= Q''(f \otimes \chi) = Q(f \otimes \chi) + Q'(f \otimes \chi) \\ &= [(\tilde{Q} + \tilde{Q}') f] \otimes \chi.\end{aligned}$$

Hence, $(\tilde{Q} + \tilde{Q}') \in \tilde{\mathfrak{Q}}$ and $Q + Q' = (\tilde{Q} + \tilde{Q}') \otimes \hat{I}$.

(iii) Let $Q'' = QQ' \in \mathfrak{Q}$. Then it follows from Theorem 2.3 that Q'' may be expressed in the form $Q'' = \tilde{Q}'' \otimes \hat{I}$, with $\tilde{Q}'' \in \tilde{\mathfrak{Q}}$, and that, if χ is a nonnull element of $\hat{\mathcal{H}}$,

$$\begin{aligned}(f \in D_{\tilde{Q}''}) &\Leftrightarrow (f \otimes \chi \in D_{Q''}) \\ &\Leftrightarrow \{(f \otimes \chi \in D_{Q'}) \quad \text{and} \quad (Q'(f \otimes \chi) \in D_Q)\} \\ &\Leftrightarrow \{(f \in D_{\tilde{Q}'}) \quad \text{and} \quad (\tilde{Q}' f \in D_{\tilde{Q}})\} \\ &\Leftrightarrow (f \in D_{\tilde{Q}\tilde{Q}'}).\end{aligned}$$

Thus $D_{\tilde{Q}} = D_{\tilde{Q}\tilde{Q}'}$. Further, if f lies in this domain, then

$$\begin{aligned}(\tilde{Q}'' f) \otimes \chi &= Q''(f \otimes \chi) = QQ'(f \otimes \chi) \\ &= Q((\tilde{Q}' f) \otimes \chi) = (\tilde{Q}\tilde{Q}' f) \otimes \chi.\end{aligned}$$

Hence $\tilde{Q}'' = \tilde{Q}\tilde{Q}'$ and, therefore, $QQ' = (\tilde{Q}\tilde{Q}') \otimes \hat{I}$.

(iv) Let $\xi \in D_{Q+Q'} \equiv D_Q \cap D_{Q'}$. Then it follows from the Corollary to Theorem 2.3 that, if

$$\xi = \sum_1^\infty g_n \otimes \theta_n, \quad \text{with} \quad \{\theta_n\} \in \hat{\mathfrak{V}},$$

then

$$Q\xi = \sum_1^\infty (\tilde{Q} g_n) \otimes \theta_n \quad \text{and} \quad Q'\xi = \sum_1^\infty (\tilde{Q}' g_n) \otimes \theta_n,$$

these sums being strongly convergent. Hence

$$(Q + Q')\xi = \sum_1^\infty (\tilde{Q} + \tilde{Q}') g_n \otimes \theta_n,$$

this latter sum also being strongly convergent. In view of this convergence, it follows from the Corollary to Theorem 2.3 that, if $(\tilde{Q} + \tilde{Q}') \in \tilde{\mathfrak{Q}}$, then $\xi \in D_{(\tilde{Q}+\tilde{Q}')\otimes \hat{I}}$ and

$$((\tilde{Q} + \tilde{Q}') \otimes \hat{I})\xi = \sum_1^\infty (\tilde{Q} + \tilde{Q}') g_n \otimes \theta_n,$$

i.e., $[(\tilde{Q} + \tilde{Q}') \otimes \hat{I}]\xi = (Q + Q')\xi, \forall\, \xi \in D_{Q+Q'}$. Thus $(Q + Q') \subseteq (\tilde{Q} + \tilde{Q}') \otimes \hat{I}$, if $\tilde{Q} + \tilde{Q}' \in \tilde{\mathfrak{Q}}$.

(iv) Let $\xi \in D_{QQ'}$, i.e., $\xi \in D_{Q'}$ and $Q'\xi \in D_Q$. It follows from the Corollary to Theorem 2.3 that, if

$$\xi = \sum_1^\infty g_n \otimes \theta_n, \quad \text{with} \quad \{\theta_n\} \in \hat{\mathfrak{V}},$$

then

$$Q'\xi = \sum_1^\infty \tilde{Q}' g_n \otimes \theta_n \quad \text{and} \quad QQ'\xi = \sum_1^\infty \tilde{Q}\tilde{Q}' g_n \otimes \theta_n,$$

this latter sum being strongly convergent. In view of this convergence, it follows from the Corollary to Theorem 2.3 that, if $\tilde{Q}\tilde{Q}' \in \tilde{\mathfrak{Q}}$, then

$$\sum_1^\infty \tilde{Q}\tilde{Q}' g_n \otimes \theta_n = (\tilde{Q}\tilde{Q}' \otimes \hat{I})\xi,$$

i.e.,

$$(\tilde{Q}\tilde{Q}' \otimes \hat{I})\xi = QQ'\xi, \quad \forall\, \xi \in D_{QQ'}.$$

Thus $QQ' \subseteq \tilde{Q}\tilde{Q}' \otimes \hat{I}$ if $\tilde{Q}\tilde{Q}' \in \tilde{\mathfrak{Q}}$. QED

Theorem 2.5: Let $Q = \tilde{Q} \otimes \hat{I}\,(Q \in \mathfrak{Q}, \tilde{Q} \in \tilde{\mathfrak{Q}})$ and let $\{E_\lambda\}$ and $\{\tilde{E}_\lambda\}$ be the families of spectral projectors for Q^*Q and $\tilde{Q}^*\tilde{Q}$, respectively. Let $Q_\lambda = QE_\lambda$ and $\tilde{Q}_\lambda = \tilde{Q}\tilde{E}_\lambda$. Then:

(i) $E_\lambda = \tilde{E}_\lambda \otimes \hat{I}$;

(ii) $Q_\lambda = \tilde{Q}_\lambda \otimes \hat{I}$;

(iii) if $\xi \in \mathcal{H}$, then $\xi \in D_{\tilde{Q}\otimes I}$ if and only if $\|(\tilde{Q}_\lambda \otimes \hat{I})\xi\|$ is a bounded function of λ, in which case $\|(\tilde{Q}_\lambda \otimes \hat{I})\xi\| \leq \|(\tilde{Q} \otimes \hat{I})\xi\|, \forall\, \lambda < \infty$;

(iv)

$$(\mathrm{s}, \mathcal{H})\text{-}\lim_{\lambda\to\infty} (\tilde{Q}_\lambda \otimes \hat{I}) = [(\mathrm{s}, \tilde{\mathcal{H}})\text{-}\lim_{\lambda\to\infty} \tilde{Q}_\lambda] \otimes \hat{I};$$

(v) $[(\tilde{Q}_\lambda)^* \otimes \hat{I}] \to \tilde{Q}^* \otimes \hat{I}$, strongly, on $D_{Q^*\otimes \hat{I}}$ as $\lambda \to \infty$.

Proof:

(i) Since $Q \in \mathfrak{Q}$, it follows from Theorem 2.4(i) that $Q^* \in \mathfrak{Q}$. Hence $\hat{I} \otimes \mathcal{B}(\hat{\mathcal{H}})$ commutes with Q and Q^* and thus with Q^*Q. Therefore, since $Q^*Q \in \mathfrak{Q}^0$, it follows that $Q^*Q \in \mathfrak{Q}$. Consequently, by Theorem 2.4(iii),

$$Q^*Q = \tilde{Q}^*\tilde{Q} \otimes \hat{I}. \tag{2.26}$$

Since $\hat{I} \otimes \mathcal{B}(\hat{\mathcal{H}})$ commutes with Q^*Q, it also commutes with $\{E_\lambda\}$. Thus $E_\lambda \in \mathcal{B}(\mathcal{H}) \otimes \hat{I}$; i.e., E_λ may be expressed in the form

$$E_\lambda = \tilde{E}'_\lambda \otimes \hat{I}, \tag{2.27}$$

where $\tilde{E}'_\lambda \in \mathcal{B}(\tilde{\mathcal{H}})$. Since E_λ is a projector in $\mathcal{H}$, it follows that $\tilde{E}'_\lambda$ is a projector in $\tilde{\mathcal{H}}$.

It follows from the definitions of Q^*Q and E_λ that Q^*QE_λ, $E_\lambda Q^*Q$, $Q^*Q(I - E_\lambda)$, and $(I - E_\lambda)Q^*Q \in \mathfrak{Q}$. Hence, by Theorem 2.4(iii) and Eqs. (2.26) and (2.27),

$$\begin{aligned} Q^*QE_\lambda = \tilde{Q}^*\tilde{Q}\tilde{E}'_\lambda \otimes \hat{I}, \quad E_\lambda Q^*Q = \tilde{E}'_\lambda \tilde{Q}^*\tilde{Q} \otimes \hat{I}, \\ Q^*Q(I - E_\lambda) = \tilde{Q}^*\tilde{Q}(\tilde{I} - \tilde{E}'_\lambda) \otimes \hat{I}, \\ (I - E_\lambda)Q^*Q = (\tilde{I} - \tilde{E}'_\lambda)\tilde{Q}^*\tilde{Q} \otimes \hat{I}. \end{aligned} \tag{2.28}$$

Now the spectral projector E_λ is uniquely defined as the projection operator for which

$$\begin{aligned} E_\lambda Q^*Q \subseteq Q^*QE_\lambda, \quad Q^*QE_\lambda \leq \lambda E_\lambda, \\ Q^*Q(I - E_\lambda) > \lambda(I - E_\lambda). \end{aligned} \tag{2.29}$$

Hence, by Eqs. (2.27)–(2.29),

$$\begin{aligned} \tilde{E}'_\lambda \tilde{Q}^*\tilde{Q} \subseteq \tilde{Q}^*\tilde{Q}\tilde{E}'_\lambda, \quad \tilde{Q}^*\tilde{Q}\tilde{E}'_\lambda \leq \lambda E'_\lambda, \\ \tilde{Q}^*\tilde{Q}(\tilde{I} - \tilde{E}'_\lambda) > \lambda(\tilde{I} - \tilde{E}'_\lambda). \end{aligned} \tag{2.30}$$

Since $\tilde{E}'_\lambda$ is a projector, it follows from Eqs. (2.30) that $\tilde{E}'_\lambda = \tilde{E}_\lambda$.

Consequently, by Eq. (2.27), $E_\lambda = \tilde{E}_\lambda \otimes \hat{I}$.

(ii) This follows from (i) and Theorem 2.4(iii).

(iii) This follows from (ii) and Theorem 2.1(iv).

(iv) This follows from (ii) and Theorem 2.1(v).

(v) This follows from (ii) and Theorems 2.1(vi) and 2.4(i). QED

3. STATES OF PHYSICAL SYSTEMS

Let Γ be a ν-dimensional Euclidean space and let L be the set of all bounded, measurable subsets Λ of Γ. We shall denote the Hilbert spaces of real square-integrable functions on Γ and Λ by $\mathfrak{L}$ and $\mathfrak{L}_\Lambda$, respectively. Points in Γ will be denoted by x or y.

In the Fock representation of $\mathfrak{L}$, corresponding to canonical commutation relations (CCR's) or canonical anticommutation relations (CAR's), each element f of

$\mathfrak{L}$ is associated with a pair of operators $a(f)$, $a^*(f)$ [$= (a(f))^*$] in a complex Hilbert space $\mathcal{H}_F$, with unit operator I_F, such that

$$[a(f), a^*(g)]_\pm = (f, g)_{\mathfrak{L}} I_F, \quad [a(f), a(g)]_\pm = 0.$$

The space $\mathcal{H}_F$ contains a "vacuum vector" Ω_F, possessing the property that $a(f)\Omega_F = 0$, $\forall f \in \mathfrak{L}$. Further, the space $\mathcal{H}_F$ may be generated by repeated application of the $a^*(f)$'s to Ω_F. Thus $\mathcal{H}_F$ may be expressed as a direct sum

$$\mathcal{H}_F = \sum_{n=0}^{\infty} \oplus \mathcal{H}_F^{(n)}, \tag{3.1}$$

where $\mathcal{H}_F^{(0)}$ consists of scalar multiples of Ω_F and where $\mathcal{H}_F^{(n)}$ is the subspace of $\mathcal{H}_F$ generated by applying monomials of order n in the $a^*(f)$'s to Ω_F. We define E_F to be I_F in the case of CCR's and to be the projection operator for $\sum_{\text{even } n} \otimes \mathcal{H}_F^{(n)}$ in the case of CAR's.

The Fock representation for $\mathfrak{L}_\Lambda$ may be embedded in the above structure, since $\mathcal{H}_F$ may be expressed as a completed tensor product of Fock spaces $\tilde{\mathcal{H}}_\Lambda$ and $\hat{\mathcal{H}}_\Lambda$, corresponding to Λ (i.e., to $\mathfrak{L}_\Lambda$) and $\Gamma \setminus \Lambda$, respectively (cf. Ref. 2):

$$\mathcal{H}_F = \tilde{\mathcal{H}}_\Lambda \otimes \hat{\mathcal{H}}_\Lambda. \tag{3.2}$$

Let $\mathfrak{U}_\Lambda$ and $\tilde{\mathfrak{U}}_\Lambda$ be the algebras of bounded operators in $\mathcal{H}_F$ and $\tilde{\mathcal{H}}_\Lambda$, defined by

$$\mathfrak{U}_\Lambda = \tilde{\mathfrak{U}}_\Lambda \otimes \hat{I}_\Lambda = [\mathfrak{B}(\tilde{\mathcal{H}}_\Lambda) \otimes I_\Lambda] \cap (E_F)', \tag{3.3}$$

where $(E_F)'$ is the commutant of E_F. Thus $\mathfrak{U}_\Lambda$ is the von Neumann algebra generated, in the case of CCR's, by $\{\exp i[a(f) + a^*(f)], \exp[a(f) - a^*(f)] \mid f \in \mathfrak{L}_\Lambda\}$ and, in the case of CAR's, by even monomials in $\{a(f), a^*(f) \mid f \in \mathfrak{L}_\Lambda\}$. We define $\mathfrak{U}$ to be the norm closure of $\mathfrak{U}_L \equiv \bigcup_{\Lambda \in L} \mathfrak{U}_\Lambda$. Thus $\mathfrak{U}_L$ is the algebra of all local bounded observables, and $\mathfrak{U}$ is the C^*-algebra of quasilocal bounded observables.

It follows from our definitions that $\mathfrak{U}_\Lambda$ is isotonic w.r.t. Λ, i.e., $(\mathfrak{U}_{\Lambda'} \supset \mathfrak{U}_\Lambda) \Leftrightarrow (\Lambda' \supset \Lambda)$. Further, $\mathfrak{U}$ has the property of local commutativity, i.e., $\mathfrak{U}_\Lambda$ commutes with $\mathfrak{U}_{\Lambda'}$ if $\Lambda \cap \Lambda'$ is void.

The set Γ is unitarily represented in $\mathcal{H}_F$ by the transformation group $\{U_F(x)\}$. defined by

$$U_F(x)\Omega_F = \Omega_F$$

and

$$U_F(x)a(f)U_F(x)^{-1} = a(f_x), \tag{3.4}$$

with

$$f_x(y) \equiv f(y - x).$$

Let

$$\gamma_x A \equiv U_F(x) A U_F(x)^{-1}, \quad \forall A \in \mathfrak{U}. \tag{3.5}$$

Then it follows that

$$\gamma_x \mathfrak{U}_\Lambda = \mathfrak{U}_{\Lambda + x}, \tag{3.6}$$

where $\Lambda + x$ is the set obtained by translating Λ through x. Hence $\gamma_x \colon \mathfrak{U} \to \mathfrak{U}$; i.e., $\{\gamma_x\}$ is a group of automorphisms of $\mathfrak{U}$, corresponding to translations in Γ. Further, it follows from Eq. (3.6) and the local commutativity of $\mathfrak{U}$ that this latter algebra is asymptotically Abelian w.r.t. Γ, i.e., $\|[\gamma_x A, B]_-\| \to 0$ as $|x| \to \infty$, $\forall A, B \in \mathfrak{U}$.

In certain cases, there is also a homomorphism τ of the real line $T = \{t\}$ onto a group of unitarily implemented automorphisms $\{\tau_t\}$ of $\mathfrak{U}$. In such cases

$$\tau_t A \equiv V_F(t) A V_F(t)^{-1}, \tag{3.7}$$

where $\{V_F(t)\}$ is a unitary representation of T. It will be assumed that the automorphisms τ_t, when they exist, correspond to time translations.

Let $\mathfrak{C}$ be the state space of $\mathfrak{U}$. Thus $\mathfrak{C}$ is the convex, w^*-compact set

$$\{\phi \mid \phi \in \mathfrak{U}^*, \phi(A^*A) \geq 0, \forall A \in \mathfrak{U}, \|\phi\|_{\mathfrak{U}^*} = 1\}.$$

The GNS representation of $\mathfrak{U}$, corresponding to the state ϕ, is a $*$-homomorphism R_ϕ of $\mathfrak{U}$ into the bounded operators in a Hilbert space $\mathfrak{H}_\phi$, with cyclical vector Ω_ϕ. This representation has the property that

$$\phi(A) = (\Omega_\phi, R_\phi(A)\Omega_\phi), \quad \forall A \in \mathfrak{U}. \tag{3.8}$$

We shall denote the projection operator for Ω_ϕ by $E(\Omega_\phi)$.

Let $\mathfrak{C}_L$ be the set of all locally normal states on $\mathfrak{U}$. Then, if $\phi \in \mathfrak{C}_L$, $\mathfrak{H}_\phi$ may be expressed[8] as a completed tensor product

$$\mathfrak{H}_\phi = \tilde{\mathfrak{H}}_\Lambda \bar{\otimes} \hat{\mathfrak{H}}_\Lambda \tag{3.9}$$

of two Hilbert spaces $\tilde{\mathfrak{H}}_\Lambda$ and $\hat{\mathfrak{H}}_\Lambda$, in such a way that

$$R_\phi(\tilde{A}_\Lambda \otimes \hat{I}_\Lambda) = W_\Lambda \tilde{A}_\Lambda W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda, \quad \forall \tilde{A}_\Lambda \in \tilde{\mathfrak{U}}_\Lambda, \tag{3.10}$$

where W_Λ is an isometry of $\tilde{\mathcal{H}}_\Lambda$ onto $\tilde{\mathfrak{H}}_\Lambda$ and $\hat{\mathfrak{J}}_\Lambda$ is the unit operator in $\hat{\mathfrak{H}}_\Lambda$.

Let $\mathfrak{C}_\Gamma^0$ be the set of all Γ-invariant states on $\mathfrak{U}$, i.e.,

$$\mathfrak{C}_\Gamma^0 = \{\phi \mid \phi \in \mathfrak{C}, \phi(\gamma_x A) = \phi(A), \forall A \in \mathfrak{U}, x \in \Gamma\}.$$

Thus, if $\phi \in \mathfrak{C}_\Gamma^0$, it follows[9] that the transformation $R_\phi(A) \to R_\phi(\gamma_x A)$ is unitarily implemented in $\mathfrak{H}_\phi$, i.e.,

$$R_\phi(\gamma_x A) = U_\phi(x) R_\phi(A) U_\phi(x)^{-1}, \quad U_\phi(x)^{-1} = U_\phi(x)^*, \tag{3.11}$$

and that

$$U_\phi(x)\Omega_\phi = \Omega_\phi. \tag{3.12}$$

We shall denote the projection operator for the subspace of $\mathfrak{H}_\phi$ spanned by all Γ-translationally variant vectors by $E^\Gamma\phi(0)$, i.e.,

$$E_\phi^\Gamma(0)\mathfrak{H}_\phi = \{\psi \mid \psi \in \mathfrak{H}_\phi, U_\phi(x)\psi = \psi, \forall x \in \Gamma\}.$$

Let $\mathcal{C}_\Gamma$ be the subset of $\mathcal{C}_\Gamma^0$ for which $U_\phi(x)$ is strongly continuous[10] w.r.t. x in $\mathfrak{H}_\phi$. We define $\mathcal{E}$ to be the subset of $\mathcal{C}_\Gamma$ for which Ω_ϕ is the only Γ-invariant vector in $\mathfrak{H}_\phi$, i.e., $\mathcal{E} = \{\phi \mid \phi \in \mathcal{C}_\Gamma, E(\Omega_\phi) = E_\phi(0)\}$. Thus $\mathcal{E}_\Gamma$ consists of Γ-ergodic states on $\mathfrak{U}$. Further, as $\mathfrak{U}$ is asymptotically Abelian w.r.t. Γ, it follows[11] that $\mathcal{E}_\Gamma$ consists precisely of the extremal elements of the convex, w^*-compact set $\mathcal{C}_\Gamma$.

In cases where the homomorphism $\tau: T \to \{\tau_t\}$ exists, we define

$$\mathcal{C}_T^0 = \{\phi \mid \phi \in \mathcal{C}, \phi(\tau_t A) = \phi(A), \forall\, t \in T, A \in \mathfrak{U}\}.$$

Thus, $\mathcal{C}_T^0$ corresponds to the set of time-translationally invariant states. It follows from our definition that, if $\phi \in \mathcal{C}_T^0$, the transformation $R_\phi(A) \to R_\phi(\tau_t A)$ is unitarily implemented in $\mathfrak{H}_\phi$, i.e.,

$$R_\phi(\tau_t A) \equiv V_\phi(t) R_\phi(A) V_\phi(t)^{-1},$$
$$V_\phi(t)^{-1} = V_\phi(-t) = V_\phi(t)^*, \tag{3.13}$$

and that

$$V_\phi(t)\Omega_\phi \equiv \Omega_\phi. \tag{3.14}$$

We shall denote by $E_\phi^T(0)$ the projection operator for the subspace of $\mathfrak{H}_\phi$ given by

$$\{\psi \mid \psi \in \mathfrak{H}_\phi, V_\phi(t)\psi = \psi, \forall\, t \in T\}.$$

We define $\mathcal{C}_T$ as the subset of $\mathcal{C}_T^0$ for which $V_\phi(t)$ is strongly continuous w.r.t. t in $\mathfrak{H}_\phi$, and we define $\mathcal{E}_T$ as the subset of $\mathcal{C}_T$ for which Ω_ϕ is the only T-invariant vector in $\mathfrak{H}_\phi$. Thus $\mathcal{E}_T$ is the T-ergodic subset of $\mathcal{C}_T$.

The subset of $\mathcal{C}_T$ that satisfies the Kubo–Martin–Schwinger boundary conditions will be denoted by $\mathcal{C}_{\mathrm{KMS}}$. As shown by Haag *et al.* (Ref. 1), these conditions may be reformulated as follows. Let f be a $\mathfrak{D}$-class test function on T, and let f_l be the associated $\mathcal{S}$-class function defined by

$$f_l(t) = \int_{-\infty}^{\infty} dw f(w) \exp w(l + it), \quad l \in T. \tag{3.15}$$

Then $\phi \in \mathcal{C}_{\mathrm{KMS}}$ if and only if there exists a real positive quantity θ such that

$$\int dt f_\theta(t)\phi(B(\tau_t A)) = \int dt \phi((\tau_t A)B) f_0(t),$$
$$\forall\, A, B \in \mathfrak{A}, \quad f \in \mathfrak{D}. \tag{3.16}$$

The quantity θ corresponds to the inverse temperature in cases where ϕ is a Gibbs state of the type formulated by Haag *et al.*

The set of all factor states on $\mathfrak{U}$ will be denoted by $\mathcal{F}$. The sets $\mathcal{F} \cap \mathcal{C}_\Gamma$ and $\mathcal{F} \cap \mathcal{C}_T$ will be denoted by $\mathcal{F}_\Gamma$ and $\mathcal{F}_T$, respectively, and the convex hull of $\mathcal{F}_\Gamma$ will be denoted by $\mathcal{F}_\Gamma^{\mathrm{C}}$. Thus $\mathcal{F}_\Gamma \subseteq \mathcal{E}_\Gamma$, $\mathcal{F}_T \subseteq \mathcal{E}_T$, $\mathcal{F}_\Gamma^{\mathrm{C}} \subseteq \mathcal{C}_\Gamma$, and $\mathcal{C}_{\mathrm{KMS}} \cap \mathcal{E}_T \subseteq \mathcal{F}_T$.[12]

We conclude this section with a definition and three lemmas.

Definition 3.1: Following Kastler and Robinson,[13] we define an M-filter[14] as a set of functions $h_l(x)$, where the index $l \in T$ and where (i) $h_l(x) \geq 0$, (ii) $\int_\Gamma dx h_l(x) = 1$, (iii) $\int_\Gamma dx\, |h_l(x + y) - h_l(x)| \to 0$ as $l \to \infty$ for any fixed $y \in \Gamma$. Then, if $g(x)$ is a measurable function on Γ such that $\int_\Gamma dx h_l(x) g(x)$ tends to a limit $\bar{g}$, as $l \to \infty$, and if $\bar{g}$ is the same for all M-filters, we say that $Mg(x)$ exists and is equal to $\bar{g}$.

Lemma 3.1:

(i) If $\phi \in \mathcal{C}_\Gamma$ and $\psi_1, \psi_2 \in \mathfrak{H}_\phi$, then $M(\psi_1, U_\phi(x)\psi_2)$ exists and $= (\psi_1, E_\phi^\Gamma(0)\psi_2)$.

(ii) If $\phi \in \mathcal{C}_T$ and $\psi_1, \psi_2 \in \mathfrak{H}_\phi$, then

$$\frac{1}{t}\int_0^t du(\psi_1, V_\phi(u)\psi_2) \to (\psi_1, E_\phi^T(0)\psi_2) \quad \text{as} \quad t \to \infty.$$

Proof: Ref. 13, Lemma 1.

Lemma 3.2: If $\phi \in \mathcal{F}_\Gamma^{\mathrm{C}}$, then $U_\phi(\lambda x) \to E_\phi^\Gamma(0)$, weakly, as $\lambda \to \infty$, $\forall\, x \neq 0$.

Proof: Let $\phi \in \mathcal{F}_\Gamma^{\mathrm{C}}$. Then ϕ may be expressed as a direct integral over $\mathcal{F}_\Gamma^{\mathrm{C}}$. Thus, denoting the elements of $\mathcal{F}$ by $\{\phi_\alpha\}$, we have

$$\phi = \int_{\mathcal{F}_\Gamma} \phi_\alpha\, d\mu(\alpha), \tag{3.17}$$

where μ is a measure on the index set $\{\alpha\}$. Correspondingly,

$$(\mathfrak{H}_\phi, \Omega_\phi, R_\phi, U_\phi(x)) = \int_{\mathcal{F}_\Gamma} \oplus\, d\mu(\alpha)(\mathfrak{H}_{\phi_\alpha}, \Omega_{\phi_\alpha}, R_{\phi_\alpha}, U_{\phi_\alpha}(x)). \tag{3.18}$$

Since $\phi_\alpha \in \mathcal{F}_\Gamma \subseteq \mathcal{E}_\Gamma$, it follows that Ω_{ϕ_α} is the only Γ-invariant vector in $\mathfrak{H}_{\phi_\alpha}$ and, consequently,

$$E_\phi^\Gamma(0) = \int \oplus\, d\mu(\alpha) E(\Omega_{\phi_\alpha}). \tag{3.19}$$

Further, since ϕ_α is a Γ-invariant factor state on the locally commutative algebra $\mathfrak{U}$, it follows from a theorem due to Araki[15] that

$$\phi_\alpha((\gamma_{\lambda x}A)B) \to \phi_\alpha(A)\phi_\alpha(B) \quad \text{as} \quad \lambda \to \infty,$$
$$\forall\, A, B \in \mathfrak{U}, \quad x \neq 0. \tag{3.20}$$

Hence, by Eq. (3.17) and Lebesgue's theorem,

$$\phi((\gamma_{\lambda x}A)B) \to \int d\mu(\alpha)\phi_\alpha(A)\phi_\alpha(B) \quad \text{as} \quad \lambda \to \infty,$$
$$\forall\, A, B \in \mathfrak{U}, \quad x \neq 0. \tag{3.21}$$

By Eqs. (3.8), (3.11), and (3.12), the lhs of Eq. (3.21) equals $(U_\phi(\lambda x)R_\phi(A^*)\Omega_\phi, R_\phi(B)\Omega_\phi)$ and, by Eqs. (3.18) and (3.19), the rhs of Eq. (3.21) equals

$$\int_{\mathcal{F}_\Gamma} d\mu(\alpha)(R_{\phi_\alpha}(A^*)\Omega_{\phi_\alpha}, \Omega_{\phi_\alpha})(\Omega_{\phi_\alpha}, R_{\phi_\alpha}(B)\Omega_{\phi_\alpha}) = (R_\phi(A^*)\Omega_\phi, E_\phi^\Gamma(0)R_\phi(B)\Omega_\phi).$$

Hence we may rewrite Eq. (3.21) as

$$(U_\phi(\lambda x)R_\phi(A^*)\Omega_\phi, R_\phi(B)\Omega_\phi) \to (R_\phi(A^*)\Omega_\phi, E_\phi^\Gamma(0)R_\phi(B)\Omega_\phi), \quad \text{as} \quad \lambda \to \infty, \forall A, B \in \mathfrak{U}, \quad x \neq 0.$$

Therefore, because $R_\phi(\mathfrak{U})\Omega_\phi$ is dense in $\mathfrak{H}_\phi$ and because $E^\Gamma(0)$ is a projection operator, it follows that $U_\phi(\lambda x) \to E_\phi^\Gamma(0)$, weakly, as $\lambda \to \infty$, $\forall\, x \neq 0$. QED

Lemma 3.3: Let ϕ_ψ be a vector state on $\mathfrak{U}$ corresponding to $\psi \in \mathfrak{H}_\phi$, i.e., $\phi_\psi(A) \equiv (\psi, R_\phi(A)\psi)$. Then $\phi_\psi \in \mathcal{C}_L$ if $\phi \in \mathcal{C}_L$.

Proof: Let $\phi \in \mathcal{C}_L$, and let $A = \tilde{A}_\Lambda \otimes I_\Lambda$ $(\in \mathfrak{U}_\Lambda)$. Then it follows from Eq. (3.10) and our definition of ϕ_ψ that

$$\phi_\psi(A) = (\psi, (W_\Lambda \tilde{A}_\Lambda W^{-1} \otimes \hat{\jmath}_\Lambda)\psi).$$

Hence, proceeding as in the theorem of Ref. 4, we find that there exists a density matrix σ_ψ in $\tilde{\mathcal{H}}_\Lambda$ such that

$$\phi_\psi(\tilde{A}_\Lambda \otimes I_\Lambda) = T\gamma_{\tilde{\mathcal{H}}_\Lambda}(\sigma_\psi \tilde{A}_\Lambda), \quad \forall\, \tilde{A}_\Lambda \in \tilde{\mathfrak{U}}_\Lambda.$$

Thus, ϕ_ψ is locally normal.

Corollary 1: If $\phi \in \mathcal{C}_L$ and $\phi = \alpha\phi_1 + (1-\alpha)\phi_2$, with $0 < \alpha < 1$ and $\phi_1, \phi_2 \in \mathcal{C}$, then $\phi_1, \phi_2 \in \mathcal{C}_L$.

Proof: Corresponding to $\phi = \alpha\phi_1 + (1-\alpha)\phi_2$, we have

$$\mathfrak{H}_\phi = \mathfrak{H}_{\phi_1} \oplus \mathfrak{H}_{\phi_2},$$
$$R_\phi = R_{\phi_1} \oplus R_{\phi_2},$$

and

$$\Omega_\phi = \alpha^{\frac{1}{2}}\Omega_{\phi_1} \oplus (1-\alpha)^{\frac{1}{2}}\Omega_{\phi_2}.$$

Thus ϕ_1, ϕ_2 are vector states corresponding to Ω_{ϕ_1}, $\Omega_{\phi_2} \in \mathfrak{H}_\phi$ and, hence, if $\phi \in \mathcal{C}_L$, then $\phi_1, \phi_2 \in \mathcal{C}_L$. QED

Corollary 2: If $\phi \in \mathcal{C}_L \cap \mathcal{C}_\Gamma$ (resp $\mathcal{C}_L \cap \mathcal{C}_T$) and if $\phi = \alpha\phi_1 + (1-\alpha)\phi_2$, where $\phi_1, \phi_2 \in \mathcal{C}_\Gamma$ (resp $\mathcal{C}_T$) and $0 < \alpha < 1$, then $\phi_1, \phi_2 \in \mathcal{C}_L \cap \mathcal{C}_\Gamma$ (resp $\mathcal{C}_L \cap \mathcal{C}_T$).

Proof: This follows immediately from Corollary 1. QED

4. REPRESENTATION OF ALL LOCAL OBSERVABLES

Let $\mathcal{Q}_F^0$ denote the set of all closed, densely defined operators in $\mathcal{H}_F$. We define $\mathcal{Q}_\Lambda$ to be the subset of $\mathcal{Q}_F^0$ affiliated to $\mathfrak{U}_\Lambda$, i.e., $\mathcal{Q}_\Lambda = \{Q \mid Q \in \mathcal{Q}_F^0,\ BQ \subseteq QB\ \forall\, B \in \mathfrak{U}_\Lambda'\}$, and we define $\mathcal{Q}_L = \bigcup_{\Lambda \in L} \mathcal{Q}_\Lambda$. Thus $\mathfrak{U}_\Lambda$ (resp $\mathfrak{U}_L$) is the set of all bounded elements of $\mathcal{Q}_\Lambda$ (resp $\mathcal{Q}_L$). It will be assumed that the self-adjoint elements of $\mathcal{Q}_L$ correspond to the local observables of the system.

It follows from the above definition that $\mathcal{Q}_\Lambda$ is isotonic w.r.t. Λ, i.e., $(\mathcal{Q}_\Lambda \supset \mathcal{Q}_{\Lambda'}) \Leftrightarrow (\Lambda \supset \Lambda')$. Corresponding to each $Q \in \mathcal{Q}_L$, we define

$$\Sigma_Q = \{\Lambda \mid \Lambda \in L,\ Q \in \mathcal{Q}_\Lambda\}.$$

Thus, in view of the isotony of $\mathcal{Q}_\Lambda$ w.r.t. Λ, it follows that, if $\Lambda \in \Sigma_Q$ and $\Lambda' \supset \Lambda$, then $\Lambda \in \Sigma_Q$.

Let $\tilde{\mathcal{Q}}_\Lambda^0$ be the set of all closed, densely defined operators in $\tilde{\mathcal{H}}_\Lambda$. Then it follows from Theorem 2.3 that $\mathcal{Q}_\Lambda$ induces a subset $\tilde{\mathcal{Q}}_\Lambda$ of $\tilde{\mathcal{Q}}_\Lambda^0$ in $\tilde{\mathcal{H}}_\Lambda$, this subset being defined[16] by $\mathcal{Q}_\Lambda = \tilde{\mathcal{Q}}_\Lambda \otimes \hat{I}_\Lambda$. Hence, if $\Lambda \in \Sigma_Q$, then Q induces an operator $\tilde{Q}_\Lambda$ $(\in \tilde{\mathcal{Q}}_\Lambda)$ in $\tilde{\mathcal{H}}_\Lambda$, where $Q = \tilde{Q}_\Lambda \otimes \hat{I}_\Lambda$.

We extend the spatial and temporal translation operators, γ_x and τ_t, from $\mathfrak{U}_L$ to $\mathcal{Q}_L$ by the prescriptions

$$\gamma_x Q = U_F(x)QU_F(x)^{-1}, \quad \forall\, Q \in \mathcal{Q}_L, \tag{4.1}$$

and

$$\tau_t Q = V_F(t)QV_F(t)^{-1}, \quad \forall\, Q \in \mathcal{Q}_L. \tag{4.2}$$

It follows from Eq. (4.1) that, since E_F commutes with $U_F(x)$, then $\gamma_x\mathcal{Q}_\Lambda = \mathcal{Q}_{\Lambda+x}$ and thus $\gamma_x\mathcal{Q}_L = \mathcal{Q}_L$. On the other hand, Eq. (4.2) does not necessarily imply that $\tau_t\mathcal{Q}_L = \mathcal{Q}_L$.

The following definition serves to extend the representation R_ϕ from $\mathfrak{U}$ to $\mathfrak{U} \bigcup \mathcal{Q}_L$, in cases where $\phi \in \mathcal{C}_L$.

Definition 4.1: Let $Q \in \mathcal{Q}_L$, $\Lambda \in \sum_Q$, $Q = \tilde{Q}_\Lambda \otimes \hat{I}_\Lambda$, and $\phi \in \mathcal{C}_L$. Then we extend Eq. (3.10) from $\mathfrak{U}_\Lambda$ to $\mathcal{Q}_\Lambda$ by defining $R_\phi(Q) = W_\Lambda \tilde{Q}_\Lambda W^{-1} \otimes \hat{\jmath}_\Lambda$.

Note: Since W_Λ is an isometry of $\tilde{\mathcal{H}}_\Lambda$ onto $\tilde{\mathfrak{H}}_\Lambda$, it follows from Theorem 2.3 that $R_\phi(Q)$ is a closed, densely defined operator in $\mathfrak{H}_\phi$.

The next theorem [specifically parts (ii), (iii), (v), (vii)] shows that Definition 4.1 provides a consistently defined $*$-homomorphism R_ϕ of $\mathcal{Q}_L$ into the closed, densely defined operators in $\mathfrak{H}_\phi$.

Theorem 4.1: Let $\phi \in \mathcal{C}_L$ and let $Q, Q' \in \mathcal{Q}_L$. Then:

(i) $R_\phi(Q) = (\mathrm{s}, \mathfrak{H}_\phi)\text{-}\lim_{\lambda \to \infty} R_\phi(Q_\lambda)$, with Q_λ defined as in Sec. 2;

(ii) $R_\phi(Q)$ is independent of the choice of Λ from Σ_Q in Ref. 4, Sec. 1;

(iii) $R_\phi(Q^*) = (R_\phi(Q))^*$;

(iv) $R_\phi((Q_\lambda)^*) \to R_\phi(Q^*)$, strongly, on $D_{R_\phi(Q^*)}$ as $\lambda \to \infty$;

(v) if $(Q + Q') \in \mathfrak{Q}_L$, then $R_\phi(Q) + R_\phi(Q') \subseteq R_\phi(Q + Q')$;

(vi) if $QQ' \in \mathfrak{Q}_L$, then $R_\phi(Q)R_\phi(Q') \subseteq R_\phi(QQ')$.

Proof:

(i) Let Q, Q_λ, $\tilde{Q}_\Lambda$, and $\tilde{Q}_{\Lambda\lambda}$ correspond to Q, Q_λ, $\tilde{Q}$, and $\tilde{Q}_\lambda$, respectively, of Theorem 2.5 (with $\mathcal{H}_F$, $\tilde{\mathcal{H}}_\Lambda$, and $\hat{\mathcal{H}}_\Lambda$ corresponding to $\mathcal{H}$, $\tilde{\mathcal{H}}_1$, and $\hat{\mathcal{H}}$). Since $Q \in \mathfrak{Q}_\Lambda$, it follows from the definition of $\mathfrak{Q}_\Lambda$ that Q^*, Q^*Q, E_λ, and $Q_\lambda \in \mathfrak{Q}_\Lambda$. Since by Theorem 2.1(ii) Q_λ is a bounded operator (for $\lambda < \infty$), it follows that $Q_\lambda \in \mathfrak{U}_\Lambda$ and, correspondingly, that $\tilde{Q}_{\Lambda\lambda} \in \mathfrak{U}_\Lambda$. Hence, by Theorem 2.5(ii) and Eq. (3.10),

$$Q_\lambda = \tilde{Q}_{\Lambda\lambda} \otimes \hat{I}_\Lambda \tag{4.3}$$

and

$$R_\phi(Q_\lambda) = W_\Lambda \tilde{Q}_{\Lambda\lambda} W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda. \tag{4.4}$$

Since W_Λ is an isometric transformation from $\tilde{\mathcal{H}}_\Lambda$ onto $\tilde{\mathfrak{H}}_\Lambda$, it follows from Theorem 2.1(v) that

$$(\mathrm{s}, \tilde{\mathfrak{H}}_\Lambda)\text{-}\lim_{\lambda\to\infty} W_\Lambda \tilde{Q}_{\Lambda\lambda} W_\Lambda^{-1} = W_\Lambda \tilde{Q}_\Lambda W_\Lambda^{-1}. \tag{4.5}$$

Moreover, we may apply Theorem 2.5(iv) to Eq. (4.4) in the form

$$(\mathrm{s}, \mathfrak{H}_\phi)\text{-}\lim_{\lambda\to\infty} R_\phi(Q_\lambda) = [(\mathrm{s}, \tilde{\mathfrak{H}}_\Lambda)\text{-}\lim_{\mu\to\infty} (W_\Lambda Q_{\Lambda\mu} W_\Lambda^{-1})] \otimes \hat{\mathfrak{J}}_\Lambda,$$

i.e., by Definition 4.1 and Eq. (4.5),

$$(\mathrm{s}, \mathfrak{H}_\phi)\text{-}\lim_{\lambda\to\infty} R_\phi(Q_\lambda) = R_\phi(Q).$$

(ii) Since $R_\phi(Q_\lambda) \in R_\phi(\mathfrak{U})$, it follows that $R_\phi(Q_\lambda)$ is independent of the choice of Λ from Σ_Q. Hence, by (i), $R_\phi(Q)$ is likewise independent of this choice.

(iii) Since $Q = \tilde{Q}_\Lambda \otimes \hat{I}_\Lambda$, it follows from Theorem 2.4(i) and Definition 4.1 that

$$Q^* = \tilde{Q}_\Lambda^* \otimes \hat{I}_\Lambda,$$
$$R_\phi(Q^*) = W_\Lambda \tilde{Q}_\Lambda^* W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda,$$

and

$$(R_\phi(Q))^* = (W_\Lambda \tilde{Q}_\Lambda W_\Lambda^{-1})^* \otimes \hat{\mathfrak{J}}_\Lambda.$$

Hence, since W_Λ is isometric, $R_\phi(Q^*) = (R_\phi(Q))^*$.

(iv) Since R_ϕ is a $*$-representation of $\mathfrak{U}$, it follows from Eq. (4.4) that $R_\phi((Q_\lambda)^*) = W_\Lambda(\tilde{Q}_{\Lambda\lambda})^* W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda$. Hence, by Theorem 2.5(v),

$$R_\phi((Q_\lambda)^*) \to R_\phi(Q^*), \quad \text{strongly, on} \quad D_{R_\phi(Q^*)} \quad \text{as} \quad \lambda \to \infty.$$

(v) Assume that Q, Q' and $(Q + Q') \in \mathfrak{Q}_L$. Let $\Lambda_1 \in \Sigma_Q$, $\Lambda_2 \in \Sigma_{Q'}$, and $\Lambda_3 \in \Sigma_{Q+Q'}$. Then it follows from the isotony of $\mathfrak{Q}_\Lambda$ w.r.t. Λ that $\Lambda_1 \cup \Lambda_2 \cup \Lambda_3 \in \Sigma_Q \cap \Sigma_{Q'} \cap \Sigma_{Q+Q'}$. Thus, denoting $\Lambda_1 \cup \Lambda_2 \cup \Lambda_3$ by Λ, we find from Theorem 2.4(ii) that

$$Q = \tilde{Q}_\Lambda \otimes \hat{I}_\Lambda, \quad Q' = \tilde{Q}' \otimes \hat{I}_\Lambda,$$

and

$$Q + Q' = (\tilde{Q}_\Lambda + \tilde{Q}'_\Lambda) \otimes \hat{I}_\Lambda.$$

Consequently, by Definition 4.1,

$$R_\phi(Q) = W_\Lambda \tilde{Q}_\Lambda W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda,$$
$$R_\phi(Q') = W_\Lambda \tilde{Q}'_\Lambda W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda,$$

and

$$R_\phi(Q + Q') = W_\Lambda(\tilde{Q}_\Lambda + \tilde{Q}'_\Lambda) W_\Lambda^{-1} \otimes \hat{\mathfrak{J}}_\Lambda.$$

Hence, by Theorem 2.4(iv), $R_\phi(Q) + R_\phi(Q') \subseteq R_\phi(Q + Q')$.

(vi) Similarly, it follows from Theorem 2.4(iii), (v) and Definition 4.1 that, if Q, Q' and $QQ' \in \mathfrak{Q}_L$, then $R_\phi(Q)R_\phi(Q') \subseteq R_\phi(QQ')$. QED

Definition 4.2:

(i) For $\phi \in \mathfrak{C}_L \cap \mathfrak{C}_\Gamma^0$, we define

$$R_\phi(\gamma_x Q) = U_\phi(x) R_\phi(Q) U_\phi(x)^{-1}, \quad \forall\, Q \in \mathfrak{Q}_L.$$

(ii) For $\phi \in \mathfrak{C}_L \cap \mathfrak{C}_\Gamma^0$, we define

$$R_\phi(\tau_t Q) = V_\phi(t) R_\phi(Q) V_\phi(t)^{-1}, \quad \forall\, Q \in \mathfrak{Q}_L.$$

Note: These definitions serve to extend Eqs. (3.11) and (3.13) for $R(\gamma_x \cdots)$, $R(\tau_t \cdots)$ from $\mathfrak{U}$ to $\mathfrak{U} \cup \mathfrak{Q}_L$. Further, these definitions are consistent with Definition 4.1. For, if $\phi \in \mathfrak{C}_L \cap \mathfrak{C}_\Gamma^0$ and $Q \in \mathfrak{Q}_L$, then $\gamma_x \in \mathfrak{Q}_L$ It follows, from Eq. (4.1) and the definition of Q_λ in Sec. 2, that $(\gamma_x Q)_\lambda = \gamma_x(Q_\lambda)$. Hence, by Theorem 4.1(i) and Eq. (3.11), the value of $R_\phi(\gamma_x Q)$ that follows from Definition 4.1 is given by

$$\begin{aligned}(\mathrm{s}, \mathfrak{H}_\phi)\text{-}\lim_{\lambda\to\infty} R_\phi((\gamma_x Q)_\lambda) &= (\mathrm{s}, \mathfrak{H}_\phi)\text{-}\lim_{\lambda\to\infty} R_\phi(\gamma_x Q_\lambda) \\ &= (\mathrm{s}, \mathfrak{H}_\phi)\text{-}\lim_{\lambda\to\infty} U_\phi(x) R_\phi(Q_\lambda) U_\phi(x)^{-1} \\ &= U_\phi(x) R_\phi(Q) U_\phi(x)^{-1},\end{aligned}$$

in accordance with Definition 4.2(i). Likewise, Definition 4.2(ii) is consistent with Definition 4.1 in cases where $\tau_t Q \in \mathfrak{Q}_L$, these being the only cases where the question of inconsistency could arise.

Definition 4.3: For $\phi \in \mathfrak{C}_L$, we define

$$\mathfrak{K}_\phi = \{Q \mid Q \in \mathfrak{Q}_L, \Omega_\phi \in D_{R_\phi(Q)}\}.$$

Thus, it follows from this definition and Eq. (3.12) that, if $\phi \in \mathfrak{C}_L \cap \mathfrak{C}_\Gamma^0$ and $Q \in \mathfrak{K}_\phi$, then $\gamma_x Q \in \mathfrak{K}_\phi$.

Likewise, if $\phi \in \mathcal{C}_L \cap \mathcal{C}_T^0$ and $Q \in \mathcal{K}_\phi$, then $\Omega_\phi \in D_{R_\phi(\tau_t Q)}$.

Definition 4.4:

(i) For $\phi \in \mathcal{C}_L$ and $Q, Q' \in \mathcal{K}_\phi$, we define

$$G_\phi(Q^*, Q') = (R_\phi(Q)\Omega_\phi, R_\phi(Q')\Omega_\phi).$$

(ii) For $\phi \in \mathcal{C}_L \cap \mathcal{C}_\Gamma^0$ and $Q, Q' \in \mathcal{K}_\phi$, we define

$$G_\phi^\Gamma(Q^*, Q' \mid x) = (R_\phi(\gamma_x Q)\Omega_\phi, R_\phi(Q')\Omega_\phi) = (U_\phi(x)R_\phi(Q)\Omega_\phi, R_\phi(Q')\Omega_\phi),$$

by Eq. (3.12) and Definition 4.2(i).

(iii) For $\phi \in \mathcal{C}_L \cap \mathcal{C}_T^0$ and $Q, Q' \in \mathcal{K}_\phi$, we define

$$G_\phi^T(Q^*, Q' \mid t) = (R_\phi(\tau_t Q)\Omega_\phi, R_\phi(Q')\Omega_\phi) = (V_\phi(t)R_\phi(Q)\Omega_\phi, R_\phi(Q')\Omega_\phi),$$

by Eq. (3.14) and Definition 4.2(ii).

(iv) For $\phi \in \mathcal{C}_L \cap \mathcal{C}_T^0$ and $Q^*, Q'^* \in \mathcal{K}_\phi$, we define

$$F_\phi^T(Q', Q^* \mid t) = \overline{(R_\phi(Q'^*)\Omega_\phi, R_\phi(\tau_t Q^*)\Omega_\phi)} = \overline{G_\phi^T(Q, Q'^* \mid t)}.$$

Note: The above definition for G_ϕ (resp G_ϕ^Γ, G_ϕ^T) represents the correlation between Q (resp $\gamma_x Q$, $\tau_t Q$) and Q' for the state ϕ. In cases where $Q, Q' \in \mathfrak{U}$, then $G_\phi(Q^*, Q)$, $G_\phi^\Gamma(Q^*, Q' \mid x)$, $G_\phi^T(Q^*, Q \mid t)$ reduce to $\phi(Q^*Q)$, $\phi((\gamma_x Q^*)Q)$, and $\phi((\tau_t Q^*)Q)$, respectively.

Lemma 4.1: If $\phi \in \mathcal{C}_L$ and $Q, Q' \in \mathfrak{A}_L$, then:

(i) $Q \in \mathcal{K}_\phi$ if and only if

$$\phi((Q_\lambda)^* Q_\lambda) \; [\equiv \|R_\phi(Q_\lambda)\Omega_\phi\|^2]$$

is a bounded function of λ.

(ii) If $Q, Q' \in \mathcal{K}_\phi$, then $\phi((Q_\lambda)^* Q'_{\lambda'}) \to G_\phi(Q^*, Q')$, as λ, λ' tend independently to ∞, and

$$|\phi((Q_\lambda)^*{}'_\lambda))| \leq \|R_\phi(Q)\Omega_\phi\| \, \|R_\phi(Q')\Omega_\phi\|.$$

(iii) If $\phi \in \mathcal{C}_\Gamma^0$ and $Q, Q' \in \mathcal{K}_\phi$, then

$$\phi((\gamma_x Q_\lambda)^* Q'_{\lambda'}) \to G_\phi^\Gamma(Q^*, Q' \mid x),$$

uniformly w.r.t. x, as λ, λ' tend independently to ∞, and $|\phi((\gamma_x Q_\lambda)^* Q'_{\lambda'})| \leq \|R_\phi(Q)\Omega_\phi\| \, \|R_\phi(Q')\Omega_\phi\|$.

(iv) If $\phi \in \mathcal{C}_T^0$ and $Q, Q' \in \mathcal{K}_\phi$, then

$$\phi((\tau_t Q_\lambda)^* Q'_{\lambda'}) \to G_\phi^T(Q^*, Q't),$$

uniformly w.r.t. t, as λ, λ' tend independently to ∞, and

$$|\phi((\tau_t Q_\lambda)^* Q'_{\lambda'})| \leq \|R_\phi(Q)\Omega_\phi\| \, \|R_\phi(Q')\Omega_\phi\|.$$

Proof: As W_Λ is an isometric transformation from $\tilde{\mathcal{H}}_\Lambda$ to $\tilde{\mathfrak{H}}_\Lambda$, then

(i) follows from Theorem 2.5(iii) and Definition 4.1,

(ii) follows from Theorem 2.5(iii), Theorem 4.1(i), Definition 4.1, and Definition 4.4(i),

(iii) follows from Theorem 2.5(iii), Theorem 4.1(i), Definition 4.1, Definition 4.4(ii), and the unitarity of $U_\phi(x)$, and

(iv) follows from Theorem 2.5(iii), Theorem 4.1(i), Definition 4.1, Definition 4.4(iii), and the unitarity of $V_\phi(t)$. QED

Theorem 4.2: If $\phi \in \mathcal{C}_L \cap \mathcal{C}_{\mathrm{KMS}}$ and if $Q, Q', Q^*, Q'^* \in \mathcal{K}_\phi$, then the KMS boundary conditions may be extended to $G_\phi^T(Q^*, Q' \mid t)$ and $F_\phi^T(Q', Q^* \mid t)$. Thus, there is a real positive θ such that:

(i) $G_\phi^T(Q^*, Q' \mid s)$ can be analytically continued into the strip $0 > \operatorname{Im} s > -\theta$ and is continuous on its boundaries;

(ii) $F_\phi^T(Q', Q'' \mid s)$ can be analytically continued into the strip $\theta > \operatorname{Im} s > 0$ and is continuous on its boundaries;

(iii) $G_\phi^T(Q^*, Q \mid t - i\theta) = F_\phi^T(Q', Q^* \mid t), \quad \forall\, t \in T.$

Proof: Let $\phi \in \mathcal{C}_{\mathrm{KMS}}$. Then, since $Q_\lambda, Q'_{\lambda'} \in \mathfrak{U}$, $\forall\, \lambda, \lambda' < \infty$, it follows from Eq. (3.16) that

$$\int dt \phi(Q'_{\lambda'}(\tau_t Q_\lambda)^*) f_\theta(t) = \int dt \phi((\tau_t Q_\lambda)^* Q'_{\lambda'}) f_\theta(t), \quad \forall\, \lambda, \lambda' < \infty, \; f \in \mathfrak{D}. \tag{4.6}$$

Further, it follows from Lemma 4.1(iv) and Lebesgue's theorem that, if $Q, Q' \in \mathcal{K}_\phi$, then

$$\int dt \phi((\tau_t Q_\lambda)^* Q'_{\lambda'}) f_\theta(t) \to \int dt G_\phi^T(Q^*, Q' \mid t) f_\theta(t) \quad \text{as} \quad \lambda, \lambda' \to \infty. \tag{4.7}$$

Likewise, it follows from Lemma 4.1(iv), Definition 4.4(iv), and Lebesgue's theorem that, if $Q^*, Q'^* \in \mathcal{K}_\phi$, then

$$\int dt \phi(Q'_{\lambda'}(\tau_t Q_\lambda)^*) f_\theta(t) \to \int dt F_\phi^T(Q', Q^* \mid t) f_\theta(t) \quad \text{as} \quad \lambda, \lambda' \to \infty. \tag{4.8}$$

Hence, by Eqs. (4.6)–(4.8),

$$\int dt F_\phi^T(Q', Q^* \mid t) f_\theta(t) = \int dt G_\phi^T(Q^*, Q' \mid t) f_\theta(t), \quad \forall\, f \in \mathfrak{D}.$$

This equation is equivalent to the above-defined KMS boundary conditions for G_ϕ^T and F_ϕ^T (cf. Ref. 1). QED

Definition 4.5: If $\phi \in \mathcal{C}_L \cap \mathcal{C}_\Gamma^0$ and C_ϕ^Γ is the space-correlation function defined by

$$C_\phi^\Gamma(Q^*, Q' \mid x) = G_\phi^\Gamma(Q^*, Q' \mid x) - G_\phi^\Gamma(Q^*, I) G_\phi^\Gamma(I, Q'), \quad \forall\, Q, Q' \in \mathcal{K}_\phi,$$

then:

(i) ϕ is said to be weakly clustering if, for all Q, $Q' \in \mathcal{K}_\phi$, $MC_\phi^\Gamma(Q^*, Q' \mid x)$ exists and is zero (M being defined as in Definition 3.1);

(ii) ϕ is said to be strongly clustering if, for all Q, $Q' \in \mathcal{K}_\phi$ and $x \neq 0$, $C_\phi^\Gamma(Q^*, Q' \mid \lambda x) \to 0$ as $\lambda \to \infty$;

(iii) ϕ is said to possess weak long-range order (WLRO) if $\exists\, Q, Q' \in \mathcal{K}_\phi$ such that $MC_\phi^\Gamma(Q^*, Q' \mid x)$ exists and is nonzero;

(iv) ϕ is said to possess long-range order (LRO) if $\exists\, Q, Q' \in \mathcal{K}_\phi$ such that, for all $x \in \Gamma \setminus 0$, $C_\phi^\Gamma(Q, Q' \mid \lambda x)$ tends, as $\lambda \to \infty$, to a nonzero limit whose value is independent of x.

Theorem 4.3:

(i) The elements of $\mathcal{C}_L \cap \mathcal{E}_\Gamma$ are weakly clustering;
(ii) the elements of $\mathcal{C}_L \cap \mathcal{F}_\Gamma$ are strongly clustering;
(iii) the elements of $\mathcal{C}_L \cap (\mathcal{C}_\Gamma \setminus \mathcal{E}_\Gamma)$ possess WLRO;
(iv) the elements of $\mathcal{C}_L \cap (\mathcal{F}_\Gamma^c \setminus \mathcal{F}_\Gamma)$ possess LRO.

Proof: Let $Q, Q' \in \mathcal{K}_\phi$. We define

$$S_\phi^\Gamma(Q^*, Q') = ([E_\phi^\Gamma(0) - E(\Omega_\phi)]R_\phi(Q)\Omega_\phi, R_\phi(Q')\Omega_\phi). \tag{4.9}$$

It follows from Lemma 3.2 and Definitions 4.4 and 4.5 that

$$MC_\phi^\Gamma(Q^*, Q' \mid x) = S_\phi^\Gamma(Q^*, Q'), \quad \forall\, \phi \in \mathcal{C}_L \cap \mathcal{C}_\Gamma, \tag{4.10}$$

and it follows from Lemma 3.1 and Definitions 4.4 and 4.5 that

$$C_\phi^\Gamma(Q^*, Q' \mid \lambda x) \to S_\phi^\Gamma(Q^*, Q'), \quad \forall\, \phi \in \mathcal{C}_L \cap \mathcal{F}_\Gamma^c, x \in \Gamma \setminus 0. \tag{4.11}$$

Further, it follows from the definition of $\mathcal{E}_\Gamma$ that $E_\phi^\Gamma(0) - E(\Omega_\phi) = 0$ if and only if $\phi \in \mathcal{E}_\Gamma$. Thus, by Eq. (4.9),

$$S_\phi^\Gamma(Q^*, Q') = 0, \quad \forall\, \phi \in \mathcal{C}_L \cap \mathcal{E}_\Gamma. \tag{4.12}$$

On the other hand, if $\phi \in \mathcal{C}_L \cap (\mathcal{C}_\Gamma \setminus \mathcal{E}_\Gamma)$, then $E_\Gamma^\phi(0) - E(\Omega_\phi) \equiv P_\phi$, say, is a nonnull projection operator in $\mathfrak{H}_\phi$. Thus, since $R_\phi(\mathcal{K}_\phi)\Omega_\phi [\supseteq R_\phi(\mathcal{U}_L)\Omega_\phi]$ is dense in $\mathfrak{H}_\phi$, it follows that $P_\phi R_\phi(\mathcal{K}_\phi)\Omega_\phi$ is dense in the proper subspace $P_\phi \mathfrak{H}_\phi$ of $\mathfrak{H}_\phi$ and, therefore, by Eq. (4.9), $\exists\, Q, Q' \in \mathcal{K}_\phi$ for which $S_\Gamma^\phi(Q^*, Q')$ [$\equiv (P_\phi R_\phi(Q)\Omega_\phi, P_\phi R_\phi(Q')\Omega_\phi)$] is nonzero.

In view of the fact that $\mathcal{F}_\Gamma \subseteq \mathcal{E}_\Gamma$ and $\mathcal{F}_\Gamma^c \setminus \mathcal{F}^\Gamma \subseteq \mathcal{C}_\Gamma \setminus \mathcal{E}_\Gamma$, it is evident that this result, together with Eqs. (4.10)–(4.12), constitutes a proof of the theorem. QED

Remark: Suppose that

(i) $\phi \in \mathcal{C}_L \cap \mathcal{C}_\Gamma$,
(ii) ϕ is invariant under some group G,
(iii) $\phi = \alpha\phi_1 + (1 - \alpha)\phi_2$, where $\phi_1, \phi_2 \in \mathcal{C}_\Gamma$, and $1 > \alpha > 0$ and where ϕ_1 and ϕ_2 are not invariant under G.

Then it follows from Theorem 4.3 that ϕ possesses WLRO (possibly LRO). Thus we have a connection between symmetry breakdown and (possibly weak) long-range order. In particular, one may base the theory of long-range order in a superfluid phase, proposed by Penrose and Onsager[17] and by Yang,[18] on the assumption of gauge symmetry breakdown.

Theorem 4.4: If $\phi \in \mathcal{C}_L \cap \mathcal{C}_T$ and C_ϕ^T is the time-correlation function defined by $C_\phi^T(Q^*, Q' \mid t) = G_\phi^T(Q^*, Q \mid t) - G_\phi(Q^*, I)G_\phi(I, Q')$, $\forall\, Q, Q' \in \mathcal{K}_\phi$, then

(i) if $\phi \in \mathcal{E}_T$,

$$\frac{1}{t_0}\int_0^{t_0} dt C_\phi^T(Q^*, Q' \mid t) \to 0 \quad \text{as} \quad t_0 \to \infty, \qquad \forall\, Q, Q' \in \mathcal{K}_\phi$$

and

(ii) $\phi \in \mathcal{C}_T \setminus \mathcal{E}_T$, then $\exists\, Q, Q' \in \mathcal{K}_\phi$ such that

$$t_0^{-1}\int_0^{t_0} dt C_\phi^T(Q^*, Q' \mid t)$$

tends to a nonzero limit as $t_0 \to \infty$.

Proof: This is easily established, using Lemma 3.1(ii), by direct analogy with Theorem 4.3(i), (iii).

5. GIBBS STATES

We shall now extend the theory of Gibbs states, as formulated by Haag *et al.*,[1] so as to include the operators $\mathfrak{A}_L$.

Thus, following Haag *et al.*, we start by constructing an increasing sequence $\{\Lambda_n\}$ of subsets of Γ, such that $\bigcup_n \Lambda_n = \Gamma$. It follows from the isotony of $\mathfrak{U}_\Lambda$ w.r.t. Λ that, if $\Lambda \in \mathfrak{U}_L$, then $\exists\, n_0$ ($< \infty$). We have $A \in \mathfrak{U}_{\Lambda_n}$, $\forall\, n > n_0$. Hence, by Eq. (3.3),

$$A = \tilde{A}_{\Lambda_n} \otimes \hat{I}_{\Lambda_n}, \quad \forall\, n > n_0. \tag{5.1}$$

We associate with each Λ_n a 1-parameter group $\{V_F^{(n)}(t)\}$ of unitary transformations of $\tilde{\mathcal{H}}_{\Lambda_n}$ and a density matrix $\rho^{(n)}$ in $\tilde{\mathcal{H}}_{\Lambda_n}$. Correspondingly, we define a group of automorphisms $\{\tau_t^{(n)}\}$ of $\mathfrak{U}_{\Lambda_n}$ and a linear

functional $\phi^{(n)}$ on $\mathfrak{U}_{\Lambda_n}$ by

$$\tau_t^{(n)}A = V_F^{(n)}(t)\tilde{A}_{\Lambda_n}[V_F^{(n)}(t)]^{-1} \otimes \hat{I}_{\Lambda_n}, \quad \forall\, A \in \mathfrak{U}_{\Lambda_n}, \tag{5.2}$$

and

$$\phi^{(n)}(A) = \mathrm{Tr}_{\mathcal{K}_{\Lambda_n}}(\rho^{(n)}\tilde{A}_{\Lambda_n}), \quad \forall\, A \in \mathfrak{U}_{\Lambda_n}. \tag{5.3}$$

We assume that $\phi^{(n)}$ and $\tau_t^{(n)}$ have the following properties:

(i) $\rho^{(n)}$ commutes with $V_F^{(n)}(t)$ and, thus, $\phi^{(n)}$ is stationary w.r.t. $\tau_t^{(n)}$:

$$\phi^{(n)}(\tau_t^{(n)}A) \equiv \phi^{(n)}(A);$$

(ii) for $A \in \mathfrak{U}_L$ and fixed t, $\tau_t^{(n)}A$ converges normwise in $\mathcal{K}_F$, as $n \to \infty$, to

$$\tau_t A \equiv V_F(t)AV_F(t)^{-1},$$

where $\{V_F(t)\}$ is a 1-parameter group of unitary transformations of $\mathcal{K}_F$, which is independent of A.

(iii) for $A \in \mathfrak{U}_L$, the sequence $\phi^{(n)}(A)$ converges, as $n \to \infty$, to a quantity $\phi(A)$, i.e.,

$$\phi^{(n)}(A) \to \phi(A) \quad \text{as} \quad n \to \infty, \quad \forall\, A \in \mathfrak{U}_L. \tag{5.4}$$

The group[19] $\{\tau_t\}$ and the functional ϕ can then be extended from $\mathfrak{U}_L$ to $\mathfrak{U}$ by continuity. We shall refer to the resultant state ϕ as a Gibbs state, thereby generalizing somewhat the sense in which this term is usually employed.[20]

It follows from the above construction that $\phi \in \mathcal{C}_T^0$ and that (ϕ, τ_t) possesses the following properties (cf. Ref. 1):

(a) if $(\phi^{(n)}, \tau_t^{(n)})$ satisfies the KMS boundary conditions, $\forall\, n > n_0$, then so too does (ϕ, τ_t);

(b) $\phi^{(n)}((\tau_t^{(n)}A)B) \to \phi((\tau_t A)B)$ as $n \to \infty$, for fixed t,

$$\forall\, A, B \in \mathfrak{U}_L. \tag{5.5}$$

It will be assumed in the sequel that $\phi \in \mathcal{C}_L$.

We now incorporate $\mathfrak{Q}_L$ into this scheme. For this purpose we note that, as $\mathfrak{Q}_\Lambda$ is isotonic w.r.t. Λ, it follows that, if $Q \in \mathfrak{Q}_L$, then $\exists\, N_0$ $(< \infty)$ such that $\Lambda_n \in \Sigma_Q$, $\forall\, n > N_0$. Thus

$$Q = \tilde{Q}_{\Lambda_n} \otimes \hat{I}_{\Lambda_n}, \quad \forall\, n > N_0. \tag{5.6}$$

Correspondingly, we define

$$\tau_t^{(n)}Q = V_F^{(n)}(t)\tilde{Q}_{\Lambda_n}[V_F^{(n)}(t)]^{-1} \otimes \hat{I}_{\Lambda_n}. \tag{5.7}$$

Let $\tilde{\mathfrak{K}}_\phi^{(n)} = \mathfrak{Q}_{\Lambda_n} \cap \Delta_\rho^{(n)}$, where Δ_ρ is defined as in Sec. 2. Then it follows from Eq. (5.6) and the commutativity of $\rho^{(n)}$ with $V_F^{(n)}(t)$ that, if $Q \in \tilde{\mathfrak{K}}_\phi^{(n)}$, then $\tau_t^{(n)}Q \in \tilde{\mathfrak{K}}_\phi^{(n)}$. It also follows that, if $Q, Q' \in \tilde{\mathfrak{K}}_\phi^{(n)}$, then $\mathrm{Tr}_{\mathcal{K}_{\Lambda_n}}(Q'_{\Lambda_n}\rho^{(n)}Q^*_{\Lambda_n})$ exists [cf. Eq. (2.6)] and, thus, we may define

$$G_\phi^{(n)}(Q^*, Q') = \mathrm{Tr}_{\mathcal{K}_{\Lambda_n}}(\tilde{Q}'_{\Lambda_n}\rho^{(n)}\tilde{Q}^*_{\Lambda_n}) \tag{5.8}$$

and

$$G_\phi^{(n)T}(Q^*, Q' \mid t) = G_\phi^{(n)}(\tau_t^{(n)}Q^*, Q'). \tag{5.9}$$

It is evident from Eqs. (5.3), (5.6), and (5.8) that $G^{(n)}(Q^*, Q')$ reduces to $\phi^{(n)}(Q^*Q')$ in cases where $Q, Q' \in \mathfrak{U}_L$. Also, as $V_F^{(n)}(t)$ commutes with $\rho^{(n)}$, it follows from Eqs. (5.7) and (5.8) that

$$G_\phi^{(n)}(\tau_t^{(n)}Q^*, \tau_t^{(n)}Q') = G_\phi^{(n)}(Q^*, Q'), \quad \forall\, t \in T. \tag{5.10}$$

It follows from Eqs. (5.3) and (5.8) and Theorems 2.2(ii) and 2.5(ii) that

$$\phi^{(n)}((Q_\lambda)^*Q_\lambda) \equiv G_\phi^{(n)}((Q_\lambda)^*, Q_\lambda) \to G_\phi^{(n)}(Q^*, Q) \quad \text{as} \quad \lambda \to \infty, \quad \forall\, Q \in \tilde{\mathfrak{K}}_\phi^{(n)}. \tag{5.11}$$

We now define $\tilde{\mathfrak{K}}_\phi$ to be the subset of $\bigcap_{N>N_0} \tilde{\mathfrak{K}}_\phi^{(n)}$ for which this convergence is uniform w.r.t. n.

Lemma 5.1: $\tilde{\mathfrak{K}}_\phi \subseteq \mathfrak{K}_\phi$.

Proof: Let $Q \in \tilde{\mathfrak{K}}_\phi$. Then it follows from our definition of this set that, given $\epsilon > 0$, $\exists$ a finite $L(\epsilon)$ independent of n, such that, for $n > N_0$,

$$|\phi^{(n)}((Q_{\lambda'})^*Q_{\lambda'}) - \phi^{(n)}((Q_\lambda)^*Q_\lambda)| < \epsilon, \quad \forall\, \lambda' > \lambda > L(\epsilon). \tag{5.12}$$

Moreover, it follows from Eq. (5.4) that, if $A \in \mathfrak{U}_L$ and $|\phi^{(n)}(A)| < \epsilon, \forall\, n > N_0$, then $|\phi(A)| \leq \epsilon$. Hence, applying this result to Eq. (5.12), with

$$A = (Q_{\lambda'})^*Q_{\lambda'} - (Q_\lambda)^*Q_\lambda,$$

we find that

$$|\phi((Q_{\lambda'})^*Q_{\lambda'}) - \phi((Q_\lambda)^*Q_\lambda)| \leq \forall\, \lambda' > \lambda > L(\epsilon).$$

Thus $\phi((Q_\lambda)^*Q)$ converges to a finite limit as $\lambda \to \infty$ and, therefore, by Lemma 4.1(i), $Q \in \mathfrak{K}_\phi$. Hence, $\tilde{\mathfrak{K}}_\phi \subseteq \mathfrak{K}_\phi$. QED

Lemma 5.2: If $Q, Q' \in \tilde{\mathfrak{K}}_\phi$, then $\exists$ some finite n_0 such that, for $n > n_0$,

(i) $G_\phi^{(n)}(Q^*, Q)$ is uniformly bounded w.r.t. n and

(ii) $|G_\phi^{(n)T}(Q^*, Q' \mid t)|$ is uniformly bounded w.r.t. n and t.

Proof:

(i) We shall prove this part of the lemma by showing that, if $Q \in \tilde{\mathfrak{K}}_\phi$, then $G_\phi^{(n)}(Q^*, Q) \to G_\phi(Q^*, Q)$ $(< \infty$, by Lemma 5.1) as $n \to \infty$.

Let $Q \in \tilde{\mathfrak{K}}_\phi$. Then it follows from the definition of $\tilde{\mathfrak{K}}_\phi$ that, given $\epsilon > 0$, $\exists$ a finite $L(\epsilon)$, independent of n, such that

$$|G_\phi^{(n)}((Q_\lambda)^*, Q_\lambda) - G_\phi^{(n)}(Q^*, Q)| < \epsilon, \quad \forall\, \lambda > L(\epsilon). \tag{5.13}$$

Further, it follows from Theorem 4.1(i), Definitions 4.3 and 4.4, and Lemma 5.1 that, given $\epsilon > 0$, $\exists$ a finite $L_1(\epsilon)$ such that

$$|G_\phi((Q_\lambda)^*, Q_\lambda) - G_\phi(Q^*, Q)| < \epsilon, \quad \forall\, \lambda > L_1(\epsilon). \tag{5.14}$$

Finally, since $Q_\lambda \in \mathfrak{U}_L$, $\forall\, \lambda < \infty$, then

$$G_\phi^{(n)}((Q_\lambda)^*, Q_\lambda) \equiv \phi^{(n)}((Q_\lambda)^* Q_\lambda)$$

and

$$G_\phi((Q_\lambda)^*, Q_\lambda) \equiv \phi((Q_\lambda{}^* Q_\lambda))$$

and, thus, it follows from Eq. (5.4) that, given $\epsilon > 0$ and $\lambda < \infty$, $\exists$ a finite $N(\epsilon, \lambda)$ such that

$$|G_\phi^{(n)}((Q_\lambda)^*, Q_\lambda) - G_\phi((Q_\lambda)^*, Q_\lambda)| < \epsilon, \quad \forall\, n > N(\epsilon, \lambda). \tag{5.15}$$

Hence, defining $L_2(\epsilon) = 1 + \max(L_1(\epsilon), L(\epsilon))$ and $\bar{N}(\epsilon) = N(\epsilon, L_2(\epsilon))$, we find from Eqs. (5.13)–(5.15) that

$$|G_\phi^{(n)}(Q^*, Q) - G_\phi(Q^*, Q)| < 3\epsilon, \quad \forall\, n > N(\epsilon).$$

Thus, $G_\phi^{(n)}(Q^*, Q) \to G_\phi(Q^*, Q)$ as $n \to \infty$, as required.

(ii) Let Q, $Q' \in \tilde{\mathfrak{K}}_\phi$. Then it follows from Eqs. (2.6) and (5.8)–(5.10) that

$$\begin{aligned} |G_\phi^{(n)T}(Q^*, Q' \mid t)| &\equiv G_\phi^{(n)}(\tau_t^{(n)} Q^*, Q') \\ &\le [G_\phi^{(n)}(\tau_t^{(n)} Q^*, \tau_t^{(n)} Q)]^{\frac{1}{2}} [G_\phi^{(n)}(Q'^*, Q')]^{\frac{1}{2}} \\ &\equiv [G_\phi^{(n)}(Q^*, Q)]^{\frac{1}{2}} [G_\phi^{(n)}(Q'^*, Q')]^{\frac{1}{2}}. \end{aligned}$$

The required result follows immediately from this inequality, together with part (i) of this lemma. QED

Lemma 5.3: If Q, $Q' \in \tilde{\mathfrak{K}}_\phi$, then

$$G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t) \to G_\phi^{(n)T}(Q^*, Q' \mid t),$$

uniformly w.r.t. n and t, as λ, λ' tend independently to ∞.

Proof: Let Q, $Q' \in \tilde{\mathfrak{K}}_\phi$. Then, by Theorem 2.5(ii) and Eqs. (2.9) and (5.8)–(5.10),

$$\begin{aligned} &|G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t) - G_\phi^{(n)T}(Q^*, Q' \mid t)| \\ &\equiv |G_\phi^{(n)}((\tau_t^{(n)} Q_\lambda)^*, Q'_{\lambda'}) - G_\phi^{(n)}((\tau_t^{(n)} Q)^*, Q')| \\ &\le [G_\phi^{(n)}(\tau_t^{(n)} Q^*, \tau_t^{(n)} Q)]^{\frac{1}{2}} \\ &\quad \times [G_\phi^{(n)}(Q'^*, Q') - G_\phi^{(n)}((Q'_{\lambda'})^*, Q'_{\lambda'})]^{\frac{1}{2}} \\ &\quad + [G_\phi^{(n)}(Q'^*, Q')]^{\frac{1}{2}} [G_\phi^{(n)}(\tau_t^{(n)} Q^*, \tau_t^{(n)} Q) \\ &\qquad - G_\phi^{(n)}(\tau_t^{(n)}(Q_\lambda)^*, \tau_t^{(n)} Q_\lambda)]^{\frac{1}{2}} \\ &\equiv [G_\phi^{(n)}(Q^*, Q)]^{\frac{1}{2}} [G_\phi^{(n)}(Q'^*, Q') - G_\phi^{(n)}((Q'_{\lambda'})^*, Q'_{\lambda'})]^{\frac{1}{2}} \\ &\quad + [G_\phi^{(n)}(Q'^*, Q')]^{\frac{1}{2}} [G_\phi^{(n)}(Q^*, Q) - G_\phi^{(n)}((Q_\lambda)^*, Q_\lambda)]^{\frac{1}{2}}. \end{aligned}$$

Thus, by definition of $\tilde{\mathfrak{K}}_\phi$, the required result follows immediately from this inequality, together with Lemma 5.2(i). QED

Theorem 5.1: If Q, $Q' \in \tilde{\mathfrak{K}}_\phi$, then:

(i) $G_\phi^{(n)}(Q^*, Q') \to G_\phi(Q^*, Q')$ as $n \to \infty$;

(ii) $G_\phi^{(n)T}(Q^*, Q' \mid t) \to G_\phi^T(Q^*, Q' \mid t)$ as $n \to \infty$, for fixed t.

Thus, the theorem states that G_ϕ and G_ϕ^T are thermodynamical limits of the corresponding quantities $G_\phi^{(n)}$ and $G_\phi^{(n)T}$, for finite systems.

Proof: Since (i) is a special case of (ii), corresponding to $t = 0$, it suffices for us to prove (ii). For this purpose we note that

$$\begin{aligned} &|G_\phi^T(Q^*, Q' \mid t) - G_\phi^{(n)T}(Q^*, Q' \mid t)| \\ &\quad \le |G_\phi^T(Q^*, Q' \mid t) - G_\phi^T((Q_\lambda)^*, Q'_{\lambda'} \mid t)| \\ &\qquad + |G_\phi^T((Q_\lambda)^*, Q'_{\lambda'} \mid t) - G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t)| \\ &\qquad + |G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t) - G_\phi^{(n)T}(Q^*, Q' \mid t)|. \end{aligned} \tag{5.16}$$

Since Q_λ, $Q'_{\lambda'} \in \mathfrak{U}$, it follows from Lemma 4.1(iv) that, given $\epsilon > 0$, $\exists$ K_ϵ and K'_ϵ, independent of t, such that

$$|G_\phi^T(Q^*, Q' \mid t) - G_\phi^T((Q_\lambda)^*, Q'_{\lambda'} \mid t)| < \epsilon, \quad \forall\, \lambda > K_\epsilon, \lambda' > K'_\epsilon. \tag{5.17}$$

Further, since Q_λ, $Q'_{\lambda'} \in \mathfrak{U}_L$, $\forall\, \lambda, \lambda' < \infty$, it follows that

$$G_\phi^T((Q_\lambda)^*, Q'_{\lambda'} \mid t) = \phi((\tau_t Q_\lambda)^* Q'_{\lambda'})$$

and

$$G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t) = \phi^{(n)}(\tau_t^{(n)}(Q_\lambda)^* Q'_{\lambda'}).$$

Hence, it follows from Eq. (5.4) that, given $\epsilon > 0$, $\exists$ a finite $N(\epsilon, \lambda, \lambda', t)$ such that

$$|G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t) - G_\phi^T((Q_\lambda)^*, Q'_{\lambda'} \mid t)| < \epsilon, \quad \forall\, n > N(\epsilon, \lambda, \lambda', t). \tag{5.18}$$

Finally, it follows from Lemma 5.3 that, given $\epsilon > 0$, $\exists$ finite L_ϵ and L'_ϵ, independent of n and t, such that

$$|G_\phi^{(n)T}((Q_\lambda)^*, Q'_{\lambda'} \mid t) - G_\phi^{(n)T}(Q^*, Q' \mid t)| < \epsilon, \quad \forall\, \lambda > L_\epsilon, \lambda' > L'_\epsilon. \tag{5.19}$$

We now define

$$M_\epsilon = \max(K_\epsilon, L_\epsilon), \quad M'_\epsilon = \max(K'_\epsilon, L'_\epsilon),$$

and

$$\bar{N}(\epsilon, t) = N(\epsilon, M_\epsilon + 1, M_\epsilon + 1, t).$$

Thus, it follows from Eqs. (5.16)–(5.19) that

$$|G_\phi^{(n)T}(Q^*, Q' \mid t) - G_\phi^T(Q^*, Q' \mid t)| < 3\epsilon, \quad \forall\, n > \bar{N}(\epsilon, t),$$

which proves the theorem. QED

The next theorem provides a representation in $\mathfrak{H}_\phi$ (more precisely on Ω_ϕ) of local equations of motion for elements of $\tilde{\mathfrak{K}}_\phi$, subject to the following assumption: The density matrix $\rho^{(n)}$ (for any $n > N_0$, say) may be expressed in the form

$$\rho^{(n)} = \sum_{r=1}^{\infty} c_{nr} E_{nr}, \quad c_{nr} > 0, \quad \sum_r c_{nr} = 1, \quad (5.20)$$

where $\{E_{nr}\}$ is the set of 1-dimensional projectors corresponding to an orthonormal set of eigenvectors $\{\psi_{nr}\}$ of $H^{(n)}$, the generator of $\{V_F^{(n)}(t)\}$.

It is evident that this assumption is satisfied in the case where the $\rho^{(n)}$ are grand canonical density matrices.

Theorem 5.2: If the assumption is valid, and if Q and S are two elements of $\tilde{\mathfrak{K}}_\phi$ such that

$$i[H^{(n)}, \tilde{Q}_{\Lambda_n}]_- = \tilde{S}_{\Lambda_n} \quad \text{on} \quad \{\psi_{nr}\}, \quad \forall\, n > N_0, \quad (5.21)$$

then

$$(\mathrm{w}, \mathfrak{H}_\phi)\text{-}\frac{d}{dt} R_\phi(\tau_t Q)\Omega_\phi = R_\phi(\tau_t S)\Omega_\phi. \quad (5.22)$$

Proof: Assume the above assumption and Eq. (5.21). Then, if ϵ_{nr} is the eigenvalue of $H^{(n)}$ for ψ_{nr}, it follows that

$$[V_F^{(n)}(t)]^{-1}\psi_{nr} = \exp(-i\epsilon_{nr}t)\psi_{nr}.$$

Consequently, by Eq. (5.21),

$$\frac{d}{dt}\{V_F^{(n)}(t)\tilde{Q}_{\Lambda_n}[V_F^{(n)}(t)]^{-1}\}\psi_{nr} = V_F^{(n)}(t)\tilde{S}_{\Lambda_n}[V_F^{(n)}(t)]^{-1}\psi_{nr}. \quad (5.23)$$

Let $A \in \mathfrak{U}_L$. Then it follows from Eqs. (5.7)–(5.9) and (5.20) that

$$G_\phi^{(n)T}(Q^*, A \mid t) = \sum_{r=1}^{\infty} c_{nr}(V_F^{(n)}(t)\tilde{Q}_{\Lambda_n}[V_F^{(n)}(t)]^{-1}\psi_{nr}, \tilde{A}_{\Lambda_n}\psi_{nr}) \quad (5.24)$$

and

$$G_\phi^{(n)T}(S^*, A \mid t) = \sum_{r=1}^{\infty} c_{nr}(V_F^{(n)}(t)\tilde{S}_{\Lambda_n}[V_F^{(n)}(t)]^{-1}\psi_{nr}, \tilde{A}_{\Lambda_n}\psi_{nr}). \quad (5.25)$$

The sums in these last two equations converge uniformly w.r.t. t; for, since $\{\psi_{nr}\}$ are eigenvectors of $H^{(n)}$,

$$\left|\sum_{r=N}^{\infty} c_{nr}(V_F^{(n)}(t)\tilde{Q}_{\Lambda_n}[V_F^{(n)}(t)]^{-1}\psi_{nr}, \tilde{A}_{\Lambda_n}\psi_{nr})\right| \leq \left(\sum_{r=N}^{\infty} c_{nr}\|\tilde{Q}_{\Lambda_n}\psi_{nr}\|^2\right)^{\frac{1}{2}}\left(\sum_{r=N}^{\infty} c_{nr}\|\tilde{A}_{\Lambda_n}\psi_{nr}\|^2\right)^{\frac{1}{2}},$$

and both of these latter factors approach zero as $N \to \infty$, since Q, $A \in \mathfrak{K}_\phi$. Hence, it follows from Eqs. (5.23)–(5.25) that, in view of the uniformity w.r.t. t of the convergence of the sums in Eqs. (5.24) and (5.25),

$$\frac{d}{dt} G_\phi^{(n)T}(Q^*, A \mid t) = G_\phi^{(n)}(S^*, A \mid t).$$

Hence, using Eq. (5.9), we obtain

$$G_\phi^{(n)T}(Q^*, A \mid t) - G_\phi^{(n)}(Q^*, A) = \int_0^t du\, G_\phi^{(n)T}(S^*, A \mid u).$$

In view of Lemma 5.2(ii), Theorem 5.1, and Lebesgue's theorem, it follows from this last equation that

$$G_\phi^T(Q^*, A \mid t) - G_\phi(Q^*, A) = \int_0^t du\, G_\phi^T(S^*, A \mid u),$$

i.e., by Definition 4.4,

$$(R_\phi(\tau_t Q)\Omega_\phi, R_\phi(A)\Omega_\phi) - (R_\phi(Q)\Omega_\phi, R_\phi(A)\Omega_\phi) = \int_0^t du(R_\phi(\tau_u S)\Omega_\phi, R_\phi(A)\Omega_\phi). \quad (5.26)$$

The derivation of this formula is valid for all $A \in \mathfrak{U}_L$. Hence, since $R_\phi(\mathfrak{U}_L)\Omega_\phi$ is dense in $\mathfrak{H}_\phi$ and since

$$\|R_\phi(\tau_t S)\Omega_\phi\| = \|R_\phi(S)\Omega_\phi\|$$

[by Eq. (3.14) and Definition 4.2(ii)] and is thus uniformly bounded, it follows that Eq. (5.26) may be extended by continuity to the form

$$(R_\phi(\tau_t Q)\Omega_\phi, \psi) - (R_\phi(Q)\Omega_\phi, \psi) = \int_0^t du(R_\phi(\tau_u S)\Omega_\phi, \psi), \quad \forall\, \psi \in \mathfrak{H}_\phi.$$

Hence,

$$\frac{d}{dt}(R_\phi(\tau_t Q)\Omega_\phi, \psi) = (R_\phi(\tau_t S)\Omega_\phi, \psi), \quad \forall\, \psi \in \mathfrak{H}_\phi,$$

which proves the theorem. QED

Corollary: Let $\phi = \alpha\phi_1 + (1 - \alpha)\phi_2$, where $0 < \alpha < 1$ and ϕ_1, $\phi_2 \in \mathfrak{C}_T$, i.e., (by Lemma 3.3, Corollary 2) ϕ_1, $\phi_2 \in \mathfrak{C}_L \cap \mathfrak{C}_T$. Then, if ϕ, Q, and S satisfy

the assumptions of Theorem 5.2, this theorem is also applicable to ϕ_1 and ϕ_2, i.e.,

$$\text{w-}\frac{d}{dt}R_{\phi_j}(\tau_t Q)\Omega_{\phi_j} = R_{\phi_j}(\tau_t S)\Omega_{\phi_j}, \quad \text{for} \quad j = 1, 2. \tag{5.27}$$

Proof: Corresponding to $\phi = \alpha\phi_1 + (1-\alpha)\phi_2$, we have

$$\mathfrak{H}_\phi = \mathfrak{H}_{\phi_1} \oplus \mathfrak{H}_{\phi_2},$$
$$\Omega_\phi = \alpha^{\frac{1}{2}}\Omega_{\phi_1} \oplus (1-\alpha)^{\frac{1}{2}}\Omega_{\phi_2},$$
$$R_\phi = R_{\phi_1} \oplus R_{\phi_2},$$
$$V_\phi(t) = V_{\phi_1}(t) \oplus V_{\phi_2}(t).$$

Let P_1 be the projection operator from $\mathfrak{H}_\phi$ to $\mathfrak{H}_{\phi_1}$. Then, for $\lambda < \infty$, $\tau_t Q_\lambda \in \mathfrak{U}$ and thus

$$P_1 R_\phi(\tau_t Q_\lambda)\Omega_\phi = \alpha^{\frac{1}{2}} R_{\phi_1}(\tau_t Q_\lambda)\Omega_{\phi_1}.$$

Hence, by Theorem 4.1(i), Definition 4.2(ii), and Eq. (3.14),

$$P_1 R_\phi(\tau_t Q)\Omega_\phi = \alpha^{\frac{1}{2}} R_{\phi_1}(\tau_t Q)\Omega_{\phi_1}.$$

Likewise,

$$P_1 R_\phi(\tau_t S)\Omega_\phi = \alpha^{\frac{1}{2}} R_{\phi_1}(\tau_t S)\Omega_{\phi_1}.$$

The required result for ϕ_1 follows immediately from these last two equations and Theorem 5.2. Similarly, we obtain the required result for ϕ_2. QED

Remark: This theorem and corollary are of significance, for example, in the theory of broken symmetries. For suppose that the assumptions of the corollary are satisfied and that

(i) Eq. (5.21) [and, correspondingly, Eqs. (5.22) and (5.27)] represents a local conservation law and

(ii) the symmetry associated with the corresponding global conservation law is broken in the states ϕ_j.

Then the representation of the local conservation law, as given by Eq. (5.27), may be used to derive[21] Goldstone's theorem for the states ϕ_j.

6. CONCLUSION

Our principal results are:

(I) If $\phi \in \mathcal{C}_L$, then R_ϕ may be extended from $\mathfrak{U}$ to $\mathfrak{U} \cup \mathfrak{Q}_L$, in such a way that $R_\phi(\mathfrak{Q}_L)$ is a $*$-homomorphism of $\mathfrak{Q}_L$ into the closed, densely defined operators in $\mathfrak{H}_\phi$ [Theorem 4.1(iii), (v), (vi)];

(II) if $\phi \in \mathcal{C}_L \cap \mathcal{C}_{\text{KMS}}$ and Q, Q^*, Q', $Q'^* \in \mathcal{K}_\phi$, then the KMS boundary conditions may be extended to $G_\phi^T(Q^*, Q' \mid t)$ and $F_\phi^T(Q', Q^* \mid t)$ (Theorem 3.2);

(III) if $\phi \in \mathcal{C}_L \cap \mathcal{C}_\Gamma$ and Q, $Q' \in \mathcal{K}_\phi$, then the clustering version long-range ordering of $G_\phi^\Gamma(Q^*, Q' \mid x)$ are given by Theorem 4.3;

(IV) if $\phi \in \mathcal{C}_L \cap \mathcal{C}_T$ and Q, $Q' \in \mathcal{K}_\phi$, then the ergodic average of $G_\phi^T(Q^*, Q' \mid t)$ is given by Theorem 4.4;

(V) if ϕ is a locally normal Gibbs state and if Q, $Q' \in \tilde{\mathcal{K}}_\phi$, then $G_\phi(Q^*, Q')$, $G_\phi^T(Q^*, Q' \mid t)$ are expressible as thermodynamical limits of corresponding correlation functions for finite systems (Theorem 5.1);

(VI) if ϕ is a locally normal Gibbs state and if Q and S are elements of $\tilde{\mathcal{K}}_\phi$ such that S is the time derivative of Q, in the sense of Eq. (5.21), then the equation of motion for $\tau_t Q$ may be represented on a domain of $\mathfrak{H}_\phi$ that includes Ω_ϕ (Theorem 5.2).

Finally, as noted in the remarks following Theorem 4.3 and the Corollary to Theorem 5.2, these latter theorems may be used to obtain significant general properties of states with broken symmetries.

[1] R. Haag, N. M. Hugenholtz, and M. Winnink, Commun. Math. Phys. **5**, 215 (1967).

[2] D. Ruelle, lecture notes, Summer School of Theoretical Physics, Cargese, Corsica, 1965.

[3] An earlier approach to the problem of representing unbounded observables by operators in the GNS space has been made by Ruelle [Commun. Math. Phys. **3**, 133 (1966), Appendix]. The present approach differs from Ruelle's in the essential respect that it is based on the assumptions of locally normal states and local observables, whereas Ruelle's treatment involves no locality principle, but rests on other assumptions, of an algebraic character, for the states and observables considered.

[4] Some general properties of locally normal states have been derived by G. F. Dell'Antonio, S. Doplicher, and D. Ruelle, Commun. Math. Phys. **2**, 223 (1966).

[5] J. Dixmier, *Les algebres d'operateurs dans l'space Hilbertien* (Gauthier-Villars, Paris, 1957), Exercise 1.1.10, p. 17.

[6] An account of the general properties of closed operators in Hilbert space is given, for example, in F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Ungar, New York, 1955), Secs. 115–119.

[7] Cf. Ref. 6, p. 305.

[8] Cf. the theorem of Ref. 4. One should note that, in the case of CAR's, the derivation of this property in Ref. 4 was designed for cases where each local algebra $\mathfrak{U}_\Lambda$ is generated by *all* monomials in $\{a(f), a^*(f) \mid f \in \mathfrak{L}_\Lambda\}$. However, one can easily extend that derivation to the present case, where $\mathfrak{U}_\Lambda$ is generated by even monomials in $\{a(f), a^*(f) \mid f \in \mathfrak{L}_\Lambda\}$, provided that the number operator (in $\mathfrak{H}_\phi$) for the region Λ, is defined to be $\sum_{\text{even } n} nE_{\Lambda,n}$, where $E_{\Lambda,n}$ is the projection operator corresponding to n particles in that region.

[9] J. Dixmier, *Les C*-algebres et leurs representations* (Gauthier-Villars, Paris, 1964), Exercises 2.12.11, p. 56.

[10] In the case of CAR's (but not CCR's), $\gamma_x A$ is norm continuous w.r.t. x, $\forall A \in \mathfrak{U}$, and, consequently, $\mathcal{C}_\Gamma' = \mathcal{C}_\Gamma^0$ in this case.

[11] This follows from Ref. 13, Lemma 1, together with Theorem 4 of the paper by S. Doplicher, R. V. Kadison, D. Kastler, and D. W. Robinson, Commun. Math. Phys. **6**, 101 (1967).

[12] S. Doplicher, D. Kastler, and D. W. Robinson, Commun. Math. Phys. **3**, 1 (1966).

[13] D. Kastler and D. W. Robinson, Commun. Math. Phys. **3**, 151 (1966)

[14] A simple example of an M-filter is given by $\{h_l(x)\}$, with $h_l(x) = X_l(x)/V_l$, where X_l and V_l, respectively, denote the characteristic function and hypervolume for the region $|x| < l$.

[15] H. Araki, Prog. Theor. Phys. **32**, 844 (1964), Proposition 4.

[16] It may readily be shown that $\tilde{\mathfrak{A}}_\Lambda$, defined in this way, is the set of all closed, densely defined operators affiliated to $\tilde{\mathfrak{U}}$ in $\tilde{\mathfrak{C}}_\Lambda$.

[17] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).
[18] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).
[19] As has been pointed out to the author, it might be desirable to weaken the above assumption (ii) to a form that does not imply the existence of the automorphisms $\{\tau_t\}$. Thus, it may be of interest to note that our subsequent theory of Gibbs states will still hold if we replace assumption (ii) by the following weaker postulate: $\exists$ a 1-parameter group $\{V_\phi(t)\}$ of unitary transformations of $\mathfrak{H}_\phi$, such that

$$V_\phi(t)\Omega_\phi = \Omega_\phi, \quad \forall t \in T,$$

and

$$\phi^{(n)}(B\tau_t(n)A) \to (R_\phi(B^*)\Omega_\phi, V_\phi(t)R_\phi(A)\Omega_\phi) \quad \text{as} \quad n \to \infty, \quad \forall A, B \in \mathfrak{U}_L, \quad t \in T.$$

In this case, the subsequent theory can be carried through provided that, for $K \in \mathfrak{U} \cup \mathfrak{A}_L$, one always replaces $R_\phi(\tau_t K)$ by

$$(R_\phi(K))_t \equiv V_\phi(t)R_\phi(K)V_\phi(t)^{-1}.$$

[20] The term "Gibbs state" is usually reserved for a state ϕ, constructed according to the above procedure, in cases where the $\rho^{(n)}$ are grand canonical density matrices corresponding to the regions Λ_n.
[21] Cf. D. Kastler, D. W. Robinson, and A. Swieca, Commun. Math. Phys. **2**, 108 (1966) and A. Swieca, Commun. Math. Phys. **4**, 1 (1967). In these papers, Goldstone's theorem was derived within the framework of local field theory, on the basis of an *a priori* assumption that the relevant local conservation laws could be represented on a domain of the GNS space that includes the cyclical vector.

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Short Proof of a Conjecture by Dyson

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(Received 26 December 1969)

Dyson made a mathematical conjecture in his work on the distribution of energy levels in complex systems. A proof is given, which is much shorter than two that have been published before.

Let $G(\mathbf{a})$ denote the constant term in the expansion of

$$F(\mathbf{x};\mathbf{a}) = \prod_{i \neq j} \left(1 - \frac{x_j}{x_i}\right)^{a_j}, \quad i, j = 1, 2, \cdots, n,$$

where $a_1, a_2, \cdots, a_n$ are nonnegative integers and where $F(\mathbf{x};\mathbf{a})$ is expanded in positive and negative powers of $x_1, x_2, \cdots, x_n$. Dyson[1] conjectured that $G(\mathbf{a}) = M(\mathbf{a})$, where $M(\mathbf{a})$ is the multinomial coefficient $(a_1 + \cdots + a_n)!/(a_1! \cdots a_n!)$. This was proved by Gunson[2] and by Wilson.[3] A much shorter proof is given here.

By applying Lagrange's interpolation formula (see, for example, Kopal[4]) to the function of x that is identically equal to 1 and then putting $x = 0$, we see that

$$\sum_j \prod_i \left(1 - \frac{x_j}{x_i}\right)^{-1} = 1, \; i = j.$$

By multiplying $F(\mathbf{x};\mathbf{a})$ by this function we see that, if $a_j \neq 0$, $j = 1, \cdots, n$, then

$$F(\mathbf{x};\mathbf{a}) = \sum_j F(\mathbf{x}; a_1, a_2, \cdots, a_{j-1}, a_j - 1, a_{j+1}, \cdots, a_n),$$

so that

$$G(\mathbf{a}) = \sum_j G(a_1, \cdots, a_{j-1}, a_j - 1, a_{j+1}, \cdots, a_n). \tag{1}$$

If $a_j = 0$, then x_j occurs only to negative powers in $F(\mathbf{x};\mathbf{a})$ so that $G(\mathbf{a})$ is then equal to the constant term in

$$F(x_1, \cdots, x_{j-1}, x_{j+1}, \cdots, x_n; a_1, \cdots, a_{j-1}, a_{j+1}, \cdots, a_n),$$

that is,

$$G(\mathbf{a}) = G(a_1, \cdots, a_{j-1}, a_{j+1}, \cdots, a_n), \quad \text{if } a_j = 0. \tag{2}$$

Also, of course,

$$G(\mathbf{0}) = 1. \tag{3}$$

Equations (1)–(3) clearly uniquely define $G(\mathbf{a})$ recursively. Moreover, they are satisfied by putting $G(\mathbf{a}) = M(\mathbf{a})$. Therefore $G(\mathbf{a}) = M(\mathbf{a})$, as conjectured by Dyson.

[1] F. J. Dyson, J. Math. Phys. **3**, 140, 157, 166 (1962).
[2] J. Gunson, J. Math. Phys. **3**, 752 (1962).
[3] K. G. Wilson, J. Math. Phys. **3**, 1040 (1962).
[4] Z. Kopal, *Numerical Analysis* (Chapman and Hall, London, 1955), p. 21.

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Degeneracy of the $SU(3)$ Direct Product and the Symmetric Representations of $SU(6) \supset SU(3) \otimes SU(2)$

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The relation between a state of $U(n)$ associated with an m-rowed Young diagram, $m \leq n$, and a state of $U(m)$ associated with an m-rowed Young diagram provides the basis for the symmetric state of $U(mn) \supset U(m) \otimes U(n)$. As an application, the state vectors associated with the irreducible representations of $SU(6)$ restricted to the subgroup $SU(3) \otimes SU(2)$ are explicitly constructed for the symmetric representation, and generalized to the case of a 2-rowed Young diagram. Expressions are given for the degeneracy of an $SU(3) \otimes SU(2)$ state in $SU(6)$, and the completeness of the obtained set of states is discussed. The direct product of symmetric $SU(6) \supset SU(3) \otimes SU(2)$ states implies a direct product of $SU(3)$ states; the operator which breaks the degeneracy of the "2-rowed" $SU(6) \supset SU(3) \otimes SU(2)$ state is shown to be Moshinsky's operator X which breaks the degeneracy of the $SU(3)$ direct product.

1. INTRODUCTION

The restriction of $U(mn)$ to the product of subgroups $U(m) \otimes U(n)$, written $U(mn) \downarrow [U(m) \otimes U(n)]$, has not been extensively studied in the literature. The case $U(4) \supset U(2) \otimes U(2)$ has been investigated,[1] but this may be considered special because $U(4) \supset O(4) \simeq O(3) \otimes O(3)$ is essentially the same problem and the restriction of $U(n)$ to $O(n)$ is known.[2] Hagen and Macfarlane[3] have studied the concept of plurality in the reduction of $SU(mn)$ with respect to the subgroup $SU(m) \otimes SU(n)$, and have tabulated the $SU(3) \otimes SU(2)$ subgroups for specific low-dimensional representations of $SU(6)$ useful in elementary particle calculations, by means of the Weyl character formula. We shall use their results in constructing the general 2-rowed state vector.

In the mathematician's side of the ledger, Robinson[4] discusses the problem of $SU(mn) \downarrow [SU(m) \otimes SU(n)]$ as the reduction of the symmetric outer product of $SU(m)$, $SU(n)$ representations. However, no implicit or explicit branching rules appear in his book; indeed, Robinson takes note of the dearth of mathematical literature on the subject.[5]

It is the purpose of this paper to examine the problem $SU(6) \downarrow [SU(3) \otimes SU(2)]$ in detail, for a general 2-rowed Young diagram, and relate the results to the $SU(3)$ direct product. The technique employed may be generalized, with all its attendant complexity, to the general 5-rowed Young diagram.

There is one essential idea which will allow construction of the symmetric $SU(6) \supset SU(3) \otimes SU(2)$ states from the $SU(3)$ states and provide the basis for much of the following analysis. The states $|\lambda; \alpha\rangle$ associated with an irreducible representation of $U(n)$ can be constructed of polynomials of the C_n vectors $\mathbf{z}_i = (z_i^1, \cdots, z_i^n)$, $i = 1, \cdots, m$, for an m-row diagram of $U(n)$. In terms of the vectors $\mathbf{z}_i$, the generators of $U(n)$ may be written[6]

$$C^{\alpha\beta} = \sum_{i=1}^{m} z_i^\alpha \frac{\partial}{\partial z_i^\beta}, \quad \alpha, \beta = 1, \cdots, n. \tag{1.1}$$

By contracting over the upper indices, the operators C_{ij} may be constructed:

$$C_{ij} = \sum_{\alpha=1}^{n} z_i^\alpha \frac{\partial}{\partial z_j^\alpha} \equiv \mathbf{z}_i \cdot \frac{\partial}{\partial \mathbf{z}_j}, \quad i, j = 1, \cdots, m. \tag{1.2}$$

The operators C_{ij} and generators $C^{\alpha\beta}$ satisfy the commutation relations of the unitary group. They also commute; hence, the operators C_{ij} may be used to construct the invariant space labeled by the Young diagram. Moshinsky[6] has proved that, if a state $|\lambda, \alpha\rangle$ satisfies the conditions

$$C_{ii} |\lambda, \alpha\rangle = h_i |\lambda, \alpha\rangle, \quad i = 1, \cdots, m \text{ (no summation)}, \tag{1.3a}$$

$$C_{ij} |\lambda, \alpha\rangle = 0, \quad i < j, \tag{1.3b}$$

this state is associated with an irreducible representation of $U(n)$. The symbol λ represents the partition $\lambda = (\lambda_1, \cdots, \lambda_m, 0, \cdots, 0)$, where λ_i are the row overhangs, $\lambda_i = h_i - h_{i-1}$, $\lambda_m = h_m$; the symbol α denotes the row labels.

Though the conditions (1.3) are sufficient to label the invariant spaces, they are not necessary. It is only necessary that the Casimir operators

$$C^p = C^{\mu_1\mu_2} C^{\mu_2\mu_3} \cdots C^{\mu_p\mu_1}, \quad p = 1, \cdots, m \tag{1.4}$$

(unless otherwise stated, the summation convention is always implied) on $|\lambda, \alpha\rangle$ be a constant

$$C^p |\lambda, \alpha\rangle = \omega^p |\lambda, \alpha\rangle, \tag{1.5}$$

where $\omega^p = f(\lambda)$.

This is what Schur's lemma requires. So, whereas it is true that if conditions (1.3) are satisfied, then Eq. (1.5) is satisfied, the converse is not, in general, true. This provides us with the freedom to use the operators C_{ij} as the generators of $U(m)$, and construct the symmetric representations of $U(mn) \supset U(n) \otimes U(m)$.

This idea, in different form, has previously appeared in the literature. Several authors[7-10] have considered upper and lower Gel'fand patterns to describe states of the symmetric representations of $U(n^2)$, restricted to the subgroup $U(n)_1 \otimes U(n)_2$. The generators of $U(n)_{1,2}$ correspond to the upper, lower indices of Eqs. (1.1) and (1.2), respectively. Brody, Moshinsky, and Renero[11] have used this decomposition to derive recursion formula for $SU(3)$ coupling coefficients. In addition to what we believe is a rather transparent construction of symmetric $SU(mn)$ states in terms of a full use of upper, lower indices, we will go on to the more complicated $SU(mn)$ states associated with the 2-rowed Young diagram.

The construction of the symmetric states and generators for $SU(mn) \downarrow [SU(m) \otimes SU(n)]$ are discussed in Sec. 2. For the case $SU(6) \supset SU(3) \otimes SU(2)$, we explicitly prove that this state is associated with the irreducible representations of $SU(3)$ and $SU(2)$. In Sec. 3, we use the results of Hagen and Macfarlane[3] to construct the fundamental states,[12] products of which yield the highest weight $SU(6) \supset SU(3) \otimes SU(2)$ state vector associated with a general 2-rowed Young diagram. Formulas are given for the degeneracy of an $SU(3) \otimes SU(2)$ multiplet in a 2-rowed $SU(6)$ representation, and completeness is discussed. In Sec. 4, an operator χ is constructed which breaks this degeneracy. We also denote a brief discussion to the coupling coefficients of the direct product of $SU(6) \supset SU(3) \otimes SU(2)$ symmetric states.

2. SYMMETRIC STATES OF $U(mn) \supset U(m) \otimes U(n)$

The state vector $|\lambda, \alpha\rangle$ associated with an irreducible representation of $U(n)$ has been constructed by Moshinsky,[6] using conditions (1.3). It has the general form

$$|\lambda; \alpha, \beta_M\rangle \equiv |\lambda, \alpha\rangle = \sum_{f_{ij}} C_{f_{ij}} (z_i^\mu)^{\lambda_1} (\Delta_{12}^{\mu\nu})^{\lambda_2} \cdots (\Delta_{12\cdots m}^{\mu\nu\cdots\gamma})^{\lambda_m}, \tag{2.1}$$

where $\Delta_{12}^{\mu\nu}$ are the 2×2 antisymmetric forms, $z_1^\mu z_2^\nu - z_1^\nu z_2^\mu = \Delta_{12}^{\mu\nu}$, $\Delta_{123}^{\mu\nu\gamma}$ are the 3×3 antisymmetric forms, and $C_{f_{ij}}$ are constants. Each factor in Eq. (2.1) is a product of factors

$$(z_1^\mu)^{\lambda_1} \equiv \prod_{\mu=1}^{n} (z_1^\mu)^{f_{1\mu}} \quad \text{with} \quad \sum_{\mu=1}^{n} f_{1\mu} = \lambda_1,$$

and similarly for the other products, suitably ordered, with $\sum_{\mu=1}^{N_i} f_{i\mu} = \lambda_i$, N_i being the total number of the ith antisymmetric forms. We introduce, in (2.1), the notation $|\lambda; \alpha\beta_M\rangle$; the symbols α, β will both represent row labels, β_M being the maximum weight state. The reason for this notation will be clear shortly.

We note that condition (1.3b) on the general polynomial of C_n vectors $\mathbf{z}_i$ requires the antisymmetric forms with lower indices appropriately ordered. That is, we first have terms $\mathbf{z}_1$ (suppressing upper indices), then antisymmetric forms Δ_{12} with vectors $\mathbf{z}_1$, $\mathbf{z}_2$, then vectors $\mathbf{z}_1$, $\mathbf{z}_2$, $\mathbf{z}_3$ in the terms Δ_{123}, and so on.

The maximum weight state α_M may be obtained from Eq. (2.1) by requiring

$$C^{\alpha\beta} |\lambda; \alpha_M, \beta_M\rangle = 0, \quad \alpha < \beta. \tag{2.2}$$

The general solution of Eq. (2.2) is

$$|\lambda; \alpha_M, \beta_M\rangle = C_{\lambda_i} (z_1^1)^{\lambda_1} (\Delta_{12}^{12})^{\lambda_2} \cdots (\Delta_{12\cdots m}^{12\cdots m})^{\lambda_m}, \tag{2.3}$$

where C_{λ_i} is the normalization. We note that (2.2) orders the *upper indices*, as condition (1.3b) ordered the lower indices. The maximum weights α_M are functions of the partition numbers λ_i, the state vector (2.3) is an eigenvector of the Casimir operators C^p, and (1.4), with eigenvalue ω^p, a function of the partition λ. For $p = 1, 2, 3$, the explicit expressions for ω^p in terms of λ have been calculated.[13] Since the Casimir operators C^p commute with the generators $C^{\alpha\beta}$, the eigenvalues ω^p hold, of course, for the general state (2.1). It is clear that there can only be m independent Casimir operators C^p for an m-rowed Young diagram since there are only m independent numbers λ_i.

We may define, in analogous fashion, the Casimir operators C_p:

$$C_p = C_{i_1 i_2} C_{i_2 i_3} \cdots C_{i_p i_1}, \quad p = 1, \cdots, m \tag{2.4}$$

(summation convention implied). Using (1.3), we have that

$$C_p |\lambda; \alpha_M, \beta_M\rangle = \omega_p |\lambda; \alpha_M, \beta_M\rangle, \tag{2.5}$$

where ω_p ($\neq \omega^p$) are also functions of the partition λ. Though the maximum weight state vector (2.3) is symmetrical in the upper, lower indices, the Casimir operators C^p, C_p differ as functions of z_k^i, hence the numbers ω^p, ω_p are not equal. However, C^p may be written as an explicit function of the operator C_p, $p = 1, \cdots, m$, or conversely, and ω^p may be written as a function of the ω_p, $p = 1, \cdots, m$. The invariant space with respect to the upper indices is the same as the invariant space with respect to the lower indices, and this is represented in the maximum weight state vector (2.3) with the same partition λ.

The Casimir operators C^p, C_p and the operators C_{ij} mutually commute. We may operate to an arbitrary weight state[14] β with the operators C_{ij},

$$|\lambda; \alpha_M, \beta\rangle = \sum_{g_{ij}} d_{g_{ij}} (z_k^1)^{\lambda_1} (\Delta_{km}^{12})^{\lambda_2} \cdots (\Delta_{km\cdots p}^{12\cdots m})^{\lambda_m} \quad (2.6)$$

similar to the state vector (2.1). Because of the mutual commutativity of the operators, this state satisfies Eqs. (1.5) and (2.5), and is associated with an irreducible representation labeled by λ. It satisfies condition (2.2), so it remains a highest weight state α_M in the upper indices. We see then that (2.6) is a polynomial of the C_m vectors $\mathbf{z}^i = (z_1^i, \cdots, z_m^i)$, $i = 1, \cdots, n$, C_{ij} are the generators, and (2.6) is the state vector of $U(m)$.

Finally, it is possible to lower (2.6) from the maximum weight state α_M of $U(n)$ to weight α. Since C_{ij}, $C^{\alpha\beta}$ commute, the weight β is unchanged under this operation. We thus obtain a state vector of weights α, β in $U(n)$ of m rows, $U(m)$, respectively, in the invariant space labeled by λ.

The state vector of weight α, β is also the symmetric state vector of $U(mn)$, labeled by the 1-rowed Young diagram. To see this more clearly, redefine the vectors z_i^α, as in Louck,[9]

$$z_i^\alpha \equiv z^{(i-1)n+\alpha} = z^\mu, \quad i = 1, \cdots, m, \quad \alpha = 1, \cdots, n, \quad \mu = 1, \cdots, mn. \quad (2.7)$$

The state vector (2.6), (2.3), or (2.1) may be written in terms of the variables z^μ. The one Casimir operator, the trace operator

$$\mathrm{Tr} = z^\mu \frac{\partial}{\partial z^\mu}, \quad (2.8a)$$

acting on the general $U(m) \otimes U(n)$ state vector, yields the eigenvalue

$$w = \lambda_1 + 2\lambda_2 + \cdots + m\lambda_m. \quad (2.8b)$$

All Casimir operators in the mn variables z^μ are functions of this one number w. This is the symmetric representation of $U(mn)$.

We illustrate the previous remarks with the symmetric state vector and generators of $SU(6) \supset SU(3) \otimes SU(2)$, and explicitly show that the state vector is associated with irreducible representations of $SU(3)$ and $SU(2)$. The generators of $SU(3)$ may be written[15]

$$I_0 = \tfrac{1}{2}(C^{11} - C^{22}), \quad Y = \tfrac{1}{3}(C^{11} + C^{22} - 2C^{33}),$$
$$I_+ = C^{12}, \quad I_- = C^{21}, C^{13}, C^{31}, C^{23}, C^{32}, \quad (2.9a)$$

where $C^{\alpha\beta}$ is given by Eq. (1.1) with $m = 2$. The explicit $SU(3)$ state vector is then

$$|\lambda_1\lambda_2; \alpha, \beta_M\rangle = N(\lambda, \alpha)(-1)^q \times \sum_k \binom{r}{k} \frac{(\lambda_2 - q)!\, p!}{(\lambda_2 - q - k)!\, [p - (r-k)]!} (z_1^\mu)^{\lambda_1} (\Delta_{12}^{\mu\nu})^{\lambda_2}, \quad (2.9b)$$

where

$$(z_1^\mu)^{\lambda_1} \equiv (z_1^1)^{p-(r-k)} (z_1^2)^{r-k} (z_1^3)^{\lambda_1 - p}$$

and

$$(\Delta_{12}^{\mu\nu})^{\lambda_2} \equiv (\Delta_{12}^{23})^k (\Delta_{12}^{13})^{\lambda_2 - q - k} (\Delta_{12}^{12})^q,$$

with row label $\alpha = (y, I, I_0)$,

$$Y = -\tfrac{1}{3}(2\lambda_1 + \lambda_2) + (p + q), \quad \mathbf{I}^2 = I(I+1),$$
$$I_0 = \tfrac{1}{2}(\lambda_2 + p - q) - r, \qquad I = \tfrac{1}{2}(\lambda_2 + p - q), \quad (2.9c)$$

and $r = 0, \cdots, 2I$, $0 \le p \le \lambda_1$, $0 \le q \le \lambda_2$. Here, $N(\lambda, \alpha)$ is the normalization

$$N(\lambda, \alpha) = \left(\frac{(\nu_1 + 1)!\, (\nu_2 + p - q + 1)!}{p!\, q!\, (\nu_2 - q)!\, (\nu_1 + p + 1)!\, (\nu_1 + \nu_2 - q + 1)!\, (\nu_1 - p)!} \right)^{\frac{1}{2}} \left(\frac{(2I - r)!}{r!\, (2I)!} \right)^{\frac{1}{2}}.$$

The generators of $SU(2)$ may be written

$$J_0 = \tfrac{1}{2}(C_{11} - C_{22}), \quad J_+ = C_{12}, \quad J_- = C_{21}, \quad (2.10)$$

where C_{ij} is given by Eq. (1.2) with $n = 3$. We note that J_+ on the $SU(3)$ state vector (2.9b) is zero, and J_0 on (2.9b) is $\frac{1}{2}\lambda_1$, the highest weight. We may operate on (2.9b) with $(J_-)^s$,

$$|\lambda_1\lambda_2; \alpha\beta\rangle = N(-1)^q \sum_{kk_i} \frac{r!\, (\lambda_2 - q)!\, p!\, (\lambda_1 - p)!\, s!}{k!\, [p - (r-k) - k_1]!\, (\lambda_2 - q - k)!\, (r - k - k_2)!\, (\lambda_1 - p - k_3)!\, k_1!\, k_2!\, k_3!} \times (z_1^\mu)^{\lambda_1 - s} (z_2^\mu)^s (\Delta_{12}^{\mu\nu})^{\lambda_2}, \quad (2.11a)$$

where

$$(z_1^\mu)^{\lambda_1 - s} \equiv (z_1^1)^{p-(r-k)-k_1} (z_1^2)^{r-k-k_2} (z_1^3)^{\lambda_1 - p - k_3},$$
$$(z_2^\mu)^s \equiv (z_2^1)^{k_1} (z_2^2)^{k_2} (z_2^3)^{k_3},$$

and $s = k_1 + k_2 + k_3$. The normalization N is $N = N(\lambda, \alpha)[(\lambda_1 - s)!/(\lambda_1)!\, s!]^{\frac{1}{2}}$. From the form of the state vector (2.11), we see that the row label α, (2.9c), remains the same. However,

$$J_0 = (\tfrac{1}{2})\lambda_1 - s \equiv m, \quad 0 \leq s \leq \lambda_1. \quad (2.11b)$$

Finally, we may see that the state vector (2.11a) is associated with the irreducible representations of $SU(3)$, $SU(2)$, respectively. Define the unitary transformations T_u, T^U:

$$T_u : z_i'^{\alpha} = u_{i'i} z_i^{\alpha}, \quad i, i' = 1, 2, \quad (2.12a)$$

$$T^U : z_i'^{\alpha} = U^{\alpha'\alpha} z_i^{\alpha'}, \quad \alpha, \alpha' = 1, 2, 3, \quad (2.12b)$$

where $U_{i'i}$, $U^{\alpha'\alpha}$ are the $SU(2)$, $SU(3)$ transformations, respectively. It is shown in Appendix A that

$$T_u |\lambda; \alpha, \beta\rangle = \mathfrak{D}^{\frac{1}{2}\lambda_1}_{\beta'\beta}(u) |\lambda; \alpha, \beta'\rangle, \quad (2.13a)$$

where $j = \frac{1}{2}\lambda_1$ and $-j \leq \beta \leq j$. It may also be shown that

$$T^U |\lambda; \alpha, \beta\rangle = \mathfrak{D}^{\lambda}_{\alpha'\alpha}(U) |\lambda; \alpha', \beta\rangle, \quad (2.13b)$$

where $\alpha' = (y', I', I_0')$, employing the $SU(3)$ representation matrices of this author.[15,16]

We may relabel the coordinates, as in Eq. (2.7),

$$z_1^1 = z^1, \quad z_1^2 = z^2, \quad z_1^3 = z^3,$$
$$z_2^1 = z^4, \quad z_2^2 = z^5, \quad z_2^3 = z^6. \quad (2.14)$$

The state (2.11a) is then associated with the symmetric representation of $SU(6)$, with maximum weight $h = \lambda_1 + 2\lambda_2$. The relabeled generators[17] of $SU(3)$ in the restriction of $SU(6)$ to $SU(3) \otimes SU(2)$ are

$$I_0 = \tfrac{1}{2}(C^{11} + C^{44} - C^{22} - C^{55}), \quad C^{13} + C^{46}, \quad C^{31} + C^{64},$$
$$I_+ = C^{12} + C^{45}, \quad I_- = C^{21} + C^{54}, \quad C^{23} + C^{56}, \quad C^{32} + C^{65}, \quad (2.15a)$$
$$Y = \tfrac{1}{3}(C^{11} + C^{22} + C^{44} + C^{55} - 2C^{33} - 2C^{66});$$

and the relabeled generators of $SU(2)$ are

$$J_0 = \tfrac{1}{2}(C^{11} + C^{22} + C^{33} - C^{44} - C^{55} - C^{66}),$$
$$J_+ = C^{14} + C^{25} + C^{36}, \quad J_- = C^{41} + C^{52} + C^{63}, \quad (2.15b)$$

where $C^{\mu\nu}$ is given by (1.1), with $m = 1$. The operator C_{11} [(1.2) with $n = 6$] is the trace operator, with eigenvalue h. The generators of $SU(6) \supset SU(3) \otimes SU(2)$ for an $m \leq 5$ rowed Young diagram have the form (2.15), with $m \leq 5$ in Eq. (1.1); and the operators C_{ij} have $n = 6$, and $i, j = 1, \cdots, m$.

3. POLYNOMIAL $SU(6) \supset SU(3) \otimes SU(2)$ STATE VECTOR

In this section, we construct the polynomial state vector of highest weight in $SU(3)$, $SU(2)$. The method of fundamental states, detailed in Ref. 1, allows one to construct the general polynomial state vector of highest weight from a knowledge of the low-dimensional representations. In the case $U(4) \supset U(2) \otimes U(2)$, the branching rules provided this information. Since there are no general branching rules for the case $SU(6) \supset SU(3) \otimes SU(2)$, we use the results of Hagen and Macfarlane,[3] particularly their Table I.[18]

Write the fundamental states S_i as $S_i = (\lambda_1\lambda_2; \nu_1\nu_2, \mu)$, where $\lambda_1\lambda_2$ are the overhang partition numbers of a 2-rowed $SU(6)$ Young diagram, $\nu_1\nu_2$ are the overhang partition numbers of an $SU(3)$ Young diagram, and $\mu = 2j$ is the 1-rowed $SU(2)$ Young diagram. The states S_i are of highest weight in $SU(3)$ and $SU(2)$. In terms of the generators (2.15), the highest weight states of $SU(3)$, $SU(2)$ are

$$I_0 = (\tfrac{1}{2})\nu_1, \quad Y = \tfrac{1}{3}(\nu_1 + 2\nu_2), \quad J_0 = j = \tfrac{1}{2}\mu. \quad (3.1)$$

Using an extension of Cartan's theorem on highest weights,[19] we have

$$(\lambda_1\lambda_2; \nu_1\nu_2, \mu)(\lambda_1'\lambda_2'; \nu_1'\nu_2', \mu')$$
$$= (\lambda_1 + \lambda_1', \lambda_2 + \lambda_2'; \nu_1 + \nu_1', \nu_2 + \nu_2', \mu + \mu'), \quad (3.2)$$

since the weights are linear forms. A state is called "fundamental" if it cannot be obtained from a product of other fundamental states [using (3.2)]. We begin with the lowest-dimensional representations of $SU(6)$, as given in Hagen and Macfarlane,[3] and obtain the fundamental states S_i, $i = 1, \cdots, 13$, using (3.2). The results are listed in Table I.

TABLE I. Fundamental states, $S_i = (\lambda_1\lambda_2; \nu_1\nu_2, \mu)$, where λ_i, ν_i, μ are the overhangs of the 2-rowed $SU(6)$, of the $SU(3)$, and of the $SU(2)$ Young diagrams, respectively.

$S_1 = (10; 10, 1)$	$S_7 = (02; 02, 0)$
$S_2 = (01; 01, 2)$	$S_8 = (02; 10, 2)$
$S_3 = (01; 20, 0)$	$S_9 = (21; 10, 0)$
$S_4 = (20; 01, 0)$	$S_{10} = (12; 01, 1)$
$S_5 = (11; 00, 1)$	$S_{11} = (03; 00, 0)$
$S_6 = (11; 11, 1)$	$S_{12} = (03; 11, 2)$
$S_{13} = (22; 11, 0)$	

Products of the fundamental state vectors S_i yield the state vector

$$P_{n_i} = \prod_{k=1}^{13} (S_k)^{n_k}, \quad n_k \geq 0. \quad (3.3)$$

TABLE II. Explicit polynomial fundamental states, where $\Delta^{ij} = z_2^i z_1^j - z_1^i z_2^j$; lower indices have been suppressed.

$$
\begin{aligned}
&S_1 = z^1, \quad S_2 = \Delta^{12}, \quad S_3 = \Delta^{14}, \quad S_4 = z^1 z^5 - z^2 z^4 \\
&S_5 = z^6\Delta^{12} + z^4\Delta^{23} - z^5\Delta^{13}, \quad S_6 = z^1(\Delta^{15} - \Delta^{24}) - 2z^4\Delta^{12} \\
&S_7 = (\Delta^{24})^2 + (\Delta^{15})^2 - 2\Delta^{12}\Delta^{45} - 2\Delta^{14}\Delta^{25}, \quad S_8 = \Delta^{14}\Delta^{23} + \Delta^{12}\Delta^{16} - \Delta^{13}\Delta^{15} \\
&S_9 = (z^1)^2\Delta^{56} + (z^4)^2\Delta^{23} + z^1 z^3\Delta^{45} - z^4 z^5\Delta^{13} + z^4 z^6\Delta^{12} - z^1 z^2\Delta^{46} \\
&S_{10} = z^4\Delta^{23}\Delta^{24} + z^5\Delta^{13}\Delta^{15} - (z^5\Delta^{16} + z^1\Delta^{56})\Delta^{12} + (z^2\Delta^{46} + z^4\Delta^{26})\Delta^{12} - (z^5\Delta^{14}\Delta^{23} + z^4\Delta^{13}\Delta^{25} + z^3\Delta^{12}\Delta^{45}) \\
&S_{11} = \Delta^{12}\Delta^{16}\Delta^{56} + \Delta^{23}\Delta^{34}\Delta^{45} - \Delta^{13}\Delta^{15}\Delta^{56} - \Delta^{12}\Delta^{26}\Delta^{46} - \Delta^{23}\Delta^{24}\Delta^{46} - \Delta^{13}\Delta^{35}\Delta^{45} \\
&\qquad + \Delta^{16}\Delta^{21}\Delta^{35} + 2\Delta^{13}\Delta^{25}\Delta^{46} - 2\Delta^{16}\Delta^{23}\Delta^{45} - \Delta^{15}\Delta^{26}\Delta^{34} \\
&S_{12} = \Delta^{12}\Delta^{15}\Delta^{16} - \Delta^{13}\Delta^{15}\Delta^{15} + 2\Delta^{13}\Delta^{14}\Delta^{25} - \Delta^{13}\Delta^{15}\Delta^{24} + \Delta^{14}\Delta^{15}\Delta^{23} \\
&\qquad - 2\Delta^{12}\Delta^{12}\Delta^{46} - \Delta^{12}\Delta^{16}\Delta^{24} - \Delta^{14}\Delta^{23}\Delta^{24} \\
&S_{13} = (z^1)^2\Delta^{15}\Delta^{56} + (z^4)^2\Delta^{23}\Delta^{24} + z^2 z^4(\Delta^{14}\Delta^{26} + \Delta^{12}\Delta^{46}) - z^1 z^6\Delta^{24}\Delta^{24} + (z^1)^2\Delta^{35}\Delta^{45} + (z^5)^2\Delta^{13}\Delta^{14} \\
&\qquad - (z^1)^2\Delta^{25}\Delta^{46} - z^2 z^5\Delta^{14}\Delta^{16} - 2z^1 z^4\Delta^{12}\Delta^{56} + z^1 z^6\Delta^{14}\Delta^{25} - (z^4)^2\Delta^{12}\Delta^{35} - z^2 z^3\Delta^{14}\Delta^{45} - 2z^4 z^5\Delta^{14}\Delta^{23} \\
&\qquad + z^1 z^4\Delta^{23}\Delta^{45}
\end{aligned}
$$

Using (3.2) and Table I, we see that the state vector P_{n_i} is of highest weight

$$
\begin{aligned}
\lambda_1 &= n_1 + 2n_4 + n_5 + n_6 + 2n_9 + n_{10} + 2n_{13}, \\
\lambda_2 &= n_2 + n_3 + n_5 + n_6 + 2n_7 + 2n_8 + n_9 \\
&\qquad + 2n_{10} + 3n_{11} + 3n_{12} + 2n_{13}, \qquad (3.4a)
\end{aligned}
$$

$$
\begin{aligned}
\nu_1 &= n_1 + 2n_3 + n_6 + n_8 + n_9 + n_{12} + n_{13}, \\
\nu_2 &= n_2 + n_4 + n_6 + 2n_7 + n_{10} + n_{12} + n_{13}, \qquad (3.4b) \\
2j = \mu &= n_1 + 2n_2 + n_5 + n_6 + 2n_8 + n_{10} + 2n_{12}.
\end{aligned}
$$

The explicit polynomials S_i may be obtained using (3.1) and the fact that S_i is of highest weight. Thus, we have

$$
(C^{13} + C^{46}, C^{12} + C^{45}, C^{23} + C^{56}, C^{14} + C^{25} + C^{36}) \times S_i = 0, \quad i = 1, \cdots, 13. \qquad (3.5)
$$

The explicit polynomials S_i are listed in Table II.

Five conditions are imposed on the 13 integers n_i by Eq. (3.4), leaving eight integers independent. However, products of polynomials S_i are dependent on other products, providing further conditions on the integers n_i. There is only one independent integer n_i, as we now show.

First, it is clear there should only be one independent integer n_i. In the restriction of $SU(6)$ to $[SU(3) \otimes SU(2)]$ for a 2-rowed Young diagram, there exists six independent Casimir operators, two in $SU(6)$, two in $SU(3)$, one in the subgroup $SU(2)$ contained in $SU(3)$, and one in the product $SU(2)$ subgroup. In addition, there exists five independent linear operators in this rank-five group. This provides a total of eleven operators on the twelve coordinates z_i^μ, $i = 1, 2$, $\mu = 1, \cdots, 6$, leaving one independent exponent.

On the other hand, products of polynomials S_i are dependent on other products. The explicit relations between products are listed in Table III. These relations imply conditions on the integers n_i, since whenever particular products occur, they may be re-expressed in terms of others. The conditions are

$$
n_6, n_{10}, n_{12}, n_{13} = 0, 1. \qquad (3.6a)
$$

If both of the sets of integers $[n_i, n_j]$ are nonzero, the term must be re-expressed as

$$
\begin{aligned}
&[(n_1, n_5, n_6, n_9, n_{10}, n_{13}), n_{12}], \\
&[(n_1, n_5, n_6, n_8, n_{10}), n_{13}], \qquad (3.6b) \\
&[n_4, n_8], \quad [n_2, n_9], \quad [n_6, n_{10}].
\end{aligned}
$$

Finally, if all three of the integers n_1, n_5, n_7 are nonzero or if $n_1 \geq 2$, $n_{11} \neq 0$, the product must be re-expressed.

Imposing these 20 conditions on the polynomial P_{n_i}, (3.3), we may classify the polynomial state

TABLE III. Relations of products of fundamental states.

$$
\begin{aligned}
(S_6)^2 &= (S_1)^2 S_7 - 4S_2S_3S_4 & (S_{12})^2 &= S_7(S_8)^2 - 4(S_2)^2S_3S_{11} \\
(S_{10})^2 &= (S_5)^2 S_7 + 4S_2S_4S_{11} & (S_{13})^2 &= S_7(S_9)^2 - 4(S_4)^2S_3S_{11} \\
S_1S_{12} &= S_6S_8 + 2S_2S_3S_5 & S_9S_{12} &= -S_3S_5S_{10} + S_1S_6S_{11} \\
S_5S_{12} &= -(S_8S_{10} + 2S_1S_2S_{11}) & S_{10}S_{12} &= -(S_5S_7S_8 + 2S_2S_6S_{11}) \\
S_6S_{12} &= 2S_2S_3S_{10} + S_1S_7S_8 & S_{13}S_{12} &= -4S_2S_3S_4S_{11} + S_7S_8S_9 - 2S_3(S_5)^2S_7 \\
S_1S_{13} &= S_6S_9 - 2S_3S_4S_5 & S_{10}S_{13} &= S_5S_7S_9 - 2S_4S_6S_{11} \\
S_5S_{13} &= S_9S_{10} + 2S_1S_4S_{11} & S_8S_{13} &= S_3S_5S_{10} + S_1S_6S_{11} \\
S_6S_{13} &= S_1S_7S_9 + 2S_3S_4S_{10} & & \\
S_4S_8 &= \tfrac{1}{2}(S_5S_6 - S_1S_{10}) & S_6S_{10} &= -(S_2S_{13} + S_4S_{12}) \\
S_2S_9 &= -\tfrac{1}{2}(S_5S_6 + S_1S_{10}) & (S_1)^2S_{11} &= S_8S_9 - S_3(S_5)^2 \\
& & S_1S_5S_7 &= -S_2S_{13} + S_4S_{12}
\end{aligned}
$$

vector into six cases:

$$
\begin{aligned}
&(1)\quad n_6 = 1, n_{10}, n_{12}, n_{13} = 0,\\
&\qquad \text{exponents: } n_1n_5n_7,\ n_4n_8,\ n_2n_9,\ n_3n_{11};\\
&(2)\quad n_{10} = 1, n_6, n_{12}, n_{13} = 0,\\
&\qquad \text{exponents: } n_1n_5n_7,\ n_4n_8,\ n_2n_9,\ n_3n_{11};\\
&(3)\quad n_{12} = 1, n_1, n_5, n_6, n_9, n_{10}, n_{13} = 0,\\
&\qquad \text{exponents: } n_4n_8,\ n_2n_3n_7n_{11};\\
&(4)\quad n_{13} = 1, n_1, n_5, n_6, n_8, n_{10}, n_{12} = 0,\\
&\qquad \text{exponents: } n_2n_9,\ n_3n_4n_7n_{11};\\
&(5)\quad n_6, n_{10}, n_{12}, n_{13} = 0,\\
&\qquad \text{exponents: } n_1n_5n_7,\ n_2n_9,\ n_4n_8,\ n_3n_{11};\\
&(6)\quad n_6, n_{10}, n_{12}, n_{13} = 0,\\
&\qquad \text{exponents: } n_1n_5n_9,\ n_2n_9,\ n_4n_8,\ n_3n_{11}.
\end{aligned}
\tag{3.7}
$$

For cases (1), (2), (5), the imposition of the conditions that n_4, $n_8 \neq 0$, n_2, $n_9 \neq 0$, and n_1, n_5, $n_7 \neq 0$ be eliminated reduces the number of independent integers to six. If the term $n_1 \geq 2$, $n_{11} \neq 0$ is present, the number of independent integers is five. Using the five conditions (3.4), we see that cases (1), (2), (5) have, at most, one independent integer. In cases (3), (4), the imposition of conditions n_4, $n_8 \neq 0$ or n_2, $n_9 \neq 0$, and (3.4), implies no independent integer n_i. These two cases are nondegenerate. Equations (3.4) together with the conditions (3.6) provide the branching rules for $SU(6) \downarrow [SU(3) \otimes SU(2)]$, that is, which representations $(\nu_1\nu_2, \mu)$ can occur, with degeneracy $g(\lambda_1\lambda_2; \nu_1\nu_2, \mu)$.

To show that this prescription gives a complete set of states, it is necessary to show that

$$
\begin{aligned}
N_{\lambda_1\lambda_2} &= \sum_{\nu_i,\mu} g(\lambda_1\lambda_2; \nu_1\nu_2, \mu) N_{\nu_1\nu_2} \cdot N_\mu\\
&= \tfrac{1}{2} \sum g(\lambda_1\lambda_2; \nu_1\nu_2, \mu)(\nu_1 + 1)(\nu_2 + 1)\\
&\quad \times (\nu_1 + \nu_2 + 2)(\mu + 1),
\end{aligned}
\tag{3.8a}
$$

where the dimension of the 2-rowed $SU(6)$ representation $N_{\lambda_1\lambda_2}$ is

$$
\begin{aligned}
N_{\lambda_1\lambda_2} &= (4!\,5!)^{-1}(\lambda_1 + 1)(\lambda_2 + 1)(\lambda_1 + \lambda_2 + 2)\\
&\quad \times (\lambda_2 + 2)(\lambda_1 + \lambda_2 + 3)(\lambda_2 + 3)\\
&\quad \times (\lambda_1 + \lambda_2 + 4)(\lambda_2 + 4)(\lambda_1 + \lambda_2 + 5).
\end{aligned}
\tag{3.8b}
$$

We then substitute Eqs. (3.4b) into (3.8a), and sum the integers n_i, subject to the conditions (3.6). This has been carried out for special cases, up to the case $\lambda_1 = 3$, $\lambda_2 = 6$, $N_{\lambda_1\lambda_2} = 168$, 168 and $\lambda_1 = 5$, $\lambda_2 = 5$, $N_{\lambda_1\lambda_2} = 206$, 388. These representations are rather large, so the completeness is assumed to hold for general λ_1, λ_2.

The method of constructing the highest weight polynomial state vector, outlined in this section, may be generalized to the case of a 5-rowed $SU(6)$ representation. It is straightforward to construct the fundamental states S_i, but the difficulty arises in determining the dependence relations of Table III.

4. DIRECT PRODUCT OF $SU(6)$ SYMMETRIC STATES

The general highest-weight polynomial state vector, associated with the 2-rowed representation, may be written

$$
|\lambda_1\lambda_2; \nu_1\nu_2\mu\rangle_\tau = \sum_{n_i} A_{n_i}(\tau) P_{n_i},
\tag{4.1}
$$

where τ is a parameter which labels the g-degenerate states and $A_{n_i}(\tau)$ are arbitrary coefficients. The polynomials P_{n_i} are not orthogonal with respect to the inner product; however, the states (4.1) may be diagonalized with respect to an operator χ which breaks the degeneracy. The method of construction of such operators χ is the same for $U(n) \downarrow O(n)$,[20] $U(4) \downarrow [U(2) \otimes U(2)]$,[1] and the present case, and so we will discuss the problem in qualitative terms.

As shown in Ref. 6, the degeneracy in the direct product of $SU(3)$ representations $SU(3)_1 \times SU(3)_2$, $(\nu_1\nu_2) \otimes (\nu_3\nu_4)$, may be broken by means of an operator χ. If we label the state vectors with the operators C_{ij}, $ij = 1, 2$ [Eq. (1.2) with $n = 3$] for the first state vector in the direct product and $i, j = 3, 4$ for the second, then we may form the operators $C_{\mu\nu}$, $\mu\nu = 1, \cdots, 4$, which operate on the direct-product state vector. The Casimir operator for the direct-product state vector

$$
C_2 = C_{\mu_1\mu_2} C_{\mu_2\mu_1}, \quad \mu_1\mu_2 = 1, \cdots, 4,
\tag{4.2a}
$$

may be written[6]

$$
C_2 = C_2(3)_1 + C_2(3)_2 + C_2(R),
\tag{4.2b}
$$

where $C_2(3)_1$ is the quadratic Casimir operator for space "1," $C_2(3)_2$ for space "2," and $C_2(R)$, a quadratic operator which commutes with the operators $C_{\mu\nu}$. The cubic operator C_3 may be expressed as a sum of operators $C_3(3)_1$, $C_3(3)_2$ [and also $C_2(3)_1$, $C_2(3)_2$] plus two additional operators constructed of $C_{\mu\nu}$ that commute with the $C_3(3)_i$, $C_2(3)_i$ operators and the generators C^{ij}. The direct-product state vector may be diagonalized with respect to one of these operators, Moshinsky's operator[6] χ.

Alternatively, it has been shown by Hecht[21] that the operator χ on the direct-product state may be expressed in terms of a mixed product of generators acting on spaces "1," "2":

$$
\chi = (C_1^{\beta\mu}(1) C^{\mu\alpha}(1) + C^{\mu\alpha}(1) C^{\beta\mu}(1)) C^{\alpha\beta}(2),
\qquad \alpha, \beta, \mu = 1, 2, 3,
\tag{4.3}
$$

where $C^{\beta\mu}(1)$, $C^{\beta\mu}(2)$ are the generators on the spaces "1," "2," respectively, and $\alpha\beta\mu = 1, 2, 3$.

We consider now the operator χ which breaks the degeneracy of $SU(3) \otimes SU(2)$ multiplets in $SU(6)$. For the symmetric representation of $SU(6)$, the $SU(3) \otimes SU(2)$ multiplets are nondegenerate. We may construct, as in (4.2a), the $SU(6)$ quadratic Casimir operator

$$C^2 = C^{\mu_1\mu_2}C^{\mu_2\mu_1} \tag{4.4}$$

which takes the form of (4.2b), a quadratic $SU(3)$ plus a quadratic $SU(2)$ Casimir operator, and a quadratic operator $C^2(R)$ constructed of the remaining $SU(6)$ generators. The operator $C^2(R)$ commutes with the $SU(3)$, $SU(2)$ quadratic Casimir operators, but, similar to (4.2b), is already diagonal with respect to Eq. (4.1). The cubic $SU(6)$ Casimir operator C^3 on the symmetric representation reduces to a sum of Casimir operators C^3, C^2 on $SU(3)$, C^2 on $SU(2)$, plus operators $C^3(R)$, $C^2(R)$, all diagonal on the symmetric state vector.

If the state vector (4.1) is associated with a 2-rowed Young diagram, the cubic Casimir operators break up as before, but $C^3(R)$ is now in two parts $C^3(R)_1$, $C^3(R)_2$ (on the symmetric representation, to within the Casimir operators, these operators are the same). Either operator $C^3(R)_i$, $i = 1, 2$, may be used to diagonalize (4.1) and determine the coefficients $A_{n_i}(\tau)$. This operator may be constructed (modulo Casimir operators) as the cubic operator contracted on the $U(2)$ lower indices C_{ij} (before relabeling).

Alternatively, in terms of the $SU(6)$ generators, we may see that the operator χ has the form (4.3). The $SU(6)$ generators, according to (1.1) with $m = 2$, may be written

$$C^{\alpha\beta} = C^{\alpha\beta}(1) + C^{\alpha\beta}(2), \quad \alpha, \beta = 1, \cdots, 6, \tag{4.5}$$

where $C^{\alpha\beta}(1)$ $[C^{\alpha\beta}(2)]$ is constructed of C_6 vectors $z_1^\alpha(z_2^\alpha)$. The cubic Casimir operator may be written

$$C^3 = C^3(1) + C^3(2) + 3C^{\mu_1\mu_2}(1)C^{\mu_2\mu_3}(1)C^{\mu_3\mu_1}(2) + 3C^{\mu_1\mu_2}(1)C^{\mu_2\mu_3}(2)C^{\mu_3\mu_1}(2). \tag{4.6}$$

The last two terms have the form of X, Eq. (4.3), up to Casimir operators.

If we consider the 2-rowed $SU(6) \supset SU(3) \otimes SU(2)$ state vector as the direct product of $SU(6)$ symmetric states, $SU(6)_1 \times SU(6)_2$, with generators $C^{\alpha\beta}(i)$, $\alpha\beta = 1, \cdots, 6$ and $i = 1, 2$ for the two spaces, then the generators have the form (4.5), and our operator χ is exactly Moshinsky's operator X (modulo Casimir operators).

Given the orthonormal state vector (4.1), it is a straightforward matter to calculate the coupling coefficients for the nondegenerate direct product

$$(\lambda_1, 0, \cdots, 0) \times (\lambda_2, 0, \cdots, 0) = \sum (\lambda_3, \mu_3, 0, \cdots, 0) \tag{4.7}$$

of $SU(6) \supset SU(3) \otimes SU(2)$ representations. We outline the steps. According to Bargmann[22] (or Ref. 15), it is necessary to construct an orthonormal polynomial h, invariant under $SU(6)$ transformations U,

$$T_u h = h.$$

Then, h may be written

$$h = \sum \begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3\mu_3 \\ \alpha_1\beta_1 & \alpha_2\beta_2 & \alpha_3\beta_3\tau \end{Bmatrix} |\lambda_1, \alpha_1\beta_1\rangle \times |\lambda_2, \alpha_2\beta_2\rangle \overline{|\lambda_3\mu_3, \alpha_3\beta_3\rangle_\tau}, \tag{4.8}$$

where $\{\ \}$ is the 3λ coupling coefficient, which may be obtained explicitly by taking the inner product (see Appendix B) of h with the 3-state vectors on the right of (4.8). The problem, then, is to find an invariant h. We state the result,

$$h = \Delta \frac{(z_2 \cdot \bar{z}_3)^{k_1}(z_1 \cdot \bar{z}_3)^{k_2}[(z_1 \times z_2) \cdot \bar{\Delta}_{34})]^{k_3}}{k_1!\, k_2!\, k_3!}, \tag{4.9}$$

where Δ is the normalization calculated in Appendix B. Finally, it is necessary to take the inner product of h, (4.9), with a product of the state vectors $|\lambda_1\alpha_1\beta_1\rangle \times |\lambda_2\alpha_2\beta_2\rangle$ [Eq. (2.11a)] and $|\lambda_3\mu_3; \alpha_3, \beta_3\rangle_\tau$ [Eq. (4.1)], to obtain the 3λ coupling coefficient.

APPENDIX A: $SU(2)$ IRREDUCIBLE REPRESENTATION

The explicit polynomial state vector for the symmetric $SU(6) \supset SU(3) \otimes SU(2)$ representation is given by (2.11a). The $SU(2)$ transformation T_u, defined in (2.12a), may be written

$$z_i'^\alpha = u_{i'i} z_{i'}^\alpha, \quad \text{where} \quad u = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}. \tag{A1}$$

We wish to prove

$$T_u |\lambda; \alpha\beta\rangle = \mathfrak{D}^j_{\beta'\beta}(u) |\lambda; \alpha\beta'\rangle, \tag{2.13a}$$

$$T_u |\lambda; \alpha\beta\rangle = N(-1)^q \sum_{\substack{\mu\nu \\ \alpha_i, \kappa_i}} \frac{r!\,(\lambda_2 - q)!\; p!\,(\lambda_1 - p)!\; s!}{k!\,(\lambda_2 - q - k)!} (\Delta_{12}^{\mu\nu})^{\lambda_2} P^{\mu\nu}_{\alpha_i\kappa_i} \cdot S^{\mu\nu}_{\alpha,\kappa_i}, \tag{A2}$$

where

$$P^{\mu\nu}_{\alpha_i\kappa_i} = (a_{11})^{\lambda_1-s-\mu}(a_{12})^{\mu}(a_{21})^{s-\nu}(a_{22})^{\nu}(z_1^1)^{\alpha_1-\kappa_1}(z_2^1)^{\kappa_1}(z_1^2)^{\alpha_2-\kappa_2}(z_2^2)^{\kappa_2}(z_1^3)^{\alpha_3-\kappa_3}(z_2^3)^{\kappa_3},$$

$$S^{\mu\nu}_{\alpha_i\kappa_i} = \sum_{\substack{a_i \\ k_1,k_2}} [a_1!\,(\alpha_1-k_1-a_1)!\,(\kappa_1-a_1)!\,(k_1-\kappa_1+a_1)!\,a_2!\,(\alpha_2-k_2-a_2)!\,(\kappa_2-a_2)!\,(k_2-\kappa_2+a_2)!]^{-1}$$
$$\times [(\mu-a_1-a_2)!\,(\alpha_3-s+k_1+k_2+a_1+a_2)!\,(\kappa_3-a_1+a_2)!\,(s-k_1-k_2-\kappa_3-a_1-a_2)!]^{-1}$$

and $\alpha_1 = p-(r-k)$, $\alpha_2 = r-k$, $\alpha_3 = \lambda_1 - p$, $\kappa_1+\kappa_2+\kappa_3 = \mu+\nu = s'$. By use of the binomial relation

$$\sum_s \frac{1}{s!\,(a-s)!\,(b-s)!\,(c+s)!} = \frac{(a+b+c)!}{a!\,b!\,(a+c)!\,(b+c)!},$$

the coefficient $S^{\mu\nu}_{\alpha_i\kappa_i}$ becomes (let $\nu' = s'-\mu'$)

$$S^{\mu\nu}_{\alpha_i\kappa_i} = \frac{(\lambda_1-s')!\,s'!}{\kappa_1!\,(\alpha_1-\kappa_1)!\,\kappa_2!\,(\alpha_2-\kappa_2)!\,\kappa_3!\,(\alpha_3-\kappa_3)!\,\mu!\,(s'-\mu)!\,[s-(s'-\mu)]!\,(\lambda_1-s-\mu)!}.$$

If we insert this result into (A2) and compare with (2.12a), we have (2.13a).

APPENDIX B: NORMALIZATION OF INVARIANT h

The inner product of h may be calculated from the generating function

$$\Phi = \sum_{ki} h\tau_1^{k_1}\tau_2^{k_2}\tau_3^{k_3}$$
$$= \exp\{\tau_1(z_2\cdot\bar z_3) + \tau_2(z_1\cdot\bar z_3) + \tau_3(z_1\times z_2)\cdot\bar\Delta_{34}\}, \tag{B1}$$

$$(\Phi',\Phi) = \sum_{k_i k_i'}(h,h)\prod_{mn}\tau_m^{km}\bar\tau'^{kn}_m \tag{B2}$$
$$= \int d\mu_{24}\exp(A), \tag{B3a}$$

where

$$A = \tau_1(z_2\cdot\bar z_3) + \tau_2(z_1\cdot\bar z_3) + \tau_3(z_1\times z_2)\cdot\bar\Delta_{34} + \bar\tau_1'(\bar z_2\cdot z_3) + \bar\tau_2'(\bar z_1\cdot z_3) + \bar\tau_3'\overline{(z_1\times z_2)}\cdot\Delta_{34} \tag{B3b}$$

and

$$d\mu_{24} = \exp(-z_\alpha^\beta\cdot z_\alpha^\beta)\prod_{i,\alpha,\beta} dx_i^\alpha\,dy_i^\beta,$$
$$\alpha = 1,\cdots,4, \quad \beta = 1,\cdots,6. \tag{B3c}$$

The exponent A may be written in the form

$$A = a_1\cdot z_3 + \overline{\bar a_2\cdot z_3} + b_1\cdot\Delta_{34} + \overline{\bar b_2\cdot\Delta_{34}},$$

using the results of Ref. 15, integrated to give

$$\int \frac{d\mu_{12}\exp\{[a_1\cdot\bar a_2 - (a_1\cdot b_1)\overline{(\bar a_2\cdot\bar b_2)}]/(1-b_1\cdot b_2)\}}{(1-b_1\cdot b_2)^5}, \tag{B4}$$

where

$$a_1 = \overline{\tau_1'z_2+\tau_2'z_1}, \quad \bar a_2 = \tau_2 z_2+\tau_2 z_1,$$
$$b_1 = \overline{\tau_3(z_1\times z_2)}, \quad \bar b_2 = \tau_3(z_1\times z_2),$$

$$(\Phi',\Phi) = \int d\mu_{12}\sum_n \frac{1}{n!}\frac{(B)^n}{(1-b_1\cdot b_2)^{n+5}}$$
$$= \sum\frac{1}{n!}\frac{(n+r+4)!}{(n+4)!\,r!}\int (B)^n(b_1\cdot b_2)^r\,d\mu_{12}, \tag{B5}$$

where

$$B = \frac{\overline{(\tau_1'z_2+\tau_2'z_1)}\cdot(\tau_1 z_2+\tau_2 z_1)}{1-\bar\tau_3'\tau_3\overline{(z_1\times z_2)}\cdot(z_1\times z_2)}.$$

To calculate the integral in (B5), we form a generating function, as in (B1),

$$\Psi' = \sum\frac{(B)^n(b_1\cdot b_2)^n}{n!\,r!}(\rho_1)^n(\rho_2)^r$$

and take the inner product of Ψ' with respect to z_2, expand out again, form a generator, and take the inner product with respect to z_1. The result is

$$(\Phi',\Phi) = \sum_{ki}(h,h)\prod_m(\tau_m\bar\tau_m')^{k_m},$$

where

$$\Delta^{-2} = (h,h) = \frac{(\lambda_3+\mu_3+5)!\,(\lambda_3+\mu_3+4)!\,(\mu_3+4)!}{\mu_3!\,(\lambda_1-\mu_3)!\,(\lambda_2-\mu_3)!\,(\lambda_3+4)!\,4!\,5!}. \tag{B6}$$

This is the normalization Δ in Eq. (4.9).

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[17] This form of the generators of $SU(6) \supset SU(3) \otimes SU(2)$ first appears in an article by M. A. B. Bég and V. Singh, Phys. Rev. Letters **13**, 418 (1964).
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(a) IR {4}, dim 126, $SU_2 \times SU_3$ content $\{2\} \otimes \{3,1\} + \{4\} \otimes \{4,0\} + \{0\} \otimes \{2,2\}$.
(b) IR {3, 1}, dim 210, $SU_2 \times SU_3$ content $\{2\} \otimes \{4\} + \{4\} \otimes \{3,1\} + \{2\} \otimes \{2,2\} + \{2\} \otimes \{3,1\} + \{2\} \otimes \{1\} + \{0\} \otimes \{3,1\} + \{0\} \otimes \{1\}$.
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Eikonal Approximation for Nonlinear Equations*

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An eikonal approximation for nonlinear equations is derived from an expansion in powers of space and time derivatives. For the special case of one dependent variable, the method is equivalent to an averaging method proposed by Whitham and derived by Luke. A general solution for each order of the expansion is obtained and discontinuous solutions are discussed.

1. INTRODUCTION

Whitham[1,2] has proposed an averaging method for treating nonlinear equations. It is based upon the existence of periodic wavetrain solutions, for which the rapid oscillations are averaged out to give equations for the relatively slow and smooth variation of the wave vectors and frequency. In the first instance, these equations were obtained by averaging conservation laws, but later it was shown that the theory could be expressed more simply in terms of an averaged Lagrangian.[2]

The derivation of the method has been considered by Luke,[3] who used an expansion procedure which had been applied to ordinary differential equations by Kuzmak[4a] and which amounts to an extension of the eikonal approximation to nonlinear equations.[4b] This work is of interest not only for the development of the theory of nonlinear equations, but also because the eikonal approximation arises frequently when there is a change of level of approximation or of physical understanding.

However, it is clear that a further study is required since part of Luke's derivation[3] referred to one particular differential equation only and, in a more general case, was restricted to second-order equations in one dependent variable, and it was found that Whitham's approach was "by no means evident from the above expansion method," but required a studied rearrangement of the equations.

The purpose of this paper is to give a more general discussion of the expansion procedure and to make certain extensions of the method, most particularly to include the important case of several coupled fields.

Two derivations will be given. In Sec. 2, the special case of one dependent variable will be considered, and it will be shown that, if one works with the conservation laws, both of Whitham's formulations[1,2] follow very simply. The content of this section is essentially the same as Luke's derivation,[3] but it is made clear that it is Hamilton's principle which permits the use of an averaged Lagrangian approach.[2] It is also shown that there is an alternative to the averaged Lagrange equations, which may be easier to use in practice.

In Sec. 3, the procedure will be extended to cover the case of coupled fields. This is accomplished by introducing several phase variables, and it allows us to consider problems in which there are "pseudo-frequencies" [2,5] and to calculate the scattering of waves in the eikonal approximation. The approach used in Sec. 3 is slightly different from that of Sec. 2. There are circumstances in which Lagrange's equations and the conservation laws are not equivalent. When the former are more fundamental, the derivation of Sec. 3 should be used; otherwise, the approach of Sec. 2 is necessary.

In Sec. 4, the higher-order equations are discussed in detail and, for one dependent variable, a general solution is found. Section 5 contains a discussion of discontinuous solutions.

No applications will be considered in this paper,

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In Sec. 4, the higher-order equations are discussed in detail and, for one dependent variable, a general solution is found. Section 5 contains a discussion of discontinuous solutions.

No applications will be considered in this paper,

and the reader will find that reference to Whitham's work[1,2,5] will make the argument more readily understandable.

2. THE EXPANSION IN LOWEST ORDER

It is assumed that the equations under consideration are Lagrange's equations for the functions v_r:

$$\frac{\partial}{\partial x_i}\left(\frac{\partial L}{\partial(\partial v_r/\partial x_i)}\right) = \frac{\partial L}{\partial v_r}. \tag{2.1}$$

Here, $r = 1, 2, \cdots, m$, and L is the Lagrangian density

$$L \equiv L\left(v_r, \frac{\partial v_r}{\partial x_i}, x_i\right). \tag{2.2}$$

The summation convention is assumed for the subscripts i, which run over the values 0, 1, 2, $\cdots$, N. Usually, we have in mind $N = 3$, with x_0 equal to the time t and (x_1, x_2, x_3) representing three space coordinates.

The Lagrangian density given in Eq. (2.2) is sufficiently general for most applications. The use of several unknown functions v_r allows us to consider systems of coupled equations and also equations which are of more than second order, provided it is possible to define a higher derivative of a function v_r as a new function v_s and still write the equations in Lagrangian form.

If L does not depend explicitly upon x_i, Eqs. (2.1) frequently have periodic wavetrain solutions of the form

$$v_r = u_r^0(\theta), \tag{2.3}$$

with

$$\theta = k_i x_i. \tag{2.4}$$

The k_i are constants, and the entire dependence of u_r upon the x_i is contained in the phase function θ. When x_0 is the time, $(-k_0)$ is the frequency and, in three space dimensions, (k_1, k_2, k_3) is the wave vector.

Substitution of Eqs. (2.3) and (2.4) into Eq. (2.1) gives

$$\frac{\partial}{\partial\theta}\left(\frac{\partial L^0}{\partial(\partial u_r^0/\partial\theta)}\right) = \frac{\partial L^0}{\partial u_r^0}, \tag{2.5}$$

where

$$L^0 \equiv L\left(u_r^0, k_i \frac{\partial u_r^0}{\partial\theta}\right). \tag{2.6}$$

Equations (2.5) are m ordinary differential equations for the functions $u_r^0(\theta)$, and they are Lagrange's equations for a dynamical system with generalized coordinates u_r^0 and Lagrangian L^0, with θ playing the role of the time. Although special solutions of Eqs. (2.1) may be found in this way, the solutions of Eqs. (2.5) generally are multiply periodic and the eikonal approximation requires the introduction of several phase variables. For this reason, to clarify the discussion and to make more direct contact with the work of Whitham[1,2] and Luke,[3] the special case of one unknown function ($m = 1$), and hence one phase variable, will be considered in this section, and the subscript will be omitted from u_r. The more general discussion will then be given in Sec. 3. Also, until later in this section, it will be assumed that there are no x_i which do not occur in θ.

The eikonal approximation consists in seeking more general solutions in which the k_i and the constants of motion occurring in $u^0(\theta)$ are slowly varying functions of the x_j. Such solutions may arise if the wave is propagating through a nonuniform medium, which varies slowly in space and time. In this case, L depends explicitly upon x_j. For a uniform medium, the slow variation of the k_i may be generated by boundary conditions, or it may correspond to the asymptotic condition of a more complicated solution, when waves of different k_i have become dispersed from one another. In this case, the approximation will not be uniformly valid for a given system, but will describe particular states of motion which may exist.[1,2]

When the k_i depend upon the x_j, Eq. (2.4) must be replaced by

$$\theta = \int_P k_i\, dx_i, \tag{2.7}$$

where the integral is taken along some path P.

Usually, it is required that

$$\frac{\partial k_i}{\partial x_j} - \frac{\partial k_j}{\partial x_i} = 0, \quad \text{for all } i, j, \tag{2.8}$$

in order that

$$\frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial^2 u}{\partial x_j \partial x_i} \tag{2.9}$$

be satisfied.

Then, provided the k_i are single valued, it follows from Stokes' theorem that, apart from a constant, θ is independent of the path P. This is not necessarily true in general. In geometrical optics,[6] for example, in the case of a point source and a plane mirror, the vector is 2-valued, one corresponding to rays from the source, the other to rays from the image. When a ray is reflected at the mirror, the wave vector jumps from one branch to the other. Thus, at each point, θ depends upon the path followed by the ray, even though Eq. (2.8) is satisfied. In this case, the path dependence of θ is one way of building the boundary conditions into the eikonal approximation.

Alternatively, it may be that $\partial v/\partial x_i$ are the basic

physical quantities and Eq. (2.9) is not satisfied. Then u may be introduced as a path-dependent variable, Eq. (2.8) need not be true, and θ is path dependent. As an example, which is discussed in Sec. 5, $\partial v/\partial x_i$ may be the components of the velocity of a fluid, and Eq. (2.9) breaks down in a region where the flow is not irrotational. For the present, it is assumed that Eq. (2.9) is required.

The object now is to find differential equations for the variation of the k_j with the x_i. The requirement that this variation be slow suggests that an expansion be made in powers of derivatives with respect to the x_i.

For any solution $v(x_i) = u(\theta, x_i)$,

$$\frac{\partial v}{\partial x_i} = k_i \frac{\partial u}{\partial \theta} + \frac{\partial u}{\partial x_i}.$$

Then, if

$$u = \sum_{n=0}^{\infty} u^n, \tag{2.10}$$

where u^n is of nth order in derivatives of u^0 with respect to x_i with θ fixed,

$$\frac{\partial v}{\partial x_i} = k_i \frac{\partial u^0}{\partial \theta} + \sum_{n=0}^{\infty} \left(k_i \frac{\partial u^{n+1}}{\partial \theta} + \frac{\partial u^n}{\partial x_i} \right), \tag{2.11}$$

with terms of the same order collected together.

In this method of phrasing the eikonal approximation, the k_j are of order zero and the derivatives are of higher order. It should be noticed that this is different from the usual approach in geometrical optics,[6] where it is assumed that the derivatives are of order zero but the k_j are large, and an expansion is made in powers of k_j^{-1}. For the electromagnetic field, the two methods yield the same result, but if the equations are not homogeneous in derivatives, or if they contain u, this is not so. The second approach is inappropriate for the present problem, since in lowest order, it does not give the equation for the periodic wave train.

Now, if the Lagrangian is expanded as

$$L = \sum_{n=0}^{\infty} L^n, \tag{2.12}$$

the successive approximations to Eqs. (2.1) may be obtained from Eqs. (2.10)–(2.12). In lowest order, Eq. (2.5) is obtained, as expected. By choice of constants of integration, the period may be assigned arbitrarily, and it will be set equal to unity. In principle, the period could be allowed to depend upon x_i, but this merely complicates the calculation, and it adds nothing since it can be absorbed into the k_j.

The equations for the variation of the k_j and the corrections may be found from the higher-order approximations to Eq. (2.1). However, it turns out that this requires quite cumbersome manipulations,[3] which can be avoided if the expansion is applied to the energy–momentum tensor.[7] Both of Whitham's formulations[1,2] follow rather easily, and the relationship between them becomes clear. In addition, there is a considerable simplification of the discussion of the corrections.

Two derivations will be given, one in the remainder of this section, the other in Sec. 3.

The energy–momentum tensor[7] is defined as

$$T_{ij} = \delta_{ij} L - \frac{\partial u}{\partial x_i} \frac{\partial L}{\partial (\partial u/\partial x_j)} \tag{2.13}$$

and, from Eqs. (2.1) and (2.9), it satisfies

$$\frac{\partial T_{ij}}{\partial x_j} = \left(\frac{\partial L}{\partial x_i} \right)_u. \tag{2.14}$$

The essential simplification in using Eqs. (2.14) instead of Eqs. (2.1) is that there are no explicit derivatives with respect to u in Eqs. (2.13) and (2.14). It may also happen that it is *essential* to use Eq. (2.14). For some systems, there is no Lagrangian, yet the equations may be written in the form of Eq. (2.14), with an appropriate change in the right-hand side.

Now, if the expansion of T_{ij} is

$$T_{ij} = \sum_{n=0}^{\infty} T_{ij}^n, \tag{2.15}$$

then

$$T_{ij}^0 = \delta_{ij} L^0 - k_i \left(\frac{\partial L^0}{\partial k_j} \right)_{u^0}, \tag{2.16}$$

where L^0 is given by Eq. (2.6), and the expansion of Eq. (2.14) is

$$k_j \frac{\partial T_{ij}^0}{\partial \theta} = 0, \tag{2.17}$$

$$k_j \frac{\partial T_{ij}^n}{\partial \theta} + \left(\frac{\partial T_{ij}^{n-1}}{\partial x_j} \right)_\theta = \left(\frac{\partial L^{n-1}}{\partial x_i} \right)_{u, k_j}, \tag{2.18}$$

for $n = 1, 2, \cdots$.

Equation (2.17) could have been obtained alternatively from Eq. (2.5) and, by using Eq. (2.16) and assuming $k_i \neq 0$, it gives the "energy equation" of Eq. (2.5),

$$k_j \frac{\partial L^0}{\partial k_j} - L^0 = \sum_r \frac{\partial u^0}{\partial \theta} \frac{\partial L^0}{\partial (\partial u^0/\partial \theta)} - L^0 = E(x_i). \tag{2.19}$$

The requirement that the period be unity gives a relation between $E(x_i)$ and the k_j, and the boundary conditions relate the other integration constants to k_i. A useful way of finding these relationships in practice[2]

is to use a particular case of Hamilton's principle for Eqs. (2.5), which states that

$$\mathfrak{L} = \langle L^0 \rangle \equiv \int_0^1 d\theta L^0 \tag{2.20}$$

is stationary with respect to variations of u. Trial functions u, with period unity, are substituted into Eq. (2.20) and $\mathfrak{L}$ is minimized with respect to parameters in u. In particular, if E is chosen as a parameter,

$$\frac{\partial \mathfrak{L}}{\partial E} = 0 \tag{2.21}$$

gives the dispersion relation between k_i and E, and if k_i are replaced by $\partial\theta/\partial x_i$, this is the eikonal differential equation.[6]

Turning now to the first-order equations, Eqs. (2.18) for $n = 1$ may be integrated with respect to θ to find

$$k_j[T^1_{ij}(\theta) - T^1_{ij}(0)] = -\int_0^\theta d\theta' \left(\frac{\partial T^0_{ij}(\theta')}{\partial x_j}\right)_{\theta'} + \int_0^\theta d\theta' \left(\frac{\partial L^0}{\partial x_i}\right)_{u^0, k_j}. \tag{2.22}$$

Now T^0_{ij} and L^0 are periodic in θ and, unless

$$\int_0^1 d\theta' \left(\frac{\partial T^0_{ij}(\theta')}{\partial x_j}\right)_{\theta'} = \int_0^1 d\theta' \left(\frac{\partial L^0}{\partial x_i}\right)_{u^0, k_j}, \tag{2.23}$$

the right-hand side of Eq. (2.22) increases without bound as θ increases. Since T^1_{ij} depends upon u^1, $\partial u^1/\partial\theta$, and x_j derivatives of u, this would imply that at least one of the u^1 would be unbounded for large θ, and the approximation would break down. Then Eq. (2.23) has to be satisfied to remove these secular terms.

Since θ' is held fixed in differentiation with respect to x_j, Eq. (2.23) may be rewritten

$$\frac{\partial}{\partial x_j} \langle T^0_{ij} \rangle = \left\langle \left(\frac{\partial L^0}{\partial x_i}\right)_{u^0, k_j} \right\rangle, \tag{2.24}$$

where $\langle \cdots \rangle$ implies averaging over θ as in Eq. (2.20). These are the required equations for the k_j, and they are one form of the averaged conservation laws introduced by Whitham.[1]

Now Hamilton's principle allows us to rewrite $\langle T^0_{ij} \rangle$ and Eqs. (2.24) in an alternative form. It follows from Eqs. (2.5) that $\mathfrak{L}$ is stationary with respect to variations of u^0, so that

$$\left\langle \left(\frac{\partial L^0}{\partial k_j}\right)_{u^0} \right\rangle = \left\langle \frac{\partial L^0}{\partial k_j} \right\rangle = \frac{\partial \mathfrak{L}}{\partial k_j} \tag{2.25}$$

and, averaging Eq. (2.16) over a period and using Eq. (2.25), we have

$$\langle T^0_{ij} \rangle = \delta_{ij}\mathfrak{L} - k_i \frac{\partial \mathfrak{L}}{\partial k_j}. \tag{2.26}$$

Using Hamilton's principle again, we see that Eq. (2.24) becomes

$$\frac{\partial}{\partial x_j} \langle T^0_{ij} \rangle = \left(\frac{\partial \mathfrak{L}}{\partial x_i}\right)_{k_j}. \tag{2.27}$$

On comparing Eqs. (2.26) and (2.27) with Eqs. (2.13) and (2.14), it can be seen that $\langle T^0_{ij} \rangle$ is the energy–momentum tensor and Eqs. (2.27) are the conservation laws of a system, for which the Lagrangian is $\mathfrak{L}$ and k_j are the derivatives of the field. That is, the Lagrangian $\mathfrak{L}$, which determines the x_j variation, is the average of the Lagrangian L^0 which determines the θ variation.

The averaged Lagrangian equations may now be obtained by substituting Eq. (2.26) into Eq. (2.27) to find

$$\frac{\partial \mathfrak{L}}{\partial k_j}\left(\frac{\partial k_j}{\partial x_i} - \frac{\partial k_i}{\partial x_j}\right) = k_i \left(\frac{\partial}{\partial x_j}\frac{\partial \mathfrak{L}}{\partial k_j}\right). \tag{2.28}$$

Then, from Eq. (2.8), provided $k_i \neq 0$, we have

$$\frac{\partial}{\partial x_j}\frac{\partial \mathfrak{L}}{\partial k_j} = 0, \tag{2.29}$$

which is the Lagrange equation corresponding to Eqs. (2.26) and (2.27), since θ does not appear explicitly in $\mathfrak{L}$.

Alternatively, Eq. (2.28) could be multiplied by $\partial\mathfrak{L}/\partial k_i$ and summed over i to obtain zero on the left-hand side. Then, provided $k_i(\partial\mathfrak{L}/\partial k_i) \neq 0$, Eq. (2.29) follows.

Equations (2.8) and (2.29) are an alternative set of equations for the k_i, and constitute the second method proposed by Whitham.[2] For linear equations,[2,4b] Eq. (2.29) becomes the transport equation of geometrical optics.[6] It can be seen from this derivation that the basic reason why the averaged Lagrangian may be used to find the variation of k_j is that the initial solutions u^0_r are extremals of $\mathfrak{L}$.

The procedure, then, is to find particular periodic solutions of Eqs. (2.5) and to calculate $\mathfrak{L}$ to find the explicit form of Eq. (2.29). However, it should be noticed that, in practice, it is often simpler to use Eq. (2.25) to rewrite Eq. (2.29) as

$$\frac{\partial}{\partial x_j}\left\langle \left(\frac{\partial L^0}{\partial k_j}\right)_{u^0} \right\rangle = 0, \tag{2.30}$$

since differentiation of u^0 (which may be a complicated function of k_j) is thereby avoided. The main advantage of using the averaged Lagrangian equation, instead of the averaged conservation laws, is that the number of equations which are peculiar to the system under consideration is reduced from $N + 1$ [Eqs. (2.27)] to one [Eq. (2.29)]. Equations (2.8) are quite general.

This advantage is preserved if Eq. (2.30) is used instead of Eq. (2.29), and, often, the calculations are simplified.

An immediate extension of the method may be obtained by assuming that $i = 0, 1, 2, \cdots, M$, and that the variables x_i for $i > N$ do not occur in θ. Slow variation with respect to these variables is not assumed and, in the expansion, by writing summations explicitly, Eqs. (2.17) and (2.18) become, for $i \leq N$,

$$\sum_{j=0}^{N} k_j \frac{\partial T_{ij}^0}{\partial \theta} + \sum_{j=N+1}^{M} \frac{\partial T_{ij}^0}{\partial x_j} = 0, \tag{2.31}$$

$$\sum_{j=0}^{N} \left[k_j \frac{\partial T_{ij}^n}{\partial \theta} + \left(\frac{\partial T_{ij}^{n-1}}{\partial x_j} \right)_\theta \right] + \sum_{j=N+1}^{M} \frac{\partial T_{ij}^n}{\partial x_j} = \left(\frac{\partial L^{n-1}}{\partial x_i} \right)_{u, k_j} \tag{2.32}$$

Equations (2.31) and (2.32) may be integrated over x_j for $j > N$ and, provided T_{ij}^n vanishes on the boundaries, Eqs. (2.17) and (2.18) are obtained, with T_{ij}^n and L^n replaced by their integrals over x_j for $j > N$.

The rest of the argument proceeds as before, except that $\mathfrak{L}$ has been averaged over x_j, for $j > N$, as well as over θ. This the procedure used by Whitham[5] in considering water waves.

3. SEVERAL PHASE VARIABLES

In general, when there are m coupled fields u_r, the solutions of Eqs. (2.5) are multiply periodic and describe the motion of many wavetrains. Then, clearly, it is too restrictive to assume that each wave train has the same wave vector k_i or that, if the wave vectors were the same initially, they would vary in the same way in space and time. In these circumstances, the procedure has to be modified, and it is necessary to introduce several phase variables θ_α. As a simple example, if the Lagrangian describes m uncoupled fields, each wavetrain has its own wave vector and requires its own phase variable.

The manner of introducing several phases will depend upon the problem, in general. Here, we describe the procedure for a special case, which, however, occurs frequently in practice. The solution of Eqs. (2.5) may be expressed in terms of angle variables $w_\alpha = \nu_\alpha \theta + \delta_\alpha$ and action variables J_β as

$$u_r^0 = u_r^0(w_\alpha, J_\beta),$$

and u_r^0 is periodic in the w_α.

Then it frequently happens that the many-phase function

$$u_r^0 = u_r^0(\nu_\alpha \beta_\alpha, J_\beta)$$

is a solution of Eqs. (2.1), even when the wave vectors

$$k_i^\alpha = \frac{\partial \theta_\alpha}{\partial x_i} \tag{3.1}$$

depend upon α. This is the situation which we consider. A special case occurs when all variables but one are cyclic. Then the solutions are periodic in one phase and linear in the remainder. This problem may also be solved with the aid of only one phase variable, and this appears to be the most general case in which this is true.[2] The recurrence of a smaller number of cyclic variables may make it possible to reduce the number of phases, but more than one will be required. The k_i^α for the cyclic variables correspond to Whitham's[1,2] pseudo-wave-vectors.

The constants δ_α which occurred in the angle variables have been absorbed into the phases θ_α. The required generalization of the procedure of Sec. 2 is to find equations for the x_j variation of the m quantities J_β as well as of the k_i^α.

One set of relations is obtained by setting the periods in θ_α equal to unity as in Sec. 2, which requires

$$\nu_j \equiv \nu_j(k_i^\alpha, J_\beta) = 2\pi.$$

For cyclic variables, the corresponding constants J_i may be absorbed into the k_i^α. The other required equations are the generalizations of Eq. (2.29), and the remainder of this section is concerned with deriving them.

In cases where the θ_α cannot be introduced in this way, more explicit methods, such as perturbation theory, must be used, and a similar accounting of the $2n$ integration constants has to be made.

For any solution $v_r(x_i) = u_r(\theta_\alpha, x_i)$,

$$\frac{\partial v_r}{\partial x_i} = k_i^\alpha \frac{\partial u_r}{\partial \theta_\alpha} + \frac{\partial u_r}{\partial x_i}, \tag{3.2}$$

where the summation convention is used for α.

If the k_i^α are constant, the Lagrangian is

$$L^0 = L\left(u_r^0, k_i^\alpha \frac{\partial u_r^0}{\partial \theta_\alpha} \right) \tag{3.3}$$

and Lagrange's equations (2.1) become

$$\frac{\partial}{\partial \theta_\alpha} \left(\frac{\partial L^0}{\partial (\partial u_r^0 / \partial \theta_\alpha)} \right) = \frac{\partial L^0}{\partial u_r^0}, \tag{3.4}$$

which is the generalization of Eq. (2.5). The uniform solutions, upon which the eikonal approximation is based, are then the special solutions of Eq. (3.4), which satisfy the requirements set out above.

Now it is possible to introduce the energy–momentum tensor and to obtain the averaged conservation equations exactly as in Sec. 2. However,

the averaged Lagrange equations for each α separately do not follow immediately. For this reason, a slightly different method is used.

Let

$$M_{\alpha\beta} = \delta_{\alpha\beta}L - \sum_r \frac{\partial u_r}{\partial\theta_\alpha}\frac{\partial L}{\partial(\partial u_r/\partial\theta_\beta)}. \tag{3.5}$$

This quantity is essentially the energy–momentum tensor for the variables θ_α. The equations for $M_{\alpha\beta}$ have the same structural advantages as the conservation equations, and they lead to the average Lagrange equations for each α. Also, we find that there is no need to take particular care of the explicit dependence of L upon x_i.

From Eq. (3.2), Lagrange's equations (2.1) become

$$\left(\frac{\partial}{\partial x_i}\frac{\partial L}{\partial(\partial u_r/\partial x_i)}\right)_\theta + k_i^\alpha \frac{\partial}{\partial\theta_\alpha}\left(\frac{\partial L}{\partial(\partial u_r/\partial x_i)}\right) = \frac{\partial L}{\partial u_r}. \tag{3.6}$$

Also, using Eq. (3.2), we have

$$\frac{\partial L}{\partial(\partial u_r/\partial\theta_\alpha)} = k_i^\alpha \frac{\partial L}{\partial(\partial u_r/\partial x_i)}, \tag{3.7}$$

$$\left(\frac{\partial L}{\partial k_i^\alpha}\right)_{u_r} = \sum_r \frac{\partial L}{\partial(\partial u_r/\partial x_i)}\frac{\partial u_r}{\partial\theta_\alpha}. \tag{3.8}$$

With the aid of these three equations, $\partial M_{\alpha\beta}/\partial\theta_\beta$ may be calculated directly from Eq. (3.5) and put into the form

$$\frac{\partial M_{\alpha\beta}}{\partial\theta_\beta} = \left[\frac{\partial}{\partial x_i}\left(\frac{\partial L}{\partial k_i^\alpha}\right)_{u_r}\right]_\theta. \tag{3.9}$$

No approximation has been made so far, but if $M_{\alpha\beta}$ is expanded as

$$M_{\alpha\beta} = \sum_n M_{\alpha\beta}^n, \tag{3.10}$$

then the lowest two orders of Eq. (3.9) are

$$\frac{\partial M_{\alpha\beta}^0}{\partial\theta_\beta} = 0, \tag{3.11}$$

$$\frac{\partial M_{\alpha\beta}^1}{\partial\theta_\beta} = \left[\frac{\partial}{\partial x_i}\left(\frac{\partial L^0}{\partial k_i^\alpha}\right)_{u_r}\right]_\theta, \tag{3.12}$$

where

$$M_{\alpha\beta}^0 = \delta_{\alpha\beta}L^0 - \sum_r \frac{\partial u_r^0}{\partial\theta_\alpha}\frac{\partial L^0}{\partial(\partial u_r^0/\partial\theta_\beta)}. \tag{3.13}$$

Equation (3.11) could be obtained from Eqs. (3.4) and (3.13) directly.

For the moment, we assume that the u_r are periodic in every θ_α. Then, when Eq. (3.12) is integrated over the θ_β, the requirement that there be no secular terms in u_r^1 for each θ_β leads to the condition

$$\frac{\partial}{\partial x_i}\left\langle\left(\frac{\partial L^0}{\partial k_i^\alpha}\right)_{u_r}\right\rangle = 0 \tag{3.14}$$

for each α, just as in Sec. 2. Here, the average is over a complete period of each θ_β. Further, if $\mathfrak{L}$ is the average Lagrangian

$$\mathfrak{L} = \int_0^1 d\theta_1\, d\theta_2 \cdots d\theta_m L^0, \tag{3.15}$$

then Hamilton's principle shows once again that the requirement of keeping u_r fixed when differentiating with respect to k_i^α may be dropped in Eq. (3.14). It may be rewritten as

$$\frac{\partial}{\partial x_i}\frac{\partial\mathfrak{L}}{\partial x_i^\alpha} = 0. \tag{3.16}$$

These are the Lagrange equations for the functions θ_α, with the Lagrangian $\mathfrak{L}$ not explicitly dependent upon θ. The conservation equations (2.27) follow immediately with the aid of Eq. (2.8).

Equations (3.16) are the appropriate generalization of Eqs. (2.29) and, in fact, the derivation is simpler than that given in Sec. 2. However, it is instructive to compare the two methods, and, furthermore, it is seen in Sec. 5 that there are circumstances in which the conservation laws (2.14) are more fundamental than Lagrange's equations; then the method of Sec. 2 should be followed.

So far, it has been assumed that the original solution was periodic in the variables $\theta_1, \theta_2, \cdots, \theta_p$. Suppose now that there is an additional variable θ_{p+1}, such that u_1^0 is linear in θ_{p+1} and that u_1^0 does not appear in L^0, which is then independent of θ_{p+1}. Then, as above, the requirement of no secular terms in $\theta_1, \cdots, \theta_m$ gives

$$\frac{\partial M_{\alpha,p+1}^{(1)}}{\partial\theta_{p+1}} = \frac{\partial}{\partial x_i}\frac{\partial\mathfrak{L}}{\partial k_i^\alpha} \tag{3.17}$$

instead of Eq. (3.16). Now the right-hand side of Eq. (3.17) is independent of θ_{p+1}, so it has to be zero if there are no secular terms in θ_{p+1} occurring in $M_{\alpha,p+1}^{(1)}$. Thus Eq. (3.16) is satisfied without integration over θ_{p+1} and the equation holds for $\alpha = p+1$ also. The k_i^{p+1} are the pseudofrequencies which were considered by Whitham[2,5] in applications to water waves.

In Eqs. (3.16), the different wave vectors are coupled together, and this equation represents an eikonal approximation for the scattering of waves.

4. HIGHER ORDERS

In this section, higher orders of the expansion are considered. In each order, coupled equations for the u_r^n are obtained. Therefore, we restrict ourselves to the case of one dependent variable, for which an explicit

solution may be found. This illustrates the procedure to be followed in the more general case. It is possible to work with T_{ij} or $M_{\alpha\beta}$ and obtain the same result, but we use the latter, since the derivation is rather simpler algebraically.

It is assumed that there is just one unknown function u and one phase variable θ. Then, instead of $M_{\alpha\beta}$ of Sec. 3, we work with

$$M = L - \frac{\partial u}{\partial\theta}\frac{\partial L}{\partial(\partial u/\partial\theta)}, \tag{4.1}$$

which satisfies

$$\frac{\partial M}{\partial\theta} = \left[\frac{\partial}{\partial x_i}\left(\frac{\partial L}{\partial k_i}\right)_u\right]_\theta, \tag{4.2}$$

as a special case of Eq. (3.9).

Now, if

$$M = \sum_{n=0}^{\infty} M^n \tag{4.3}$$

and L is expanded according to Eq. (2.12), then

$$\frac{\partial M^n}{\partial\theta} = \frac{\partial}{\partial x_i}\left(\frac{\partial L^{n-1}}{\partial k_i}\right)_u, \tag{4.4}$$

so that

$$M^n(\theta) - M^n(0) = \int_0^\theta d\theta'\left[\frac{\partial}{\partial x_i}\left(\frac{\partial L^{n-1}}{\partial k_i}\right)_u\right]_{\theta'}. \tag{4.5}$$

Now M^n depends upon u^n, $\partial u^n/\partial\theta$, and the mth derivatives of u^{n-m} and $\partial u^{n-m}/\partial\theta$ with respect to x_j and, in order to rewrite Eq. (4.5) as an equation for u^n, M^n will be rewritten

$$M^n(\theta) = \left(u^n\frac{\partial}{\partial u^0} + \frac{\partial u^n}{\partial\theta}\frac{\partial}{\partial(\partial u^0/\partial\theta)}\right)M^0(\theta) + \mu^n(\theta), \tag{4.6}$$

where, by definition, $\mu^n(\theta)$ is the part of M^n which does not contain u^n or $u^n(\theta)$.

Then, from Eqs. (4.1) and (4.6), using Eqs. (2.5), we have

$$\begin{aligned} M^n - \mu^n &= u^n\left(\frac{\partial}{\partial\theta}\frac{\partial L^0}{\partial(\partial u^0/\partial\theta)} - \frac{\partial u^0}{\partial\theta}\frac{\partial^2 L^0}{\partial u^0\partial(\partial u^0/\partial\theta)}\right) \\ &\quad - \frac{\partial u^n}{\partial\theta}\frac{\partial u^0}{\partial\theta}\frac{\partial^2 L^0}{\partial(\partial u^0/\partial\theta)^2} \\ &= \frac{\partial^2 L^0}{\partial(\partial u^0/\partial\theta)^2}\left(u^n\frac{\partial^2 u^0}{\partial\theta^2} - \frac{\partial u^n}{\partial\theta}\frac{\partial u^0}{\partial\theta}\right). \end{aligned} \tag{4.7}$$

If this expression is substituted into Eq. (4.5), the resulting equation may be integrated at once to give

$$\begin{aligned} u^n(\theta) - u^n(0) &= -\frac{\partial u^0}{\partial\theta} \\ &\times \int_0^\theta d\theta'\left\{\int_0^{\theta'} d\theta''\left(\left[\frac{\partial}{\partial x_i}\left(\frac{\partial L^{n-1}}{\partial k_i}\right)_u\right]_{\theta''} + M^n(0) - \mu^n(\theta')\right)\Big/ \right. \\ &\qquad \left.\left(\frac{\partial u^0}{\partial\theta'}\right)^2\frac{\partial^2 L^0}{\partial(\partial u^0/\partial\theta')^2}\right\} \end{aligned} \tag{4.8}$$

$$= -\frac{\partial u^0}{\partial\theta}F^n(\theta), \tag{4.9}$$

say.

This is an explicit solution for $u^n(\theta)$, since the right-hand side depends upon u^m for $m < n$ and $M^n(0)$, which is an integration constant.

Now, if u^m for $m < n$ are periodic with unit period, it follows from Eqs. (4.5), (4.8), and (4.9) that u^n will have secular terms in θ unless

$$\int_0^1 d\theta'\left[\frac{\partial}{\partial x_i}\left(\frac{\partial L^{n-1}}{\partial k_i}\right)_u\right]_{\theta'} = 0 \tag{4.10}$$

and

$$F^n(1) = 0. \tag{4.11}$$

Then, from Eqs. (4.9) and (4.11), $u^n(\theta)$ is periodic with unit period and, since this is true of $u^0(\theta)$, it follows by induction that it is true of all $u^n(\theta)$, and Eqs. (4.10) and (4.11) are satisfied for all n.

Equation (4.10) determines $u^{n-1}(0)$, and Eq. (4.11) is a condition for $M^n(0)$. Thus, the solution is completely specified. Luke[3] used a different method to find $u^n(\theta)$ for a particular Lagrangian, and it can be shown that the general solution given by Eq. (4.8) applied to that special case can be transformed into Luke's solution.

The accuracy of the lowest-order approximation could be estimated by means of the expansion, but each individual case must be considered separately, since the assumption of slow variation is expected to be good only for particular times or boundary conditions.

5. DISCONTINUOUS SOLUTIONS

The solutions of Eq. (2.29) may become many-valued or singular if the medium has a discontinuity or if, for example, the group velocity decreases along the direction of propagation, so that a given segment of the wave tends to catch up with the wave ahead of it. When this happens, the theory is strictly invalid, but it may still be possible to make use of it by introducing discontinuous solutions.[8] However, a difficulty arises in that there are different sets of conditions which might be used to determine the discontinuities. Whitham[1] suggested a particular choice

[Eq. (5.3) below]. In this section, the problem will be reconsidered, since the derivations given above suggest different possibilities.

From Eqs. (2.8) and (2.29), it is straightforward to derive[9] expressions for changes across a surface of discontinuity S, and they are, respectively,

$$[k_i]n_j = [k_j]n_i, \tag{5.1}$$

$$\left[\frac{\partial \mathfrak{L}}{\partial k_j}\right]n_j = 0, \tag{5.2}$$

where the n_j are the space and time direction cosines of the normal to S and $[v]$ is the change in a function v across S.

For continuous solutions, Eqs. (2.8) and (2.29) are equivalent to Eqs. (2.27), but the discontinuity conditions

$$[\langle T^0_{ij}\rangle]n_j = 0 \tag{5.3}$$

which come from Eqs. (2.27) are not equivalent to Eqs. (5.1) and (5.2); thus, a choice has to be made.

In the linear case,[6] Eq. (5.1) is satisfied and leads to Snell's law, but it is difficult to give meaning to Eqs. (5.2) and (5.3) since the solution becomes 2-valued as both a reflected and a transmitted wave appear.

For nonlinear problems, Whitham[1] has suggested that a shock wave might appear and that Eqs. (5.3) rather than (5.1) and (5.2) should give the discontinuity across the shock. The reason for this choice was that the approximation breaks down because of the rapid changes, but the conservation equations (2.14) still hold across the shock.

However, according to the discussion of Sec. 4, Eqs. (2.8) and (2.29) do not become invalid when there are rapid changes. What happens is that the higher corrections u^m become important and Eqs. (2.27) are no longer good approximations to the original conservation equations (2.14). Thus, from this point of view, the breakdown of the eikonal approximation favors Eqs. (5.1) and (5.2).

Furthermore, if the *mathematical* problem posed is to find solutions of Lagrange's equations (2.1), then the conservation laws (2.14) can be derived from Eqs. (2.1) only if Eq. (2.9) is satisfied and u is continuous. It is therefore inconsistent to start with Eqs. (2.14), then, for discontinuous solutions, derive Eq. (5.3) and find that Eqs. (5.1) and (5.2), which come from Eqs. (2.1) and (2.9), are invalid.

However, in any application, we wish to know which discontinuity conditions are most closely realized experimentally, and, for this purpose, it is usually possible to decide on physical grounds that one set of equations is more fundamental.

As an example, we consider the case of water waves, for which it turns out that Eq. (5.3) are appropriate. The starting point is the set of conservation equations for energy and momentum which may be written[10] in the form of Eqs. (2.14). If the flow is irrotational, it is possible to introduce a velocity potential ϕ and Lagrangian density[11] L and so to derive Eqs. (2.1) from (2.14). But Eqs. (2.1) cannot be derived if ϕ is discontinuous or if the flow is rotational so that ϕ is a path-dependent variable and does not satisfy Eq. (2.9). Therefore, one would expect that Eq. (5.3) are the appropriate shock conditions and then, since Eqs. (5.1) are not satisfied, vorticity is developed within the shock. In this example, the choice of Eq. (5.3) is the same as that made by Whitham[1]; but it was based upon a physical argument and not upon the validity of the eikonal approximation, and it seems possible that Eqs. (5.1) and (5.2) may be appropriate in other cases.

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$$\rho = \rho_0 H(y + h_0)H(\eta - y),$$

where ρ_0 is the constant density of the water, y is a vertical coordinate, $y = -h_0$ is the fixed bottom, and $y = \eta$ is the free surface. $H(\tau)$ is 1 for $\tau > 0$ and 0 for $\tau < 0$. Then the variation of ρ is obtained by varying ρ_0 and η in Bateman's variation principle, and the usual equations for surface waves are obtained. This formulation of the problem, rather than Luke's, is an essential starting point for the eikonal approximation as derived here.

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Quantum Theory of the Generalized Wave Equations. I*

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We have made a systematic analysis of the quantum theory of the infinite-component fields that transform under the combined representations of $SL(2, C)$ (Majorana) $\otimes$ Dirac. A complete set of solutions of the wave equation includes solutions with timelike and spacelike momenta. We have explicitly calculated the mass spectra for the timelike and spacelike cases. Our method makes use of the decomposition of the product representation into reducible representations of the "little" groups $SU(2)$ and $SU(1, 1)$. Finally, the quantization of the generalized fields is presented.

1. INTRODUCTION

Recent investigations of the infinite-component field equations and their algebraic formalisms have added a lot to our understanding of strong-interaction dynamics.[1–4] Models based on these equations have many interesting consequences of direct experimental interest. Attempts have been made to obtain solutions for the algebra of local current densities.[5] Unlike the case of the finite-component field equations, one is able to treat here infinitely many mass and spin states satisfying the same wave equation. Quantum systems described by such equations, indeed, possess "internal structure."[3] However, the theory is plagued with so-called "diseases." These speculative and malign pathologies are rather irrelevant! The existence of the redundant or unphysical spacelike solutions finds its way in describing an entirely new kind of phenomena of radiation involving "faster-than-light particles."[6] A systematic formulation of quantum field theory compatible with the substitution law and with the right spin–statistics relations has also been furnished.[1]

The concept of infinite-component field equations is not of recent origin. In the thirties, Majorana discovered a type of wave equation describing both the infinite-component spinor and tensor fields.[7] These field equations possess both discrete and continuous solutions (the lightlike solutions can be treated as a limiting case of the spacelike solutions). Detailed analyses of the quantum theory of these Majorana fields have been done elsewhere.[1,2] We just want to make a passing remark that these field equations have solutions for masses which are quite unrealistic in hadron physics: The masses vary inversely as the spin. Subsequently, attempts have been made to avert this situation. We will analyze an interesting field equation first proposed by Abers, Grodsky, and Norton and subsequently studied by others in the context of obtaining solutions for the current algebra at infinite momentum.[5,8] We confine ourselves to formulating a systematic quantization scheme for this generalized field equation.

The contents of the paper are arranged as follows. In Sec. 2, we describe the field equation. The fields transform as infinite-component column vectors under the product representation of $SL(2, C)$ (Majorana) $\otimes$ D (Dirac). The algebraic properties of $SL(2, C) \otimes D$ representations under various subgroups of interest are discussed in Sec. 3. We classify the field equation under each "little group" and then have summarized the corresponding mass–spin spectra in Sec. 4. In Sec. 5, we display the complete set of solutions of the field equation. Finally, we have furnished the quantization scheme for these infinite-component generalized fields.

2. THE WAVE EQUATION

Let

$$\mathfrak{L} = \int d^4x \bar{\psi}(x)(i\gamma_\mu \partial^\mu - m_0 - \tfrac{1}{2}m_1\sigma_{\mu\nu}\Gamma^{\mu\nu})\psi(x), \quad (2.1)$$

be the Lagrangian for a theory of a set $\{\psi_{\sigma n}(x)\}$ of fields. The generators of the Poincaré transformations are

$$P_\mu, J_{\mu\nu} = \tfrac{1}{2}\sigma_{\mu\nu} + \Gamma_{\mu\nu} + \Gamma^x_{\mu\nu}, \quad (2.2)$$

where $\Gamma_{\mu\nu}$ and $\frac{1}{2}\sigma_{\mu\nu}$ generate the infinite-dimensional representation and finite-dimensional (nonunitary) Dirac representation of $SL(2, C)$, respectively; $\Gamma^x_{\mu\nu}$ is the orbital part of $J_{\mu\nu}$ which is given by

$$\Gamma^x_{\mu\nu} = i(x_\mu \partial^\nu - x_\nu \partial^\mu).$$

In the rest system, $J_{\mu\nu}$ provides us the total angular momentum of the quantum system.

The fields $\{\psi_{\sigma n}(x)\}$ are labeled by two indices: The Greek index σ and the Latin index n characterize the infinite-dimensional Majorana representation and the finite-dimensional (nonunitary) Dirac representation, respectively. Thus, the transformation property

of the fields $\{\psi_{\sigma n}(x)\}$ is given by

$$\psi_{\sigma n}(x) \to \psi'_{\sigma n}(x) = U(\Lambda)^{\sigma'}_{\sigma} V(\Lambda)^{n'}_{n} \psi_{\sigma' n'}[\Lambda^{-1}(x - a)]. \tag{2.3}$$

The equation of motion follows from the given Lagrangian (2.1)

$$(i\gamma_\mu \partial^\mu - M)\psi(x) = 0, \tag{2.4}$$

where M is now a Lorentz-invariant mass matrix given by

$$M = m_0 + \tfrac{1}{2} m_1 \sigma_{\mu\nu} \Gamma^{\mu\nu}. \tag{2.5}$$

Note that M is now a matrix and no longer a constant and, hence, does not commute with γ_μ. However, it commutes with p_μ, a condition necessary to describe free-particle motion. In the limit $m_1 = 0$, the wave equation (2.4) reduces to the ordinary Dirac equation. We come to this point in detail in Sec. 4.

3. PROPERTIES OF THE $SL(2, C)$ (MAJORANA) $\otimes$ DIRAC REPRESENTATIONS

In this section, we first briefly recapitulate the mathematical properties of the two Majorana representations, the Dirac representation, and then display in detail the representation of the product space namely $X = \mathcal{K}_{SL(2,C)} \otimes \mathcal{K}_D$ under various subgroups of interest.

A. The Majorana Representations

The generators of the homogeneous Lorentz group $\Gamma_{\mu\nu}$ satisfy the commutation relations

$$[\Gamma_{\mu\nu}, \Gamma_{\rho\sigma}] = i(g_{\nu\rho}\Gamma_{\mu\sigma} - g_{\mu\sigma}\Gamma_{\nu\rho} + g_{\nu\sigma}\Gamma_{\rho\mu} - g_{\rho\mu}\Gamma_{\nu\sigma}), \tag{3.1}$$

where

$$\mu, \nu, \rho, \sigma = 0, 1, 2, 3,$$
$$g_{00} = -g_{kk} = 1, \quad k = 1, 2, 3,$$
$$g_{\mu\nu} = 0, \quad \mu \neq \nu.$$

To obtain the Majorana representations, we introduce, as usual, the operators a_α and a^+_α, $\alpha = 1, 2$, which satisfy the Bose commutation relations

$$[a_\alpha, a_\beta] = [a^+_\alpha, a^+_\beta] = 0,$$
$$[a_\alpha, a^+_\beta] = \delta_{\alpha\beta}, \quad \alpha, \beta = 1, 2. \tag{3.2}$$

Explicitly, we can express the generators $\Gamma_{\mu\nu}$ in terms of a_α and a^+_α as

$$\Gamma_{ij} = \epsilon_{ijk}\Sigma_k = \tfrac{1}{2}\epsilon_{ijk} a^+ \sigma_k a,$$
$$\Gamma_{i0} = \Lambda_i = \tfrac{1}{4}(a^+ \sigma_i C a^+ - a C \sigma_i a), \tag{3.3}$$

where $C = i\sigma_2$, the σ_i are the usual Pauli matrices. The Casimir operators of the Lorentz group C_0 and C_1 are given by

$$C_0 = \tfrac{1}{2}\Gamma_{\mu\nu}\Gamma^{\mu\nu} = \mathbf{\Sigma}^2 - \mathbf{\Lambda}^2$$
$$= \tfrac{1}{2}a^+a(\tfrac{1}{2}a^+a + 1) - [\tfrac{1}{2}a^+a(\tfrac{1}{2}a^+a + 1) + \tfrac{3}{4}]$$
$$= -\tfrac{3}{4} \tag{3.4a}$$

and

$$C_1 = \tfrac{1}{4}\epsilon^{\alpha\beta\gamma\delta}\Gamma_{\alpha\beta}\Gamma_{\gamma\delta} = \mathbf{\Sigma} \cdot \mathbf{\Lambda} \equiv 0. \tag{3.4b}$$

Thus we find that (j_0, ν) or, equivalently, $(-j_0, -\nu)$ label the unitary irreducible representations of $SL(2, C)$ as

$$C_0 = j_0^2 + \nu^2 - 1 = -\tfrac{3}{4},$$
$$C_1 = -ij_0\nu = 0. \tag{3.5}$$

From (3.5), we find that the solutions for j_0 and ν are

$$j_0 = \tfrac{1}{2}, \quad \nu = 0, \tag{3.6a}$$
$$j_0 = 0, \quad \nu = \tfrac{1}{2}. \tag{3.6b}$$

Equations (3.6a) and (3.6b) characterize the principal-series and supplementary-series representations of $SL(2, C)$, respectively. In (3.6a), the ranges of Σ are given by

$$\Sigma = \tfrac{1}{2}, \tfrac{3}{2}, \tfrac{5}{2}, \cdots,$$

and, from (3.6b), the values of Σ are

$$\Sigma = 0, 1, 2, \cdots.$$

In either case,

$$\Sigma = j_0 + k, \quad k = 0, 1, 2, 3, \cdots,$$
$$\Sigma_3 = -\Sigma, -\Sigma + 1, \cdots, +\Sigma.$$

Thus, we have obtained the Majorana representations for the infinite-component Fermi fields and Bose fields.

B. The Dirac Representation

The generators of the Dirac representation satisfy the commutation relation

$$[\tfrac{1}{2}\sigma_{\mu\nu}, \tfrac{1}{2}\sigma_{\rho\tau}] = \tfrac{1}{2}i[g_{\nu\rho}\sigma_{\mu\tau} - g_{\mu\tau}\sigma_{\nu\rho} + g_{\nu\tau}\sigma_{\rho\mu} - g_{\rho\mu}\sigma_{\nu\tau}]. \tag{3.7}$$

To obtain the representation of D, we look for the ranges of j_0 and ν, which characterize the proper Lorentz group. The representation is finite if[9] (i) j_0 and ν are simultaneously half-integral or integral, and (ii) $|\nu| > |j_0|$. The ranges of spin values are given by

$$j = j_0 + n$$
$$= |j_0| \cdots |\nu| - 1.$$

The finite-component Dirac fields belong to the coupled representation (if parity is admitted) $(\tfrac{1}{2}, \nu) + (-\tfrac{1}{2}, \nu)$, $\nu = \pm\tfrac{3}{2}$ (real!).

C. The Properties of $SL(2, C)$ (Majorana) $\otimes$ D Representations[9]

Define

$$S_{\mu\nu} = \tfrac{1}{2}\sigma_{\mu\nu} + \Gamma_{\mu\nu}. \tag{3.8}$$

Then

$$J_{\mu\nu} = S_{\mu\nu} + \Gamma^{x}_{\mu\nu}. \tag{3.9}$$

We consider the case

$$[\Gamma_{\mu\nu}, \tfrac{1}{2}\sigma_{\mu\nu}] = 0. \tag{3.10}$$

The generators $S_{\mu\nu}$ satisfy the commutation relation

$$[S_{\mu\nu}, S_{\rho\sigma}] = i(g_{\nu\rho}S_{\mu\sigma} - g_{\mu\sigma}S_{\nu\rho} + g_{\nu\sigma}S_{\rho\mu} - g_{\rho\mu}S_{\nu\sigma}). \tag{3.11}$$

To obtain the representations of $G = SL(2, C) \otimes D$, we proceed as follows. Let us define

$$\mathbf{J} = \mathbf{\Sigma} + \tfrac{1}{2}\sigma, \quad \mathbf{K} = \mathbf{\Lambda} + \tfrac{1}{2}\boldsymbol{\tau} = \mathbf{\Lambda} + \tfrac{1}{2}i\boldsymbol{\alpha}, \tag{3.12}$$

where we have identified

$$\begin{aligned} \Gamma_{ij} &= \epsilon_{ijk}\Sigma_k, \\ \Gamma_{i0} &= \Lambda_i, \\ \tfrac{1}{2}\sigma_{ij} &= \tfrac{1}{2}\epsilon_{ijk}\sigma_k, \end{aligned} \tag{3.13}$$

and

$$\tfrac{1}{2}\sigma_{i0} = \tfrac{1}{2}\tau_i = \tfrac{1}{2}i\alpha_i, \quad i, j, k = 1, 2, 3.$$

Further,

$$\begin{aligned} [\Sigma_i, \Sigma_j] &= i\epsilon_{ijk}\Sigma_k, \\ [\Sigma_i, \Lambda_j] &= i\epsilon_{ijk}\Lambda_k, \end{aligned} \tag{3.14}$$

and

$$[\Lambda_i, \Lambda_j] = -i\epsilon_{ijk}\Sigma_k.$$

Also,

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij},$$

$$\alpha_i^2 = \sigma_i^2 = 1 \quad \text{(no summation over } i\text{)},$$

and

$$[\tfrac{1}{2}\tau_i, \tfrac{1}{2}\tau_j] = -i\epsilon_{ijk}(\tfrac{1}{2}\sigma_k), \quad [\tfrac{1}{2}\tau_i, \tfrac{1}{2}\sigma_j] = i\epsilon_{ijk}(\tfrac{1}{2}\tau_k). \tag{3.15}$$

The two Casimir operators Q_0 and Q_1 are given by

$$Q_0 = \mathbf{J}^2 - \mathbf{K}^2$$

and

$$Q_1 = \mathbf{J} \cdot \mathbf{K}. \tag{3.16}$$

Now,

$$Q_0 = \mathbf{J}^2 - \mathbf{K}^2 = (\mathbf{\Sigma} + \tfrac{1}{2}\boldsymbol{\sigma})^2 - (\mathbf{\Lambda} + \tfrac{1}{2}i\boldsymbol{\alpha})^2$$

or,

$$\begin{aligned} Q_0 &= (\mathbf{\Sigma}^2 - \mathbf{\Lambda}^2) + \tfrac{3}{2} + (\boldsymbol{\sigma} \cdot \mathbf{\Sigma} - i\boldsymbol{\alpha} \cdot \mathbf{\Lambda}) \\ &= -\tfrac{3}{4} + \tfrac{3}{2} + (\boldsymbol{\sigma} \cdot \mathbf{\Sigma} - i\boldsymbol{\alpha} \cdot \mathbf{\Lambda}). \end{aligned}$$

(For Majorana representations, $C_0 = \mathbf{\Sigma}^2 - \mathbf{\Lambda}^2 = -\tfrac{3}{4}$, while for Dirac representations, $C_0 = \tfrac{3}{2}$.) Thus,

$$(Q_0 - \tfrac{3}{4}) = (\boldsymbol{\sigma} \cdot \mathbf{\Sigma} - i\boldsymbol{\alpha} \cdot \mathbf{\Lambda}). \tag{3.17}$$

Squaring both sides of (3.17), we solve for Q_0:

$$(Q_0 - \tfrac{3}{4})^2 = \tfrac{3}{4} - 2Q_0,$$

or

$$(Q_0 + \tfrac{3}{4})(Q_0 - \tfrac{1}{4}) = 0.$$

That is,

$$Q_0 = -\tfrac{3}{4} \tag{3.18a}$$

or

$$Q_0 = \tfrac{1}{4}. \tag{3.18b}$$

Similarly,

$$\begin{aligned} Q_1 = \mathbf{J} \cdot \mathbf{K} &= (\mathbf{\Sigma} + \tfrac{1}{2}\boldsymbol{\sigma})(\mathbf{\Lambda} + \tfrac{1}{2}i\boldsymbol{\alpha}) \\ &= -\tfrac{1}{2}i\gamma_5(Q_0 + \tfrac{3}{4}). \end{aligned} \tag{3.19}$$

In obtaining (3.19), we have made use of the property $C_1 = \mathbf{\Sigma} \cdot \mathbf{\Lambda} = 0$. Thus, from (3.18) and (3.19) we obtain

$$Q_1 = 0, \quad \text{for} \quad Q_0 = -\tfrac{3}{4}, \tag{3.20a}$$

$$Q_1 = -\tfrac{1}{2}i\gamma_5, \quad \text{for} \quad Q_0 = \tfrac{1}{4}. \tag{3.20b}$$

It then follows that, since D is nonunitary, the two representations (3.20) characterizing G are also nonunitary and also reducible. Since each $\mathbf{J}^2 = (\mathbf{\Sigma} + \tfrac{1}{2}\boldsymbol{\sigma})^2$ value appears *twice* in the generalized fields, these two nonunitary representations (3.20) exhaust the total reduction.

1. Reduction of G with Respect to SU(1, 1)

The $SU(1, 1)$ subgroup of G may be taken to be generated by the elements J_3, K_1, and K_2. They obey the commutation rules

$$\begin{aligned} [J_3, K_1] &= iK_2, \\ [J_3, K_2] &= -iK_1, \\ [K_1, K_2] &= -iJ_3. \end{aligned} \tag{3.21}$$

Note that $J_3 = \Sigma_3 + \tfrac{1}{2}\sigma_3$, $K_1 = \Lambda_1 + \tfrac{1}{2}\tau_1$, and $K_2 = \Lambda_2 + \tfrac{1}{2}\tau_2$. The quadratic Casimir operator of $SU(1, 1)$ is given by

$$\begin{aligned} Q &= J_3^2 - K_1^2 - K_2^2 \\ &= (\Sigma_3 + \tfrac{1}{2}\sigma_3)^2 - (\Lambda_i + \tfrac{1}{2}i\alpha_1)^2 - (\Lambda_2 + \tfrac{1}{2}i\alpha_2)^2 \\ &= (\Sigma_3^2 - \Lambda_1^2 - \Lambda_2^2) + \tfrac{3}{4} + (\sigma_3\Sigma_3 - \tau_1\Lambda_1 - \tau_2\Lambda_2) \\ &= \mathcal{C} + \tfrac{3}{4} + (\sigma_3\Sigma_3 - \tau_1\Lambda_1 - \tau_2\Lambda_2), \end{aligned} \tag{3.22}$$

where $\mathcal{C} = \Sigma_3^2 - \Lambda_1^2 - \Lambda_2^2$ is the quadratic Casimir operator of $SU(1, 1) \subset SL(2, C)$. Thus, we have

$$(Q - \mathcal{C} - \tfrac{3}{4}) = \sigma_3\Sigma_3 - \tau_1\Lambda_1 - \tau_2\Lambda_2. \tag{3.23}$$

Squaring both sides of (3.23), and after a little algebraic manipulation, we obtain

$$(Q - \mathcal{C} - \tfrac{3}{4})^2 = 2\mathcal{C} - Q + \tfrac{3}{4}.$$

Solving for $\mathcal{C}$, we have

$$\mathcal{C} = (Q + \tfrac{1}{4}) \pm (Q + \tfrac{1}{4})^{\frac{1}{2}} \tag{3.24}$$

or, solving for Q,

$$Q = (\mathcal{C} + \tfrac{1}{4}) \pm (\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}}. \qquad (3.24')$$

Using $Q = \tilde{J}(\tilde{J}+1)$ and $\mathcal{C} = \tilde{\Sigma}(\tilde{\Sigma}+1)$, we obtain from Eq. (3.24) two sets of values for $\tilde{J}$, namely,

$$\begin{aligned} \tilde{J}^{(1)} &= \tilde{\Sigma} + \tfrac{1}{2}, & \tilde{\Sigma} - \tfrac{1}{2}, \\ \tilde{J}^{(2)} &= -\tilde{\Sigma} - \tfrac{1}{2}, & -\tilde{\Sigma} - \tfrac{3}{2}. \end{aligned} \qquad (3.25)$$

Thus, we find that, for each value of Q, there are two values of $\mathcal{C}$, i.e., Eq. (3.24). Since the Dirac representation is nonunitary, $SU(1,1) \subset SL(2,C)$ multiplied by the Dirac spinor is a reducible nonunitary representation and reduces precisely to the above forms (3.25). This could have been formally checked from the fact that each value of $(\tilde{\mathbf{J}})^2 = (\tilde{\mathbf{\Sigma}} + \frac{1}{2}\tilde{\boldsymbol{\sigma}})^2$ appears twice in the generalized fields. To find the possible states, we recall some of the properties of the unitary irreducible representation of $SU(1,1)$. They fall into three classes:

Class (i) The continuous nonexceptional class:

(a) $\frac{1}{4} \leq -\mathcal{C} < \infty$, $\Sigma_3 = 0, \pm 1, \pm 2, \cdots$,

or

(b) $\frac{1}{4} \leq -\mathcal{C} < \infty$, $\Sigma_3 = \pm\frac{1}{2}, \pm\frac{3}{2}, \cdots$.

Class (ii) Continuous exceptional class:

$$0 < -\mathcal{C} < \tfrac{1}{4}, \quad \Sigma_3 = 0, \pm 1, \pm 2, \cdots.$$

Class (iii) Discrete class:

$$\begin{aligned} &\mathcal{C} = k(k-1), \quad k = \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \cdots, \\ &\Sigma_3 = k, k+1, \cdots, \infty, \quad \text{for} \quad D_k^{(+)}, \\ &\Sigma_3 = -k, -k-1, \cdots, -\infty, \quad \text{for} \quad D_k^{(-)}. \end{aligned}$$

We will see in the next section that, for the (mass)^2 to be $-ve$ (spacelike solution), the *only* values of $\tilde{J}$ admitted are given by combining Dirac representation with the class (i) representation.

2. *Some Properties of the Continuous Nonexceptional Nonunitary Representations of* $SU(1,1) \subset G$

We know that each UIR of $SL(2,C)$ characterized by (m, ρ) contains each UIR of $SU(1,1)$ of the continuous nonexceptional class *twice*. Correspondingly, the representation space $\mathcal{H}(SL(2,C))$ decomposes into $\mathcal{H}_{+m}(SU(1,1)) + \mathcal{H}_{-m}(SU(1,1))$. Thus, on restricting $SL(2,C) \otimes D$ to $SU(1,1)$, we obtain two sets of reducible representations defined by (3.25), and each reducible set, furthermore, contains two irreducible parts. We have to note here that the representations characterized by $\tilde{J}^{(1)}$ and $\tilde{J}^{(2)}$ in (3.25) are equivalent.

Thus, we have obtained all the possible irreducible representations when we restrict the group $SL(2,C) \otimes D$ with respect to its subgroup $SU(1,1)$.

4. CLASSIFICATION OF THE PLANE-WAVE SOLUTIONS AND THE MASS SPECTRA

Let us consider the field equation (2.4), that is,

$$[i\gamma_\mu \partial^\mu - m_0 - \tfrac{1}{2}m_1 \sigma_{\mu\nu}\Gamma^{\mu\nu}]\psi(x) = 0.$$

In the momentum representation,

$$\psi(x) = \frac{1}{(2\pi)^2}\int d^4p e^{-ipx}\psi(p),$$

and so we can rewrite Eq. (2.4) as

$$(\gamma_\mu p^\mu - m_0 - \tfrac{1}{2}m_1\sigma_{\mu\nu}\Gamma^{\mu\nu})\psi(p) = 0. \qquad (4.1)$$

Depending on whether p_μ is timelike, spacelike, or lightlike (i.e., $\mathbf{p}^2 - p_0^2 > 0$, $\mathbf{p}^2 - p_0^2 < 0$, or $\mathbf{p}^2 - p_0^2 = 0$), we have, in general, three classes of solutions for Eq. (4.1). We discuss these solutions and their corresponding mass spectra below.

Class I: Timelike Case (Slower-than-Light Particles)

Let us rewrite Eq. (4.1) as

$$(E - \boldsymbol{\alpha}\cdot\mathbf{p} - \beta M)\psi(p) = 0$$

or

$$H\psi(p) = E\psi(p) = (\boldsymbol{\alpha}\cdot\mathbf{p} + \beta M)\psi(p), \qquad (4.2)$$

where H is the Hamiltonian of the system. In general, the spinors $\psi(p)$ can be labeled by the eigenvalues of β, σ_3, Σ^2, and Σ_3 or, alternatively, by $|\beta, J, \lambda\Sigma\rangle$, where β, J, λ, and Σ are the eigenvalues of β, the total spin $\mathbf{J}^2 = (\mathbf{\Sigma} + \frac{1}{2}\boldsymbol{\sigma})^2$, J_3, and $\mathbf{\Sigma}^2$, respectively. That is,

$$\psi(p) \sim \psi(p, \Sigma, \Sigma_3) \otimes \chi(p, \sigma).$$

Thus, solving for the eigenvalues of H in Eq. (4.2), we obtain the masses m_J. In the rest system,

$$\begin{aligned} \mathcal{M} &= \beta M = \beta m_0 + \tfrac{1}{2}m_1\beta\sigma_{\mu\nu}\Gamma^{\mu\nu} \\ &= \beta m_0 + m_1\beta(\boldsymbol{\sigma}\cdot\mathbf{\Sigma} - \boldsymbol{\tau}\cdot\mathbf{\Lambda}). \end{aligned} \qquad (4.3)$$

Note that, for $\mathcal{M}$ to be self-adjoint, we choose β, $\beta\boldsymbol{\sigma}$, and $\beta\boldsymbol{\tau}$ to be Hermitian, and for the Majorana representations, $\mathbf{\Sigma}$ and $\mathbf{\Lambda}$ are also Hermitian. Since β does not commute with $\mathcal{M}$, the states $|\beta, J, \lambda, \Sigma\rangle$ are not the eigenstates of $\mathcal{M}$. Nonetheless, the mass matrix can be written as (for a detailed derivation of $\mathcal{M}$, see the Appendix)

$$\mathcal{M} = \begin{pmatrix} m_0 - m_1(J+\frac{3}{2}) & -im_1[J(J+1)]^{\frac{1}{2}} \\ im_1[J(J+1)]^{\frac{1}{2}} & -[m_0 + m_1(J-\frac{1}{2})] \end{pmatrix}. \qquad (4.4)$$

Diagonalizing the above matrix, we obtain

$$\begin{aligned} m_J &= m_1(J+\tfrac{1}{2}) \\ &\quad \pm [(m_0 - m_1)^2 + m_1^2(J+\tfrac{1}{2})^2 - \tfrac{1}{4}m_1^2]^{\frac{1}{2}} \end{aligned} \qquad (4.5)$$

or

$$(m_J)^2 = 2m_1^2)J + \tfrac{1}{2})^2 + (m_0 - m_1)^2 - \tfrac{1}{4}m_1^2 \pm 2m_1(J + \tfrac{1}{2})[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2 + m_1^2(J + \tfrac{1}{2})^2]^{\frac{1}{2}}. \quad (4.6)$$

Thus, we find from expression (4.5) that there are two values of m_J for each value of J. A detailed discussion of this mass matrix will be presented at the end of this section.

Class II: Spacelike Solutions (Faster-than-Light Particles)

Let us choose the frame

$$p_\mu = (\tilde{m}\sinh\zeta; 0, 0, \tilde{m}\cosh\zeta), \quad \tilde{m} > 0.$$

Then, in the rest-system ($\zeta = 0$), we obtain, from Eq. (4.1),

$$(\tilde{m} - \gamma_3 M)\psi(0, \tilde{\alpha}) = 0$$

or

$$\tilde{m}\psi(0, \tilde{\alpha}) = \gamma_3 M\psi(0, \tilde{\alpha}). \quad (4.7)$$

Thus, the mass operator is given by

$$\tilde{m} = m_0\gamma_3 + m_1\gamma_3(\tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}} - \tilde{\boldsymbol{\tau}}\cdot\tilde{\boldsymbol{\Lambda}}), \quad (4.8)$$

where

$$\tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}} = (\sigma_3\Sigma_3 - \tau_1\Lambda_1 - \tau_2\Lambda_2),$$
$$\tilde{\boldsymbol{\tau}}\cdot\tilde{\boldsymbol{\Lambda}} = (\tau_3\Lambda_3 - \sigma_1\Sigma_1 - \sigma_2\Sigma_2),$$

and

$$\tilde{\boldsymbol{\sigma}} = (\sigma_3, \tau_1, \tau_2), \quad \tilde{\boldsymbol{\tau}} = (\tau_3, \sigma_1, \sigma_2),$$
$$\tilde{\boldsymbol{\Sigma}} = (\Sigma_3, \Lambda_1, \Lambda_2), \quad \tilde{\boldsymbol{\Lambda}} = (\Lambda_3, \Sigma_1, \Sigma_2).$$

The spinors $\psi(0, \tilde{\alpha})$ are labeled by the quantum numbers $\tilde{\alpha}$, which, in general, represent γ_3, $\tilde{J}$, J_3, and $\tilde{\Sigma}$, where $\tilde{J}$, J_3, and $\tilde{\Sigma}$ are the eigenvalues of $(\tilde{\mathbf{J}})^2 = (\tilde{\boldsymbol{\Sigma}} + \frac{1}{2}\tilde{\boldsymbol{\sigma}})^2$, J_3, and $(\tilde{\boldsymbol{\Sigma}})^2 = (\Sigma_3^2 - \Lambda_1^2 - \Lambda_2^2)$, respectively. Rewriting (4.8) as

$$\tilde{m} = (m_0 - m_1)\gamma_3 + m_1\gamma_3[(\tfrac{1}{2} + \tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}}) - (\tilde{\boldsymbol{\tau}}\cdot\tilde{\boldsymbol{\Lambda}} - \tfrac{1}{2})], \quad (4.8')$$

we obtain

$$\tilde{m} = \begin{pmatrix} i(m_0 - m_1) + im_1(\mathcal{C} + \frac{1}{4})^{\frac{1}{2}} & im_1[(\mathcal{C} + \frac{1}{4})^{\frac{1}{2}} - \frac{1}{2}] \\ -im_1[(\mathcal{C} + \frac{1}{4})^{\frac{1}{2}} + \frac{1}{2}] & -i(m_0 - m_1) + im_1(\mathcal{C} + \frac{1}{4})^{\frac{1}{2}} \end{pmatrix}. \quad (4.9)$$

[For a detailed derivation of (4.9), see the Appendix.] Diagonalizing the above matrix, we obtain

$$\tilde{m}_J = i\{m_1(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}} \pm [m_1^2(\mathcal{C} + \tfrac{1}{4}) + (m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]^{\frac{1}{2}}\}. \quad (4.10)$$

Using $\mathcal{C} = \tilde{\Sigma}(\tilde{\Sigma} + 1)$, we obtain

$$(\tilde{m}_J)^2 = -2m_1^2(\tilde{\Sigma} + \tfrac{1}{2})^2 - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] \mp 2m_1(\tilde{\Sigma} + \tfrac{1}{2})[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2 + m_1^2(\tilde{\Sigma} + \tfrac{1}{2})^2]^{\frac{1}{2}}. \quad (4.11)$$

Writing $\tilde{\Sigma} = -\frac{1}{2} + iv$, we find, from Eq. (4.11),

$$(m_v)^2 = 2m_1^2v^2 - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] \pm 2m_1v\{m_1^2v^2 - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]\}^{\frac{1}{2}}. \quad (4.11')$$

For the mass $\tilde{m}$ to be *purely imaginary*, we obtain the following ranges of v:

$$(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2 \leq m_1^2v^2 < \infty$$

or

$$(m_0/m_1 - 1)^2 - \tfrac{1}{4} \leq v^2 < \infty.$$

That is,

$$[(m_0/m_1 - 1)^2 - \tfrac{1}{4}]^{\frac{1}{2}} \leq v < \infty \quad (4.12a)$$

or

$$-\infty < v \leq -[(m_0/m_1 - 1)^2 - \tfrac{1}{4}]^{\frac{1}{2}}. \quad (4.12b)$$

Class III: Lightlike Solutions

Let us choose the frame

$$p_\mu = (p; 0, 0, p). \quad (4.13)$$

The little group which leaves this configuration invariant is generated by J_3, $K_2 - J_1$, and $K_1 + J_2$. These generators satisfy the commutation relations of the $E(2)$ algebra, namely,

$$[J_3, E_1] = iE_2, \quad [J_3, E_2] = -iE_1, \quad [E_1, E_2] = 0, \quad (4.14)$$

$$\mathcal{E} = (E_1, E_2), J_3,$$
$$E_1 = K_1 + J_2 = (\Lambda_1 + \tfrac{1}{2}\tau_1) + (\Sigma_2 + \tfrac{1}{2}\sigma_2), \quad (4.15)$$
$$E_2 = K_2 - J_1 = (\Lambda_2 + \tfrac{1}{2}\tau_2) - (\Sigma_1 + \tfrac{1}{2}\sigma_1)$$

and where the invariant Casimir operator is given by

$$\mathcal{E}^2 = E_1^2 + E_2^2. \quad (4.16)$$

Let us consider the wave equation

$$E\psi = [\boldsymbol{\alpha}\cdot\mathbf{p} + m_0\gamma_0 + m_1\gamma_0(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda})]\psi.$$

Substituting (4.13) in the above equation, we have

$$p - \alpha_3 p = m_0\gamma_0 + m_1\gamma_0(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda}). \quad (4.17)$$

Multiplying Eq. (4.17) from the left by $1 + \alpha_3$, we then have

$$0 = m_0(1 + \alpha_3)\gamma_0 + m_1(1 + \alpha_3)\gamma_0(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda})$$

or

$$0 = m_0(\gamma_0 + \gamma_3) + m_1(\gamma_0 + \gamma_3)(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda}). \tag{4.18}$$

Multiplying (4.18) by $\gamma_0 - \gamma_3$ from the left throughout, we obtain

$$0 = 2m_0 + 2m_1(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda});$$

that is,

$$m_0 + m_1(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda}) = 0$$

or

$$m_0\gamma_0 = -m_1\gamma_0(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda}). \tag{4.19}$$

We can proceed exactly as in the previous cases, and obtain the mass matrix as

$$-m_0\gamma_0 = \begin{pmatrix} -m_1(J+\frac{3}{2}) & -im_1[J(J+1)]^{\frac{1}{2}} \\ im_1[J(J+1)]^{\frac{1}{2}} & -m_1(J-\frac{1}{2}) \end{pmatrix}.$$

Diagonalizing the right-hand side, we have

$$-m_0\gamma_0 = \begin{pmatrix} m_1\{(J+\frac{1}{2}) + [(J+\frac{1}{2})^2 + \frac{3}{4}]^{\frac{1}{2}}\} & 0 \\ 0 & m_1\{(J+\frac{1}{2}) - [(J+\frac{1}{2})^2 + \frac{3}{4}]^{\frac{1}{2}}\} \end{pmatrix},$$

or

$$-m_0 = m_1(J+\tfrac{1}{2}) + m_1[(J+\tfrac{1}{2})^2 + \tfrac{3}{4}]^{\frac{1}{2}} \tag{4.20a}$$

and

$$m_0 = m_1(J+\tfrac{1}{2}) - m_1[(J+\tfrac{1}{2})^2 + \tfrac{3}{4}]^{\frac{1}{2}}. \tag{4.20b}$$

Equations (4.20) are simultaneously true if and only if $m_0 \equiv 0$ and $m_1 \equiv 0$. Thus, there are no lightlike solutions of our wave equation.

Some Further Discussions on the Mass Spectra

A. Timelike Case

From Eq. (4.5), we have

$$\begin{aligned} &[m_J - m_1(J+\tfrac{1}{2})]^2 \\ &\qquad = (m_0 - m_1)^2 - \tfrac{1}{4}m_1^2 + m_1^2(J+\tfrac{1}{2})^2, \\ &m_J^2 - 2m_1m_J(J+\tfrac{1}{2}) - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] = 0, \\ &\{m_J^2 - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]\}^2 = 4m_1^2m_J^2(J+\tfrac{1}{2})^2. \end{aligned} \tag{4.21}$$

Let $y = m_J^2$ and $x = (J+\frac{1}{2})^2$. Then, we have, from (4.21),

$$\{y - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]\}^2 = 4m_1^2yx$$

or

$$y^2 - 2y[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] + [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]^2 = 4m_1^2yx. \tag{4.22}$$

Equation (4.22) is the equation of a hyperbola.

(i) If $m_1 = 0$, we obtain, from (4.22),

$$y^2 - 2m_0^2y + m_0^4 = 0 \quad \text{or} \quad (y - m_0^2)^2 = 0,$$

i.e.,

$$y = m_0^2 \quad \text{or} \quad m_J = \pm m_0.$$

This gives the equation of a straight line parallel to the x axis (pure Dirac case).

(ii) Rewriting Eq. (4.22),

$$y\{y - 2[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] - 4m_1^2x\} = [\tfrac{1}{4}m_1^2 - (m_0 - m_1)^2]^2,$$

we obtain for the equations of the asymptotes as

$$y\{y - 2[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] - 4m_1^2x\} = 0;$$

that is,

$$y_1 = 0, \tag{4.23a}$$

$$y_2 = 4m_1^2x + 2[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]. \tag{4.23b}$$

Equations (4.23) define the boundary of the timelike curve.

(iii) We have, for $x \to \infty$, (a) $y \to 0$, (b) $y \to 4m_1^2x$. That is, one branch of the mass curve monotonically rises to infinity and the other branch goes to zero. Thus, there is no discrete lowest mass; the mass spectrum has only an accumulation point.

B. Spacelike Case

The interpretation of the mass spectrum can be carried out in a completely analogous fashion to that of our previous case by studying the variation of $(m\tilde{J})^2$ vs ν^2. We take $(m\tilde{J})^2$ along the negative ordinate and ν^2 along the negative abscissa. We discuss in this section some of the distinct features.

(i) If $m_1 = 0$, from Eq. (4.11), we get

$$(m_J)^2 = -(m\tilde{J})^2 = m_0^2$$

or

$$m_J = \pm m_0.$$

This corresponds to the familiar Dirac case, the particle having constant mass m_0 ($+m_0$ is interpreted as the rest mass of the particle and $-m_0$ as the rest mass of the antiparticle).

(ii) If $m_0 = 0$, we have the mass spectrum arising purely from the symmetry-breaking term $\frac{1}{2}m_1\sigma_{\mu\nu}\Gamma^{\mu\nu}$, namely,

$$\begin{aligned} (m\tilde{J})^2 &= -2m_1^2(\tilde{\Sigma} + \tfrac{1}{2})^2 - \tfrac{3}{4}m_1^2 \\ &\quad \mp 2m_1^2(\tilde{\Sigma} + \tfrac{1}{2})[(\tilde{\Sigma} + \tfrac{1}{2})^2 + \tfrac{3}{4}]^{\frac{1}{2}} \end{aligned}$$

or

$$(m_\nu)^2 = 2m_1^2\nu^2 - \tfrac{3}{4}m_1^2 \pm 2m_1^2\nu(\nu^2 - \tfrac{3}{4})^{\frac{1}{2}}. \tag{4.24}$$

Equation (4.24) admits solutions of the wave equation *only* in the range

$$\tfrac{3}{4} \leq \nu^2 < \infty; \tag{4.25}$$

that is,

$$\sqrt{\tfrac{3}{4}} \leq \nu < \infty, \tag{4.26a}$$

$$-\infty < \nu \leq -\sqrt{\tfrac{3}{4}}. \tag{4.26b}$$

(iii) The case of $m_0 = 0$ and $m_1 = 0$ does not admit any solution of the wave equation (cf. the lightlike solution).

(iv) Finally, the mass spectrum (4.11) is degenerate in ν. This is evident from the fact that we get the same mass spectrum for each of the ranges (4.12a) and (4.12b).

5. CONSTRUCTION OF THE BASIS VECTORS, THE NORMALIZATION, AND THE COMPLETENESS OF THE SOLUTIONS OF THE FIELD EQUATION

1. Timelike Case

We have noted earlier that, in the representation space $\mathcal{H}_G = \mathcal{H}_{SL(2,C)} \oplus \mathcal{H}_D$, the fields transform as double-indexed infinite-component column vectors; i.e., we label each field component by the total spin J, the spin production J_3, and Σ. Then, in an arbitrary frame, the spinor wavefunctions are given by

$$\begin{aligned}\Psi(\mathbf{p}, JJ_3, \Sigma) &= \chi_D(\sigma, \mathbf{p}) \otimes \psi(\mathbf{p}, \Sigma, \Sigma_3) \\ &= \sum_\sigma C(\tfrac{1}{2}, \Sigma; \sigma, \Sigma_3 \,|\, JJ_3)\chi_D(\sigma, \mathbf{p})\psi(\mathbf{p}, \Sigma, \Sigma_3),\end{aligned} \tag{5.1}$$

where $C(\frac{1}{2}, \Sigma; \sigma, \Sigma_3 \,|\, J, J_3)$ is the usual Wigner coefficient, and $\chi_D(\sigma, \mathbf{p})$ and $\psi(\mathbf{p}, \Sigma, \Sigma_3)$ represent the Dirac spinor and the Majorana spinor wavefunctions, respectively. $\chi_D(\sigma, \mathbf{p})$ and $\psi(\mathbf{p}, \Sigma, \Sigma_3)$ are obtained from their rest states by applying the Lorentz boosters: i.e.,

$$\begin{aligned}\Psi(\mathbf{p}, J, J_3, \Sigma) &= e^{i\boldsymbol{\zeta}\cdot\mathbf{K}}\psi(J, J_3, \Sigma) \\ &= e^{i\boldsymbol{\zeta}(\mathbf{A}+\frac{1}{2}\boldsymbol{\tau})}\psi(J, J_3, \Sigma) \\ &= \sum_\sigma C(\tfrac{1}{2}, \Sigma; \sigma, \Sigma_3 \,|\, JJ_3) \\ &\quad \times (e^{\frac{1}{2}i\boldsymbol{\zeta}\cdot\boldsymbol{\tau}}\chi_D)[e^{i\boldsymbol{\zeta}\cdot\mathbf{A}}\psi(\Sigma, \Sigma_3)],\end{aligned} \tag{5.2}$$

where

$$\boldsymbol{\zeta} = \hat{\boldsymbol{\zeta}} \operatorname{arc\,tanh}(\mathbf{p}/E_J)$$

and

$$E_J = (\mathbf{p}^2 + m_J^2)^{\frac{1}{2}}. \tag{5.3}$$

We have to note further here that, for each value of J, there are two values for the masses; thus, we introduce an additional index ϵ to distinguish the two branches of the mass spectrum. We have

$$\begin{aligned}&e^{\frac{1}{2}i\boldsymbol{\zeta}\cdot\boldsymbol{\tau}}\chi_D(\sigma) \\ &\quad = (\cosh\tfrac{1}{2}\zeta - \tfrac{1}{2}\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\zeta}}\sinh\zeta)\chi_D(\sigma) \\ &\quad = \left[\left(\frac{E_J + m_J}{2m_J}\right)^{\frac{1}{2}} - \frac{\boldsymbol{\alpha}\cdot\mathbf{p}}{[2m_J(E_J + m_J)]^{\frac{1}{2}}}\right]\chi_\sigma(0) \\ &\quad = \frac{E_J + m_J - \boldsymbol{\alpha}\cdot\mathbf{p}}{[2m_J(E_J + m_J)]^{\frac{1}{2}}}\chi_\sigma(0).\end{aligned} \tag{5.4}$$

Again,

$$\begin{aligned}\psi(\mathbf{p}, \Sigma, \Sigma_3) &= e^{i\boldsymbol{\zeta}\cdot\mathbf{A}}\psi(\Sigma, \Sigma_3) \\ &= V(B_p)_{\Sigma\Sigma_3}^{\Sigma'\Sigma_3'}.\end{aligned} \tag{5.5}$$

Because of the unitarity of V, the spinors (5.5) are orthonormalized for all $\mathbf{p}$, that is,

$$(\psi(\mathbf{p}, \Sigma, \Sigma_3), \psi(\mathbf{p}, \Sigma', \Sigma_3')) = \delta_{\Sigma\Sigma'}\delta_{\Sigma_3\Sigma_3'}. \tag{5.6}$$

Without any loss of generality, we can choose the frame $\mathbf{p} = \mathbf{e}_z p$. Then (5.5) assumes a very familiar form:

$$V(B_p)_{\Sigma\Sigma_3}^{\Sigma'\Sigma_3'} = \delta_{\Sigma_3\Sigma_3'}V_{\Sigma\Sigma'}^{\Sigma_3}(\zeta), \tag{5.7}$$

where

$$\begin{aligned}V_{\Sigma\Sigma'}(\zeta) = \theta_{\Sigma\Sigma'}&(\cosh\tfrac{1}{2}\zeta)^{-(\Sigma+\Sigma')}(\sinh\tfrac{1}{2}\zeta)^{\Sigma-\Sigma'} \\ &\times F(\Sigma_3 - \Sigma, 1 - \Sigma - \Sigma_3, 1 + \Sigma + \Sigma'; \\ &\qquad -\sinh^2\tfrac{1}{2}\zeta)\end{aligned}$$

and

$$\theta_{\Sigma\Sigma'} = \frac{1}{(\Sigma - \Sigma')!}\left(\frac{\Gamma(\Sigma' - \Sigma_3 + 1)\Gamma(\Sigma' + \Sigma_3)}{\Gamma(\Sigma - \Sigma_3 + 1)\Gamma(\Sigma + \Sigma_3)}\right)^{\frac{1}{2}}. \tag{5.8}$$

(For $\Sigma' > \Sigma$, replace $\zeta \to -\zeta$.) To obtain the expression for the arbitrary Lorentz transformation, we can make a spatial rotation on the state vectors and compute the corresponding matrix elements $V(B_p)$. Thus, we obtain, from Eqs. (5.2), (5.4), (5.7), and (5.8),

$$\begin{aligned}&\psi_\mathcal{E}(p, J, J_3, \Sigma) \\ &= \sum_{\Sigma', \Sigma_3'} C(\tfrac{1}{2}, \Sigma'; \sigma, \Sigma_4' \,|\, JJ_3) \\ &\quad \times \left(\frac{E_J + m_J - \alpha_3 p}{[2m_J(E_J + m_J)]^{\frac{1}{2}}}\right)\chi_\sigma(0)\delta_{\Sigma_3\Sigma_3'} \\ &\quad \times [\theta_{\Sigma\Sigma'}(\cosh\tfrac{1}{2}\zeta)^{-(\Sigma+\Sigma')}(\sinh\tfrac{1}{2}\zeta)^{\Sigma-\Sigma'} \\ &\quad \times F(\Sigma_3 - \Sigma, 1 - \Sigma - \Sigma_3, 1 + \Sigma + \Sigma'; -\sinh\tfrac{1}{2}\zeta)],\end{aligned} \tag{5.9}$$

where $\mathcal{E} = \pm$ denotes the upper or lower branch of the mass spectrum (for $\Sigma < \Sigma'$, replace $\zeta \to -\zeta$ and $\Sigma \leftrightarrow \Sigma'$). In terms of the Jacobi polynomials, the

expression (5.9) can be rewritten as

$$\psi_{\mathcal{E}}(p, J, J_3, \Sigma) = \sum_{\Sigma', \Sigma_3'} C(\tfrac{1}{2}, \Sigma'; \sigma, \Sigma_3' \mid J, J_3) \times \frac{(E_J + m_J - \alpha_3 p)}{[2m_J(E_J + m_J)]^{\frac{1}{2}}} \chi_\sigma(0)\delta_{\Sigma_3\Sigma_3'} \times \left(\frac{(\Sigma - |\Sigma_3|)!(\Sigma' + |\Sigma_3|)!}{(\Sigma + |\Sigma_3|)!(\Sigma' - |\Sigma_3|)!}\right)^{\frac{1}{2}} \times \frac{(-\tanh \frac{1}{2}\zeta)^{\Sigma'-\Sigma}}{(\cosh \frac{1}{2}\zeta)^{2|\Sigma_3|+1}} P^{(\Sigma'-\Sigma, 2|\Sigma_3|)}_{\Sigma-|\Sigma_3|}\left(\frac{1}{\cosh \zeta}\right), \quad (5.10)$$

where

$$P_n^{(\alpha\beta)}(x) = \frac{1}{2^n}\sum_{s=0}^{n}\binom{n+\alpha}{s}\binom{n+\beta}{n-s}(x-1)^{n-s}(x+1)^s,$$

or

$$\psi_{\mathcal{E}}(p, J, J_3, \Sigma) = \sum_{\Sigma', \Sigma_3'} C(\tfrac{1}{2}, \Sigma'; \sigma, \Sigma_3' \mid J, J_3) \times \left(\frac{(E_J + m_J - \alpha_3 p)\chi_\sigma(0)}{[2m_J(E_J + m_J)]^{\frac{1}{2}}}\right)\delta_{\Sigma_3\Sigma_3'} \times \left(\frac{(\Sigma - |\Sigma_3|)!(\Sigma' + |\Sigma_3|)!}{(\Sigma + |\Sigma_3|)!(\Sigma' - |\Sigma_3|)!}\right)^{\frac{1}{2}} \times \left(\frac{(2m_J)^{-2|\Sigma_3|-1}(-p)}{(E_J + m_J)^{\Sigma'-\Sigma+2|\Sigma_3|+1}}\right) P^{(\Sigma'-\Sigma, 2|\Sigma_3|)}_{\Sigma-|\Sigma_3|}\left(\frac{m_{\tilde{J}}}{E_J}\right). \quad (5.11)$$

B. Spacelike Case

We label the spinor wavefunctions as $\tilde{J}, J_3$, and $\tilde{\Sigma}$. Then, in an arbitrary frame, we have

$$\psi_{\mathcal{E}}(p, \tilde{J}, J_3, \tilde{\Sigma}) = \chi_D(\mathbf{p}, \sigma, \mathcal{E}) \otimes \psi(\mathbf{p}, \tilde{\Sigma}, \Sigma_3, \mathcal{E}) = \sum C(\tfrac{1}{2}, \tilde{\Sigma}; \sigma, \Sigma_3 \mid \tilde{J}, J_3)\chi_\sigma(\mathbf{p}, \mathcal{E})\psi(\mathbf{p}, \tilde{\Sigma}, \Sigma_3). \quad (5.12)$$

As usual, we assume $\mathbf{p} = p\mathbf{e}_z$. Then,

$$\psi_{\mathcal{E}}(p, \tilde{J}, J_3, \tilde{\Sigma}) = e^{i\zeta K_3}\chi_\sigma(0, \mathcal{E}) \otimes \psi(\tilde{\Sigma}, \Sigma_3, \mathcal{E}) = \sum C(\tfrac{1}{2}, \tilde{\Sigma}; \sigma, \Sigma_3 \mid \tilde{J}, J_3)[e^{\frac{1}{2}i\zeta\tau_3}\chi_\sigma(0, \mathcal{E})] \times [e^{i\zeta\Lambda_3}\psi(\tilde{\Sigma}, \Sigma_3, \mathcal{E})], \quad (5.13)$$

where

$$\zeta = \operatorname{arc\,tanh}(E_{\tilde{J}}/p), \quad \text{and} \quad (E_{\tilde{J}})^2 = \mathbf{p}^2 - m_\nu^2, \quad (5.14)$$

$$m_\nu^2 = 2m_1^2\nu^2 - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] \pm 2m_1\nu\{m_1^2\nu^2 - [(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2]\}^{\frac{1}{2}}$$
$$m_1^{-2}[(m_0 - m_1)^2 - \tfrac{1}{4}m_1^2] \leq \nu^2 < \infty. \quad (5.15)$$

Furthermore, we have

$$e^{\frac{1}{2}i\zeta\tau_3}\chi_\sigma(0) = (\cosh \tfrac{1}{2}\zeta - \alpha_3 \sinh \tfrac{1}{2}\zeta)\chi_\sigma(0) = \{[(p + m_{\tilde{J}}) + \alpha_3 E_{\tilde{J}}]/[2m_{\tilde{J}}(p + m_{\tilde{J}})]^{\frac{1}{2}}\}\chi_\sigma(0) \quad (5.16)$$

and

$$e^{i\zeta\Lambda_3}\psi(\tilde{\Sigma}, \Sigma_3) = V_{\tilde{\Sigma},\tilde{\Sigma}'}(\zeta)\delta_{\Sigma_3\Sigma_3'}, \quad (5.17)$$

where the $V_{\tilde{\Sigma},\tilde{\Sigma}'}(\zeta)$ are those given by Bargmann. Explicitly, they can be written as in (5.8). [We have to just replace $\Sigma, \Sigma' \to \tilde{\Sigma}, \tilde{\Sigma}'$ in (5.8).] Thus, we obtain the expression for spinor wavefunctions as

$$\psi_{\mathcal{E}}(p, \tilde{J}, J_3, \tilde{\Sigma}) = \sum_{\Sigma', \Sigma_3'} C(\tfrac{1}{2}, \tilde{\Sigma}'; \sigma, \Sigma_3' \mid \tilde{J}, J_3) \times \left(\frac{(p + m_{\tilde{J}}) + \alpha_3 E_{\tilde{J}}}{[2m_{\tilde{J}}(p + m_{\tilde{J}})]^{\frac{1}{2}}}\right)\chi_\sigma(0) \times \left(\frac{(\tilde{\Sigma} - |\Sigma_3|)!(\tilde{\Sigma}' - |\Sigma_3|)!}{(\tilde{\Sigma} + |\Sigma_3|)!(\tilde{\Sigma}' - |\Sigma_3|)!}\right)^{\frac{1}{2}} \times \left(\frac{(2m_{\tilde{J}})^{-2|\Sigma_3|-1}(-E_{\tilde{J}})^{\tilde{\Sigma}'-\tilde{\Sigma}}}{(p + m_{\tilde{J}})^{\tilde{\Sigma}'-\tilde{\Sigma}+2|\Sigma_3|+1}}\right) P^{(\tilde{\Sigma}'-\tilde{\Sigma}, 2|\Sigma_3|)}_{\tilde{\Sigma}-|\Sigma_3|}\left(\frac{m_{\tilde{J}}}{p}\right). \quad (5.18)$$

As usual $\mathcal{E} = \pm$ denotes the two branches of the mass spectrum for each value of $\tilde{J} + \frac{1}{2}$ or ν.

To summarize our results in this section, we explicitly constructed spinor wavefunctions for the timelike and spacelike solutions of our wave equation. The spinors are orthonormalized as

$$(\psi_{\mathcal{E}}(p, J, J_3), \psi_{\mathcal{E}'}(p, J', J_3')) = (E_J/m_J)\delta_{J_3J_3'}\delta_{JJ'}\delta_{\mathcal{E}\mathcal{E}'}, \quad (5.19)$$

$$(\psi_{\mathcal{E}}(p, \tilde{J}, J_3), \psi_{\mathcal{E}'}(p, \tilde{J}', J_3')) = (E_{\tilde{J}}/m_{\tilde{J}})\delta_{J_3J_3'}\delta(\nu - \nu')\delta_{\mathcal{E}\mathcal{E}'}, \quad (5.20)$$

(note that these spinors have been normalized in the continuum), and

$$(\psi_{\mathcal{E}}(p, J, J_3), \psi_{\mathcal{E}'}(p, \tilde{J}, J_3)) = 0. \quad (5.21)$$

Further, we should note that each of the orthonormal conditions are separately satisfied by the $+ve$ and $-ve$ energy spinor wavefunctions. As usual, $\mathcal{E} = \pm$ denotes the upper and lower branches of the mass spectra.

Then, the completeness relation for any eigenvector ψ in the reducible representation space of

$$SL(2, C) \otimes D\left(X = \sum_\alpha \int_\oplus d\tilde{\alpha}\{\alpha, \tilde{\alpha}\}\right)$$

may be written as

$$\psi(p) = \sum_\alpha (\bar{\psi}_\alpha(p), \psi(p))\psi_\alpha(p) + \int_{-i\infty}^{+i\infty} d\tilde{\alpha}(\bar{\psi}_{\tilde{\alpha}}(p), \psi(p))\psi_{\tilde{\alpha}}(p), \quad (5.22)$$

where α represents the total spin and takes discrete values, and where $\tilde{\alpha}$ represents the continuous spin of the system.

6. QUANTIZATION OF THE INFINITE-COMPONENT GENERALIZED FIELDS

As shown in Sec. 2, the generalized field equation

$$(i\gamma_\mu\partial^\mu - M)\Psi(x) = 0, \quad M = m_0 + \tfrac{1}{2}m_1\sigma_{\mu\nu}\Gamma^{\mu\nu} \tag{6.1}$$

follows from the Lagrangian density

$$\mathfrak{L} = \bar{\Psi}(x)(-i\gamma_\mu\partial^\mu + M)\Psi(x),$$

with

$$\bar{\Psi}(x) = \Psi^+(x)\gamma_0. \tag{6.2}$$

The equation conjugate to (5.1) is given by

$$[i\partial_\mu\bar{\Psi}\gamma_\mu + \bar{\psi}M] = 0. \tag{6.3}$$

Thus, we define a conserved density

$$J_\mu(x) = \bar{\Psi}(x)\gamma_\mu\Psi(x). \tag{6.4}$$

The momentum conjugate to Ψ is given by

$$\pi_\sigma = \frac{\partial\mathfrak{L}}{\partial\dot{\psi}_\sigma} = i\psi^+_\sigma. \tag{6.5}$$

Then, the Hamiltonian density $\mathcal{H}$ is obtained from (6.1) and (6.3) as

$$\begin{aligned}\mathcal{H} &= \pi\dot{\Psi} - \mathfrak{L}\\ &= \Psi^+(x)(-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \gamma_0 M)\Psi(x)\\ &= \Psi^+(x)\left(i\frac{\partial}{\partial t}\right)\Psi(x).\end{aligned} \tag{6.6}$$

We can obtain the expressions for the energy–momentum 4-vector and the generalized angular-momentum tensor in the standard manner from the conservation principle, namely,

$$\mathbf{P} = :\int d^3x\bar{\Psi}\gamma_0(-i\omega)\boldsymbol{\nabla}:, \tag{6.7}$$

$$\begin{aligned}H &= :\int\mathcal{H}(x)\,d^3x:\\ &= :\int d^3x\Psi^+(-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + M)\Psi:,\end{aligned} \tag{6.8}$$

$$J_{\mu\nu} = :\int d^3x\Psi^+[\Gamma_{\mu\nu} + \tfrac{1}{2}\sigma_{\mu\nu} + i(x_\mu\partial_\nu - x_\nu\partial_\mu)]\Psi:. \tag{6.9}$$

For the space components of $J_{\mu\nu}$, in particular, we have

$$\begin{aligned}\mathbf{J} &= (J_{23}, J_{31}, J_{12})\\ &= :\int d^3x\Psi^+[-i\mathbf{r}\times\boldsymbol{\nabla} + \boldsymbol{\Sigma} + \tfrac{1}{2}\boldsymbol{\sigma}]\Psi:.\end{aligned} \tag{6.10}$$

The double dots on both sides of the above expressions denote, as usual, that the normal-ordered products are obtained by moving all destruction operators to the right. From (5.4), we obtain an additional conserved quantity, the charge Q,

$$Q = :\int d^3x\Psi^+(x)\Psi(x):. \tag{6.11}$$

To establish the second quantized theory for the generalized fields, we make use of the relations obtained in Sec. 5. We define the general solution of Eq. (6.1) as

$$\begin{aligned}&\Psi_\mathcal{E}(x)\\ &= \sum_{J,J_3}\int\frac{d^3p}{(2\pi)^{\frac{3}{2}}}\left(\frac{m_J}{E_J}\right)^{\frac{1}{2}}(\exp\{-i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 + m_J^2)^{\frac{1}{2}}t]\}\\ &\quad\times u(\mathbf{p}, J, J_3, \mathcal{E})b(\mathbf{p}, J, J_3, \mathcal{E})\\ &\quad + \exp\{i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 + m_J^2)^{\frac{1}{2}}t]\}\\ &\quad\times v(\mathbf{p}, J, J_3, \mathcal{E})d^+(\mathbf{p}, J, J_3, \mathcal{E}))\\ &\quad + \sum_{J_3}\int d\nu\int\frac{d^3p}{(2\pi)^{\frac{3}{2}}}\left(\frac{m_\nu}{E_\nu}\right)^{\frac{1}{2}}(\exp\{i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 - m_\nu^2)^{\frac{1}{2}}t]\}\\ &\quad\times u(\mathbf{p}, \nu, J_3, \mathcal{E})b(\mathbf{p}, \nu, J_3, \mathcal{E})\\ &\quad + \exp\{-i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 - m_\nu^2)^{\frac{1}{2}}t]\}\\ &\quad\times v(\mathbf{p}, \nu, J_3, \mathcal{E})d^+(\mathbf{p}, \nu, J_3, \mathcal{E})).\end{aligned} \tag{6.12}$$

Similarly, the adjoint field $\Psi^+(x)$ is given by

$$\begin{aligned}&\Psi^+_\mathcal{E}(x)\\ &= \sum_{J,J_3}\int\frac{d^3p}{(2\pi)^{\frac{3}{2}}}\left(\frac{m_J}{E_J}\right)^{\frac{1}{2}}(\exp\{i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 + m_J^2)^{\frac{1}{2}}t]\}\\ &\quad\times u^+(\mathbf{p}, J, J_3, \mathcal{E})b^+(\mathbf{p}, J, J_3, \mathcal{E})\\ &\quad + \exp\{-i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 + m_J^2)^{\frac{1}{2}}t]\}\\ &\quad\times v^+(\mathbf{p}, J, J_3, \mathcal{E})d(\mathbf{p}, J, J_3, \mathcal{E}))\\ &\quad + \sum_{J_3}\int d\nu\int\frac{d^3p}{(2\pi)^{\frac{3}{2}}}\left(\frac{m_\nu}{E_\nu}\right)^{\frac{1}{2}}(\exp\{i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 - m_\nu^2)^{\frac{1}{2}}t]\}\\ &\quad\times u^+(\mathbf{p}, \nu, J_3, \mathcal{E})b^+(\mathbf{p}, \nu, J_3, \mathcal{E})\\ &\quad + \exp\{-i[\mathbf{p}\cdot\mathbf{x} - (\mathbf{p}^2 - m_\nu^2)^{\frac{1}{2}}t]\}\\ &\quad\times v^+(\mathbf{p}, \nu, J_3, \mathcal{E})d(\mathbf{p}, \nu, J_3, \mathcal{E})),\end{aligned} \tag{6.13}$$

with

$$E_J = p_J^0 = (\mathbf{p}^2 + m_J^2)^{\frac{1}{2}}$$

and

$$(E_J)^2 = (\mathbf{p}^2 + m_J^2)$$

or

$$E_\nu^2 = (\mathbf{p}^2 - m_\nu^2).$$

We then postulate the canonical anticommutation relations between b_α, b_α^+, d_α, and d_α^+ as

$$\begin{aligned}&[b(\mathbf{p}, J, J_3, \mathcal{E}), b^+(\mathbf{p}', J', J_3', \mathcal{E}')]_+\\ &\qquad = \delta^3(\mathbf{p} - \mathbf{p}')\delta_{\mathcal{E}\mathcal{E}'}\delta_{JJ'}\delta_{J_3J_3'},\\ &[d(\mathbf{p}, J, J_3, \mathcal{E}), d^+(\mathbf{p}', J', J_3', \mathcal{E}')]_+\\ &\qquad = \delta^3(\mathbf{p} - \mathbf{p}')\delta_{\mathcal{E}\mathcal{E}'}\delta_{JJ'}\delta_{J_3J_3'},\\ &[b(\mathbf{p}, \nu, J_3, \mathcal{E}), b^+(\mathbf{p}', \nu', J_3', \mathcal{E}')]_+\\ &\qquad = \delta^3(\mathbf{p} - \mathbf{p}')\delta_{\mathcal{E}\mathcal{E}'}\delta(\nu - \nu')\delta_{J_3J_3'},\\ &[d(\mathbf{p}, \nu, J_3, \mathcal{E}), d^+(\mathbf{p}', \nu', J_3', \mathcal{E}')]_+\\ &\qquad = \delta^3(\mathbf{p} - \mathbf{p}')\delta_{\mathcal{E}\mathcal{E}'}\delta(\nu - \nu')\delta_{J_3J_3'},\end{aligned} \tag{6.14}$$

and all other commutators vanish. From the relations (6.14) and the completeness relation (5.22), we obtain the *local* commutation relations for the generalized fields as

$$[\Psi_\alpha(t, \mathbf{x}), \Psi^+_\beta(t, \mathbf{x}')]_+ = \delta^3(\mathbf{x} - \mathbf{x}')\delta_{\alpha\beta}. \quad (6.15)$$

As observed by some authors, since the "spectral conditions" are no more true for generalized infinite component fields, we have constructed a local field $\Psi(x)$, which annihilates the vacuum.[2] We have to note further that, contrary to earlier observations, our fields constructed in the above fashion are local. This arises from the fact that our mass spectra is no longer bounded from below: We just have an accumulation point at the minima.

Another interesting feature is the expression for the charge Q. We can, after a little manipulation, derive the charge operator as

$$\begin{aligned} Q &= \int d^3x :\Psi^+\Psi: \\ &= \sum_{J,J_3} \int d^3p :[b^+(p, J, J_3, \mathcal{E})b(p, J, J_3, \mathcal{E}) \\ &\quad + d^+(p, J, J_3, \mathcal{E})d(p, J, J_3, \mathcal{E})]: \\ &\quad + \sum_{J_3} \int d\nu \int d^3p :[b^+(p, \nu, J_3, \mathcal{E})b(p, \nu, J_3, \mathcal{E}) \\ &\quad + d^+(p, \nu, J_3, \mathcal{E})d(p, \nu, J_3, \mathcal{E})]:. \end{aligned} \quad (6.16)$$

Better still, we can express Q in terms of particle number operators. Define

$$\begin{aligned} N_+(p, \alpha, J_3, \mathcal{E}) &= b^+(p, \alpha, J_3, \mathcal{E})b(p, \alpha, J_3, \mathcal{E}), \\ N_-(p, \alpha, J_3, \mathcal{E}) &= d^+(p, \alpha, J_3, \mathcal{E})d(p, \alpha, J_3, \mathcal{E}), \end{aligned} \quad (6.17)$$

where α denotes either J or ν. Then

$$\begin{aligned} Q &= \sum_{J,J} \int d^3p[N_+(p, J, J_3, \mathcal{E}) - N_-(p, J, J_3, \mathcal{E})] \\ &\quad + \sum_{J_3} \int d\nu \int d^3p[N_+(p, \nu, J_3, \mathcal{E}) - N_-(p, \nu, J_3, \mathcal{E})]. \end{aligned} \quad (6.18)$$

N_+ and N_- are interpreted as number operators for $+ve$ energy particles and antiparticles, respectively. Note further that, in the case $m_1 = 0$, the fields only contain the timelike parts and, correspondingly, the charge Q has the first terms in the rhs of Eq. (6.18).

We would like to bring out some salient features of our fields. In the general solution of (6.1), the fields $\Psi(x)$ contain both the $+ve$ and $-ve$ frequency solutions which in turn are associated with annihilation and creation operators for particles and antiparticles, respectively. We have explicitly displayed the $+ve$ frequency solutions in Sec. 5. To obtain the $-ve$ frequency solutions, we just have to replace $\Psi(x)$ by $\gamma_5\Psi(x)$. Thus, the fields $\psi(x)$ explicitly contain both $\Psi(x)$ and $\gamma_5\Psi(x)$ parts. This is very similar to the familiar *pure* Dirac fields. In either case, we note, the S principle is automatically satisfied.[10] Contrary to the pure Dirac fields or the generalized Dirac fields of our present discussion, the Majorana fields $\Psi(x)$ contain *only* the annihilation operators. Hence, it necessitates the introduction of the conjugate fields with the creation operators. However, the quantized fields so constructed do not possess any symmetry between the $+ve$ and $-ve$ frequency solutions. To redress this difficulty, one demands rather that (i) $\Psi(x)$ and $\Psi^{-T}(x)$ to be treated on the same footing, and (ii) the action is invariant under the interchange of $\Psi(x)$ and $V\Psi^{+T}(x)$, where $V = e^{(i\pi J_2)}$. By constructing the fields in the above manner, one then restores the usual spin–statistics relation. (For a detailed discussion, see Refs. 1 and 10.)

We make no secret of the fact that we have been able to formulate the second quantized theory of the infinite-component Fermi fields in accordance with the substitution principle and satisfying the usual spin–statistics relations. The pathologies diagnosed by earlier work[8] have been redressed in our present discussion. Further, we note that an identical procedure can be carried out for the quantization of the infinite-component Bose fields.

7. CONCLUSIONS

To conclude our discussions, we constructed quantum theory of the infinite-component generalized fields satisfying local commutativity. Since the fields explicitly contain particle and antiparticle solutions, the conventional *TCP* invariance is also preserved! Like other infinite-component field theories, our field equation possesses timelike and spacelike solutions. The former gives rise to discrete-spin spectra and the latter to continuous-spin spectra for the masses. The continuous-spin spectrum, which is rather a peculiar characteristic of infinite-component field theories satisfying linear covariant field equations, gives rise to an entirely new kind of radiation involving spacelike particles.[1,10] The special features of this phenomenon have been discussed by Sudarshan, and the possible implications have been also discussed from the point of view of finite-component field theories.[10]

Another feature of the mass spectrum is that, for each value of the "spin," there are two values for the masses. One is an ascending branch and the other asymptotically goes to zero. In fact, the former one is rather attractive for hadron spectra. To be more

optimistic, the two branches of the discrete spectra can be interpreted as the mass spectrum of the "electron" and the "muon" by cleverly adjusting the parameters m_0 and m_1.

Finally, we believe that such a formulation of the field equation has some added advantage over the *pure* Majorana wave equation. Some more interesting cases of field equations and a systematic study of their solutions and quantization schemes will be reported elsewhere.

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APPENDIX A

1. Timelike Case

We wish to derive the expression for the mass matrix (4.4), i.e.,

$$\mathcal{M} = \begin{pmatrix} m_0 - m_1(J+\frac{3}{2}) & -im_1[J(J+1)]^{\frac{1}{2}} \\ im_1[J(J+1)]^{\frac{1}{2}} & -m_0 - m_1(J-\frac{1}{2}) \end{pmatrix}.$$

Let us consider the mass operator (4.3):

$$\mathcal{M} = m_0\gamma_0 + m_1\gamma_0(\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda}).$$

We have seen that the basis vectors can be labeled by the eigenvalues of γ_0, σ_3, $\boldsymbol{\Sigma}^2$, and Σ_3 or, alternatively, by $|\beta, J, \lambda, \Sigma\rangle$, where β, J, and λ are the eigenvalues of γ_0, the total spin $\mathbf{J}^2 = (\boldsymbol{\Sigma} + \frac{1}{2}\boldsymbol{\sigma})^2$, and $J_3 = (\frac{1}{2}\sigma_3 + \Sigma_3)$, respectively. We note further that, since γ_0 does not commute with $\mathcal{M}$, these do not furnish the eigenstates of mass. To write down the mass matrix, we find that, since for a unitary representation $\boldsymbol{\Lambda}$ behaves like a vector under $\boldsymbol{\Sigma}$, the $\boldsymbol{\tau}\cdot\boldsymbol{\Lambda}$ term in the mass matrix will contribute to the off-diagonal matrix elements, whereas $\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma}$ will contribute for the diagonal ones. We have, $\mathbf{J} = \boldsymbol{\Sigma} + \frac{1}{2}\boldsymbol{\sigma}$. Squaring both sides, we get

$$\mathbf{J}^2 = J(J+1) = \boldsymbol{\Sigma}^2 + \tfrac{3}{4} + \boldsymbol{\sigma}\cdot\boldsymbol{\Sigma}$$

or

$$\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} = J(J+1) - \Sigma(\Sigma+1) - \tfrac{3}{4}. \tag{A1}$$

For $\Sigma = J + \frac{1}{2}$, we have

$$\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} = -(J+\tfrac{3}{2}),$$

while, for $\Sigma = J - \frac{1}{2}$,

$$\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} = J - \tfrac{1}{2}.$$

Now,

$$\begin{aligned}(\boldsymbol{\tau}\cdot\boldsymbol{\Lambda})(\boldsymbol{\tau}\cdot\boldsymbol{\Lambda}) &= -(\boldsymbol{\alpha}\cdot\boldsymbol{\Lambda})(\boldsymbol{\alpha}\cdot\boldsymbol{\Lambda}) \\ &= -\boldsymbol{\Lambda}^2 - \boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} \\ &= -\boldsymbol{\Lambda}^2(\mathbf{J}^2 - \boldsymbol{\Sigma}^2 - \tfrac{3}{4}) \\ &= (\boldsymbol{\Sigma}^2 - \boldsymbol{\Lambda}^2) - \mathbf{J}^2 + \tfrac{3}{4} = -\mathbf{J}^2 \\ &= -J(J+1). \end{aligned} \tag{A2}$$

Thus,

$$\mathcal{M} = \begin{pmatrix} m_0 - m_1(J-\frac{3}{2}) & -im_1[J(J+1)]^{\frac{1}{2}} \\ im_1[J(J+1)]^{\frac{1}{2}} & -m_0 - m_1(J-\frac{1}{2}) \end{pmatrix}.$$

2. Spacelike Case

In this case, the basic vectors are labeled by $\gamma_3, \tilde{J}, \lambda$, and $\tilde{\Sigma}$, where $\gamma_3, \tilde{J}, \lambda$, and $\tilde{\Sigma}$ are the eigenvalues of γ_3, $\tilde{\mathbf{J}} = (\tilde{\boldsymbol{\Sigma}} + \frac{1}{2}\boldsymbol{\sigma})^2$, $J_3 = (\Sigma_3 + \frac{1}{2}\sigma_3)$ and $\mathcal{C} = (\Sigma_3^2 - \Lambda_1^2 - \Lambda_2^2) = \tilde{\boldsymbol{\Sigma}}^2$, respectively.

Defining

$$\begin{aligned} J_3 &= \Sigma_3 + \tfrac{1}{2}\sigma_3, \\ K_1 &= \Lambda_1 + \tfrac{1}{2}\tau_1, \\ K_2 &= \Lambda_2 + \tfrac{1}{2}\tau_2, \end{aligned}$$

we find the following expression for the second-order Casimir operator:

$$\begin{aligned} Q &= J_3^2 - K_1^2 - K_2^2 \\ &= (\Sigma_3 + \tfrac{1}{2}\sigma_3)^2 - (\Lambda_1 + \tfrac{1}{2}\tau_1)^2 - (\Lambda_2 + \tfrac{1}{2}\tau_2)^2 \\ &= (\Sigma_3^2 - \Lambda_1^2 - \Lambda_2^2) + \tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}} + \tfrac{3}{4} \\ &= \mathcal{C} + \tfrac{3}{4} + \tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}}, \end{aligned} \tag{A3}$$

where

$$\begin{aligned} \tilde{\boldsymbol{\sigma}} &= (\sigma_3, \tau_1, \tau_2), & \tilde{\boldsymbol{\tau}} &= (\tau_3, \sigma_1, \sigma_2), \\ \tilde{\boldsymbol{\Sigma}} &= (\Sigma_3, \Lambda_1, \Lambda_2), & \tilde{\boldsymbol{\Lambda}} &= (\Lambda_3, \Sigma_1, \Sigma_2). \end{aligned}$$

Note that, under $\tilde{\boldsymbol{\Sigma}}$ and $\tilde{\boldsymbol{\sigma}}$, $\tilde{\boldsymbol{\Lambda}}$ and $\tilde{\boldsymbol{\tau}}$ respectively transform like vectors. Furthermore, we have

$$\begin{aligned}(\tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}} - \tilde{\boldsymbol{\tau}}\cdot\tilde{\boldsymbol{\Lambda}}) &= (\sigma_3\Sigma_3 - \tau_1\Lambda_1 - \tau_2\Lambda_2) \\ &\quad - (\tau_3\Lambda_3 - \sigma_1\Sigma_1 - \sigma_2\Sigma_2) \\ &= (\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} - \boldsymbol{\tau}\cdot\boldsymbol{\Lambda}),\end{aligned}$$

as it should.

From (A3), we have

$$(Q - \mathcal{C} - \tfrac{3}{4}) = \tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}}. \tag{A4}$$

Squaring both sides of (A4) and simplifying, we obtain

$$(Q - \mathcal{C} - \tfrac{3}{4})^2 = 2\mathcal{C} - Q + \tfrac{3}{4}$$

or, solving for Q,

$$Q = (\mathcal{C} + \tfrac{1}{4}) \pm (\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}}. \tag{A5}$$

Furthermore, from (A3), we have

$$\tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\Sigma}} = Q - \mathcal{C} - \tfrac{3}{4}.$$

Substituting for Q, we obtain

$$\tilde{\sigma}\cdot\tilde{\Sigma} = -\tfrac{1}{2} \pm (\mathcal{C}+\tfrac{1}{4})^{\frac{1}{2}}$$

or

$$(\tfrac{1}{2} + \tilde{\sigma}\cdot\tilde{\Sigma}) = \pm(\mathcal{C}+\tfrac{1}{4})^{\frac{1}{2}}. \quad \text{(A6)}$$

Again,

$$(\tilde{\tau}\cdot\tilde{\Lambda})(\tilde{\tau}\cdot\tilde{\Lambda}) = (\Sigma_1^2+\Sigma_2^2-\Lambda_3^2) - \tilde{\sigma}\cdot\tilde{\Sigma}$$
$$= (-\tfrac{3}{4}-\mathcal{C}) - (Q-\mathcal{C}-\tfrac{3}{4}), \quad \text{(A7)}$$

since

$$C_0 = -\tfrac{3}{4} = \mathbf{\Sigma}^2 - \mathbf{\Lambda}^2$$
$$= (\Sigma_3^2-\Lambda_1^2-\Lambda_2^2) - (\Lambda_3^2-\Sigma_1^2-\Sigma_2^2).$$

Equation (A7) may be written as

$$(\tilde{\tau}\cdot\tilde{\Lambda})(\tilde{\tau}\cdot\tilde{\Lambda}) = -Q,$$

since

$$(-\tfrac{1}{2}+\tilde{\tau}\cdot\tilde{\Lambda})(-\tfrac{1}{2}-\tilde{\tau}\cdot\tilde{\Lambda}) = \tfrac{1}{4} - (\tilde{\tau}\cdot\tilde{\Lambda})(\tilde{\tau}\cdot\tilde{\Lambda})$$
$$= \tfrac{1}{4} + Q$$
$$= [(\mathcal{C}+\tfrac{1}{4})^{\frac{1}{2}} \pm \tfrac{1}{2}]^2. \quad \text{(A8)}$$

Note further that $\frac{1}{2} + \tilde{\sigma}\cdot\tilde{\Sigma}$ contributes to the diagonal elements of the mass matrix, whereas $-\frac{1}{2} + \tilde{\tau}\cdot\tilde{\Lambda}$ contributes to the off-diagonal ones. Thus the matrix $\tilde{m}$ can be written as

$$\tilde{m} = \begin{pmatrix} i(m_0-m_1) + im_1(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} & im_1[(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} - \frac{1}{2}] \\ -im_1[(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} + \frac{1}{2}] & -i(m_0-m_1) + im_1(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} \end{pmatrix}.$$

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Convolution Approximation for the n-Particle Distribution Function

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The convolution approximation introduced by Jackson and Feenberg for the 3-particle distribution function is extended to the n-particle distribution function g_n. It is shown that the generalized convolution form satisfies the limiting and the recursion relations connecting g_n and g_{n+1}.

I. INTRODUCTION

An important problem in the quantum mechanical and statistical consideration of many-particle systems is the approximation of the n-particle correlation function g_n by lower-order ones, usually the pair distribution function g_2. Many years ago, Kirkwood[1] introduced in the theory of classical fluid the superposition approximation for the 3-particle distribution function. The idea of superposition has been widely accepted and its extension to the n-particle distribution function has also been used.[2] An alternate approximation for the 3-particle distribution function,

Substituting for Q, we obtain

$$\tilde{\sigma}\cdot\tilde{\Sigma} = -\tfrac{1}{2} \pm (\mathcal{C}+\tfrac{1}{4})^{\frac{1}{2}}$$

or

$$(\tfrac{1}{2} + \tilde{\sigma}\cdot\tilde{\Sigma}) = \pm(\mathcal{C}+\tfrac{1}{4})^{\frac{1}{2}}. \quad \text{(A6)}$$

Again,

$$(\tilde{\tau}\cdot\tilde{\Lambda})(\tilde{\tau}\cdot\tilde{\Lambda}) = (\Sigma_1^2+\Sigma_2^2-\Lambda_3^2) - \tilde{\sigma}\cdot\tilde{\Sigma}$$
$$= (-\tfrac{3}{4}-\mathcal{C}) - (Q-\mathcal{C}-\tfrac{3}{4}), \quad \text{(A7)}$$

since

$$C_0 = -\tfrac{3}{4} = \mathbf{\Sigma}^2 - \mathbf{\Lambda}^2$$
$$= (\Sigma_3^2-\Lambda_1^2-\Lambda_2^2) - (\Lambda_3^2-\Sigma_1^2-\Sigma_2^2).$$

Equation (A7) may be written as

$$(\tilde{\tau}\cdot\tilde{\Lambda})(\tilde{\tau}\cdot\tilde{\Lambda}) = -Q,$$

since

$$(-\tfrac{1}{2}+\tilde{\tau}\cdot\tilde{\Lambda})(-\tfrac{1}{2}-\tilde{\tau}\cdot\tilde{\Lambda}) = \tfrac{1}{4} - (\tilde{\tau}\cdot\tilde{\Lambda})(\tilde{\tau}\cdot\tilde{\Lambda})$$
$$= \tfrac{1}{4} + Q$$
$$= [(\mathcal{C}+\tfrac{1}{4})^{\frac{1}{2}} \pm \tfrac{1}{2}]^2. \quad \text{(A8)}$$

Note further that $\frac{1}{2} + \tilde{\sigma}\cdot\tilde{\Sigma}$ contributes to the diagonal elements of the mass matrix, whereas $-\frac{1}{2} + \tilde{\tau}\cdot\tilde{\Lambda}$ contributes to the off-diagonal ones. Thus the matrix $\tilde{m}$ can be written as

$$\tilde{m} = \begin{pmatrix} i(m_0-m_1) + im_1(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} & im_1[(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} - \frac{1}{2}] \\ -im_1[(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} + \frac{1}{2}] & -i(m_0-m_1) + im_1(\mathcal{C}+\frac{1}{4})^{\frac{1}{2}} \end{pmatrix}.$$

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I. INTRODUCTION

An important problem in the quantum mechanical and statistical consideration of many-particle systems is the approximation of the n-particle correlation function g_n by lower-order ones, usually the pair distribution function g_2. Many years ago, Kirkwood[1] introduced in the theory of classical fluid the superposition approximation for the 3-particle distribution function. The idea of superposition has been widely accepted and its extension to the n-particle distribution function has also been used.[2] An alternate approximation for the 3-particle distribution function,

the convolution form, was proposed by Jackson and Feenberg[3] in the correlated basis function (CBF) approach to the theory of quantum fluids. The convolution form has proven to be more convenient to use in the evaluation of matrix elements occurring in the CBF formalism. In the evaluation of the excitation spectrum of He II, for example, the convolution form largely reduces the amount of numerical works while yielding results comparable to those obtained using the superposition approximation.[3] Similar simplifications have also been observed in its application to the theory of fermion liquids.[4,5] In the further perturbative treatments in the CBF formalism, convolution forms of higher-distribution functions are also needed. Thus Lee[6] has obtained and used the convolution form of g_4 to compute the second-order correction to the excitation spectrum of He II. More recently, calculations have been carried out for liquid ^{3}He and ^{3}He–^{4}He mixtures with partial contributions from g_5 and g_6 included.[7] It would then be of practical as well as theoretical interests to extend the previous results on the convolution approximation. Lee[6] used intuitive reasonings to generate the convolution form of g_4. However, we find it very difficult to go further beyond in the absence of precise statement of generalization. It is the purpose of the present paper to make the rule precise and generalize the convolution approximation to the n-particle distribution function.

II. PRELIMINARIES

Consider a system of N identical particles confined in a volume Ω. The thermodynamic limit $N \to \infty$, $\Omega \to \infty$ will be taken, if necessary, with the density $N/\Omega = \rho$ kept constant. We define as usual[8] the n-particle distribution function

$$g_n(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n) = \frac{N!}{(N-n)!}\rho^{-n}\frac{\int W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)\, d\mathbf{r}_{n+1}\cdots d\mathbf{r}_N}{\int W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)\, d\mathbf{r}_1 \cdots d\mathbf{r}_N}, \tag{1}$$

with $W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n)$ a function symmetric in the coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n$. Explicitly, we have

$$W = \exp\left[-V(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)/kT\right], \quad \text{for a classical system,}$$
$$= |\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2, \quad \text{for a quantal system.}$$

Here V is the total potential energy and ψ the wavefunction describing the system. Physically,

$$\Omega^{-n} g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n)$$

is the probability density function for n ($\ll N$) particles to situate at $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n$.

Some implications now follow as consequences of the definition. It is clear that $g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ is nonnegative, symmetric in its n coordinates, and vanishes for strongly interacting systems when two particle coordinates coincide. The definition (1) also implies the recursion relation

$$\rho\int g_{n+1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1})\, d\mathbf{r}_{n+1} = (N-n)g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) \tag{2}$$

and hence the normalization condition

$$\rho^n\int g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n)\, d\mathbf{r}_1 \cdots d\mathbf{r}_n = \frac{N!}{(N-n)!}. \tag{3}$$

Furthermore, taking a particle to infinity is equivalent to removing one particle from the system. As a consequence, we expect the limiting condition

$$\lim_{r_{n+1}\to\infty} g_{n+1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1}) = g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) \tag{4}$$

to hold. Any approximate form for the n-particle distribution function should be tested against these necessary conditions.

For a uniform system, we expect g_1 to be a constant. Normalization then requires

$$g_1(\mathbf{r}) = 1. \tag{5}$$

We also expect the pair distribution function g_2 to depend on the distance $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ only. We define the f function as

$$f_{12} = f(r_{12}) = g_2(r_{12}) - 1. \tag{6}$$

The normalization condition (3) then implies the following conditions on f:

$$\rho\int f(r)\, d\mathbf{r} = -1, \tag{7}$$

$$f(\infty) = 0. \tag{8}$$

In the following discussions, f is assumed to satisfy both (7) and (8).

The Kirkwood superposition approximation[1] $g_3^{(s)}$ for the 3-particle distribution function is

$$g_3^{(s)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = g_2(r_{12})g_2(r_{23})g_2(r_{31}). \tag{9}$$

This approximate form satisfies most of the necessary conditions on g_3 except the recursion and the normalization relations (2) and (3). In fact, explicit evaluations using (7) yield the results

$$\rho\int g_3^{(s)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\, d\mathbf{r}_3 = g_2(r_{12})\left(N - 2 + \rho\int f_{13}f_{23}\, d\mathbf{r}_3\right) \tag{10}$$

and

$$\rho^3\int g_3^{(s)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3$$
$$= N(N-1)(N-2) - N + \rho^3\int f_{12}f_{23}f_{31}\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3. \tag{11}$$

The remainder term in (10) is deceptively small and, as it turns out, proves to be of primary importance in applications.[3] The generalized superposition form for the n-particle distribution function,

$$g_n^{(s)}(\mathbf{r}_1,\cdots,\mathbf{r}_n) = \prod_{1\le i<j\le n} g_2(r_{ij}), \tag{12}$$

also fails to meet the requirements (2) and (3).

An alternate approximation of g_3 which exactly satisfies the recursion and the normalization relations is the convolution form[3]

$$g_3^{(c)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = 1 + f_{12} + f_{23} + f_{31} + f_{12}f_{23} + f_{23}f_{31} + f_{31}f_{12} + \rho\int f_{14}f_{24}f_{34}\,d\mathbf{r}_4. \tag{13}$$

It is easy to see that $g_3^{(c)}$ is symmetric in the particle coordinates and satisfies the recursion and the limiting conditions (2) and (4). However, it fails in the other tests. Namely, $g_3^{(c)}$ is not necessarily nonnegative and the approximation is poor for strongly interacting systems when the particle coordinates are close. But these are not critical objections in view of its convenience in applications. In fact, it is not known in actual calculations which approximation using $g_3^{(s)}$ or $g_3^{(c)}$ is more accurate.[3] With nothing better available, the convolution form remains a useful approximation in evaluating integrals involving nonsingular operators. Lee[6] has extended the convolution form to g_4 and obtained the explicit expression of $g_4^{(c)}$ which yields $g_3^{(c)}$ upon integrating over one particle coordinate. In the next section we shall generalize further to the n-particle distribution function. The resulting form is a generalization of the known expressions of $g_3^{(c)}$ and $g_4^{(c)}$ and satisfies both the recursion and the limiting relations (2) and (4).

III. CONVOLUTION APPROXIMATION FOR g_n

It is convenient to introduce a diagrammatic representation which will facilitate our discussions. We first give some definitions in the language of linear graphs.[9]

A linear graph is a collection of points with lines joining certain pairs of points. Examples of linear graphs are given in Fig. 1. A graph is said to be disconnected if it is possible to separate the points of the graph into two or more groups such that there is no line joining a point of one group with a point of the other. Otherwise the graph is said to be connected. Thus, Fig. 1(a) is disconnected and Figs. 1(b), 1(c) are connected. A line successively joining a set of points is called a path. If the final and the initial points of a path coincide, we speak of a cycle. For instance, points 2, 3, and 4 in Fig. 1(c) form a cycle. A Cayley tree is a connected linear graph containing no cycles. Figure 1(b) is an example of a Cayley tree. An isolated (unconnected) point is also a Cayley tree. The number of lines incident at each point is called the degree of the point. Therefore, the degree of the black point in Fig. 1(b) is three, and the degrees of all other points in the same graph are all one. If a point of the graph is given a numerical label, $1, 2, \cdots$, we call this point a root point and speak of a rooted graph. In the following, all root points will be denoted by open circles or open points, and all unlabeled points by black circles or black points, as shown in Fig. 1.

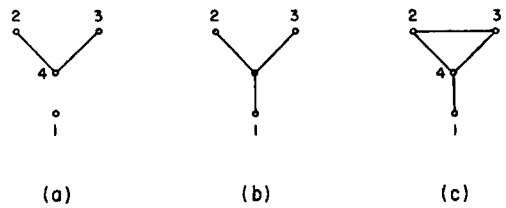

FIG. 1. Examples of linear graphs.

A diagrammatic representation for mathematical expressions is now in order. A factor f_{ij} is represented by a line joining two points with labels i and j. The point i is a black one if the coordinate $\mathbf{r}_i$ appears as the integration variable under an integral sign; otherwise it is an open point. In other words, a black point represents a factor $\rho\int d\mathbf{r}_k$ with the label k deleted from the graph. All isolated open points are taken to represent a numerical factor of 1. Thus, the graphs of Fig. 1 represent the following expressions:

$$f_{24}f_{34}, \qquad \text{for Fig. 1(a)},$$
$$\rho\int f_{14}f_{24}f_{34}\,d\mathbf{r}_4, \qquad \text{for Fig. 1(b)},$$
$$f_{14}f_{42}f_{23}f_{34}, \qquad \text{for Fig. 1(c)}.$$

As another example, the convolution approximation $g_3^{(c)}$ for the 3-particle distribution function given by (13) has the diagrammatic representation of Fig. 2.

In these notations, we now define the convolution approximation $g_n^{(c)}$ for the n-particle distribution

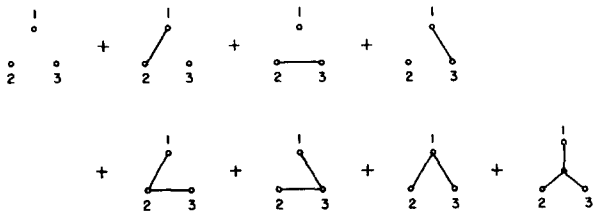

FIG. 2. Diagrammatic representation of the convolution approximation $g_3^{(c)}$ given by Eq. (13).

function as

$$g_n^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n) = \text{the collection of all distinct graphs of rooted Cayley trees (connected and disconnected) with each graph consisting of } n \text{ root points, labeled } 1, \cdots, n, \text{ and any number of unlabeled points provided that the degree of each unlabeled point is at least three.} \quad (14)$$

Clearly, $g_n^{(c)}$ is symmetric in the coordinates $\mathbf{r}_1$, $\mathbf{r}_2, \cdots, \mathbf{r}_n$. We now show that $g_n^{(c)}$ satisfies the limiting relation

$$\lim_{r_{n+1}\to\infty} g_{n+1}^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1}) = g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n) \quad (15)$$

and the recursion relation

$$\rho \int g_{n+1}^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1})\, d\mathbf{r}_{n+1} = (N - n) g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (16)$$

It is convenient to classify the graphs of $g_{n+1}^{(c)}$ according to the connectivity of the root point with the label $n + 1$ [the $(n + 1)$th root point]. We write

$$g_{n+1}^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_{n+1}) = G_1 + G_2 + G_3 + G_4, \quad (17)$$

where

G_1 = the collection of graphs of $g_{n+1}^{(c)}$ in which the $(n + 1)$th root point is isolated,

G_2 = the collection of graphs of $g_{n+1}^{(c)}$ in which the $(n + 1)$th root point is connected to precisely one open point,

G_3 = the collection of graphs of $g_{n+1}^{(c)}$ in which the $(n + 1)$th root point is connected to precisely one black point,

G_4 = the remaining graphs of $g_{n+1}^{(c)}$ in which the degree of the $(n + 1)$th root point is at least two.

First we note that G_1 contains precisely the graphs of $g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ with the addition of isolated $(n + 1)$th root points. Since all isolated root points represent the same numerical factor 1, we then recognize the identity

$$G_1 = g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (18)$$

Now, G_2, G_3, and G_4 contain all graphs in which the $(n + 1)$th root point is connected. It follows then from (8) that all graphs of G_2, G_3, and G_4 vanish on taking the limit $r_{n+1} \to \infty$. Only G_1 survives on the left-hand side of (15) and this completes the proof of the limiting relation.

To prove the recursion relation (16), we note that the integration over an isolated point simply yields a numerical factor $\rho \int d\mathbf{r} = N$. Hence from (18) we have

$$\rho \int G_1\, d\mathbf{r}_{n+1} = N g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (19)$$

Next, since G_2 contains all rooted Cayley trees in which the $(n + 1)$th root point is connected to precisely one root point, one may generate *all* graphs of G_2 by joining in graphs of G_1 the $(n + 1)$th root point to one of the n other root points. In fact, by joining to the n other root points in succession, n different graphs of G_2 are generated from a given graph of G_1. However, because of (7), these n graphs are all equivalent upon integrating over $d\mathbf{r}_{n+1}$. It follows then, using (7),

$$\rho \int G_2\, d\mathbf{r}_{n+1} = -nG_1 = -ng_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (20)$$

We remark that we have, in the above, used the fact that G_1, or $g_n^{(c)}$, contains the collection of *all* rooted Cayley trees with n root points so that all graphs of G_2 are generated from G_1. Finally, we note that there exists a one-to-one correspondence between the graphs of G_3 and G_4. For each graph G of G_3, we may generate a graph G' of G_4 by first removing the $(n + 1)$th root point in G and then converting the black point originally connected to this $(n + 1)$th point into a root point with the label $n + 1$. Since the degree of the original black point is at least three, the degree of the new root point will be at least two and the resulting graph will certainly be contained in G_4. Conversely, for each graph of G_4, a unique graph of G_3 can be generated by the reversing process. An example of this correspondence is shown in Fig. 3. Now the integration over $\rho \int d\mathbf{r}_{n+1}$ simply changes the $(n + 1)$th root point into a black point in G' and

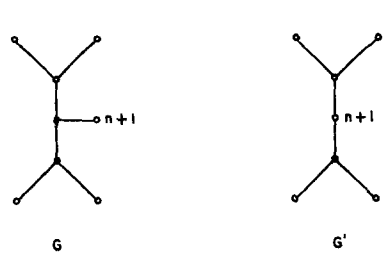

FIG. 3. An example of the one-to-one correspondence between graphs $G \in G_3$ and $G' \in G_4$. All labels of the root points have been deleted in G and G' except the label $n + 1$.

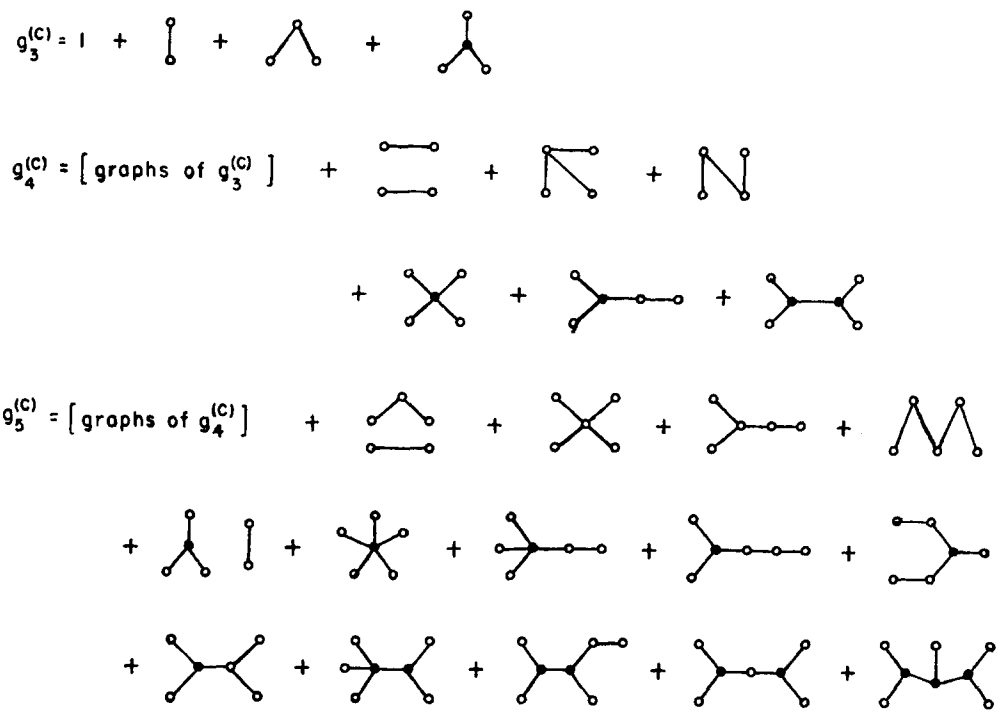

FIG. 4. A compact diagrammatic representation of $g_3^{(c)}$, $g_4^{(c)}$, and $g_5^{(c)}$. Only the topologically distinct graphs are included with all the labels and isolated points deleted.

removes the $(n+1)$th root point in G, the following relation between G and G' then follows from (7):

$$\rho\int G\, d\mathbf{r}_{n+1} = -\rho\int G'\, d\mathbf{r}_{n+1}$$

or

$$\rho\int (G + G')\, d\mathbf{r}_{n+1} = 0.$$

The one-to-one correspondence of the graphs of G_3 and G_4 then ensures

$$\rho\int (G_3 + G_4)\, d\mathbf{r}_{n+1} = 0. \tag{21}$$

The recursion relation (16) now follows as a result on combining (19)–(21).

IV. CONCLUSION

We have shown that the convolution approximation of the n-particle distribution function given by (14) satisfies the limiting relation (15) and the recursion relation (16). The explicit expressions of $g_3^{(c)}$, $g_4^{(c)}$, and $g_5^{(c)}$ are collected in Fig. 4 in a more compact graphical notation in which only the topologically distinct graphs are shown with all labels and isolated points deleted.[10] For example, all the $\binom{n}{2}$ terms of the form f_{ij} are represented by a single graph. Thus the 4 graphs of $g_3^{(c)}$ represent a total of 8 terms, the 10 graphs of $g_4^{(c)}$ represent 58 terms and the 24 graphs of $g_5^{(c)}$ represent a total of 617 terms. In this simplified notation, the expression (14) for $g_n^{(c)}$ can be rewritten as

$g_n^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n) =$ the collection of all distinct graphs of connected and disconnected Cayley trees excluding isolated points and consisting of n or less open points and any number of black points, provided that the degree of each black point is at least three.

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[10] This is also the notation used in Ref. 6.

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Infinite-Dimensional Representations of the Lorentz Group

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The method used by Naimark to obtain symmetrical spinors and their transformation law from finite-dimensional representations of the group $SL(2, C)$ is extended to infinite-dimensional representations. As an infinite-dimensional representation, we use the principal series of representations realized by means of the special unitary group SU_2. As a result another form of the principal series of representations of $SL(2, C)$ is obtained which describes the transformation law of an infinite set of numbers under the group transformation in a way which is very similar, but as a generalization, to the way spinors appear in the finite-dimensional case.

Two component spinors[1] are associated with finite-dimensional representations of the group $SL(2, C)$ when realized in the space of polynomials. $SL(2, C)$ is the group of all 2×2 complex matrices with determinant unity, and it is the covering group of the restricted Lorentz group describing homogeneous Lorentz transformations which are orthochroneous and proper.[2] Spinors appear (up to factorial terms) as the coefficients of the polynomials of the space in which the representation is realized. Their transformation law then provides another form for the representation.[3]

However, the group $SL(2, C)$ has also infinite-dimensional representations the most notable of which is the principal series of representations.[3,4] In this paper, we define an infinite set of numbers which can be associated with the principal series of representations in a way which is very similar, but as a generalization, to the way spinors appear in describing the finite-dimensional representations. The transformation law of these numbers, at the same time, defines another form of the principal series of representations of $SL(2, C)$. Just as in the spinor case, these numbers become functions of space–time when applied in physics.

The principal series of representations of $SL(2, C)$ is an irreducible unitary representation, which can be realized in several ways according to the space of realization. For our purpose, we employ that particular realization of it by means of the special unitary group SU_2.

We denote by $L_2^{2s}(SU_2)$ the set of all functions $\phi(u)$, where $u \in SU_2$, which are measurable and satisfy the conditions

$$\phi(\gamma u) = e^{is\psi}\phi(u), \tag{1}$$

$$\int |\phi(u)|^2 \, du < \infty, \tag{2}$$

where $\gamma \in SU_2$ is given by

$$\gamma = \begin{pmatrix} e^{-\frac{1}{2}i\psi} & 0 \\ 0 & e^{\frac{1}{2}i\psi} \end{pmatrix}. \tag{3}$$

$L_2^{2s}(SU_2)$ provides a Hilbert space[3,5] where the scalar product is defined by

$$(\phi_1, \phi_2) = \int \phi_1(u)\overline{\phi_2}(u) \, du. \tag{4}$$

The principal series of representations is then given by the formula[3]

$$V_g\phi(u) = [\alpha(ug)/\alpha(u\bar{g})]\phi(u\bar{g}), \tag{5}$$

where

$$g = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}$$

is an element of the group $SL(2, C)$ and $\alpha(g)$ is a function given by

$$\alpha(g) = g_{22}^{2s}\,|g_{22}|^{i\rho-2s-2}. \tag{6}$$

Here ρ is a real number and $2s$ is an integer.[6]

Consider now all possible systems of numbers ϕ_n^j, where $n = -j, -j+1, \cdots, j$ and $j = |s|, |s|+1, |s|+2, \cdots$, with the condition

$$\sum_{j=|s|}^{\infty} (2j+1) \sum_{n=-j}^{j} |\phi_n^j|^2 < \infty. \tag{7}$$

The aggregate of all such systems ϕ_n^j forms a Hilbert space, which we denote by l_2^{2s}, where the scalar product is defined by

$$\sum_{j=|s|}^{\infty} (2j+1) \sum_{n=-j}^{j} \phi_n^j\overline{\psi_n^j}, \tag{8}$$

for any two vectors ϕ_n^j and ψ_m^k of l_2^{2s}. With each vector $\phi_n^j \in l_2^{2s}$, we associate the function

$$\phi(u) = \sum_{j=|s|}^{\infty} (2j+1) \sum_{n=-j}^{j} \phi_n^j T_n^j(u), \tag{9}$$

where $T_n^j(u)$ is the matrix element $T_{sn}^j(u)$ of the irreducible representation of SU_2. Since[3]

$$T_n^j(\gamma u) = e^{is\psi}T_n^j(u),$$

the function given by Eq. (9) belongs to the space $L_2^{2s}(SU_2)$. On the other hand, every function in

$L_2^{2s}(SU_2)$ can be written in the form (9), since the $T_n^j(u)$ provide a complete orthogonal set.[5,7] The two spaces $L_2^{2s}(SU_2)$ and l_2^{2s} are, in fact, isometric where the transition from one space to the other can be made by means of the generalized Fourier transform

$$\phi_n^j = \int \phi(u)\bar{T}_n^j(u)\,du. \tag{10}$$

Similarly to spinors, which appear as coefficients in the polynomials of the space of representation, we see that the numbers ϕ_n^j appear as coefficients in the expansion given by Eq. (9) of the functions $\phi(u)$ of the space $L_2^{2s}(SU_2)$. By means of the mapping (10), the operator V_g of the representation (5) may also be regarded as an operator in the space l_2^{2s}, whose explicit expression we find below. This expression also defines another form of the principal series of representations.

Applying the operator V_g to the function $\phi(u)$ as given by Eq. (9), we obtain

$$V_g\phi(u) = \sum_j (2j+1) \sum_n \phi_n^j \frac{\alpha(ug)}{\alpha(u\bar{g})} T_n^j(u\bar{g}) \tag{11}$$

or

$$V_g\phi(u) = \sum_j (2j+1) \sum_n \phi_n^j \sum_{j'} (2j'+1) \times \sum_{n'} V_{nn'}^{jj'}(g; s, \rho) T_{n'}^{j'}(u), \tag{12}$$

where

$$V_{nn'}^{jj'}(g; s, \rho) = \int \frac{\alpha(ug)}{\alpha(u\bar{g})} T_n^j(u\bar{g})\bar{T}_{n'}^{j'}(u)\,du. \tag{13}$$

Accordingly, we obtain

$$V_g\phi(u) = \sum_j (2j+1) \sum_n \phi_n'^j T_n^j(u), \tag{14}$$

where, using Eq. (12), we have

$$\phi_{n'}'^{j'} = \sum_{j=|s|}^{\infty} (2j+1) \sum_{n=-j}^{j} V_{nn'}^{jj'}(g; s, \rho)\phi_n^j. \tag{15}$$

Thus, the operator V_g of the principal series of representations of $SL(2, C)$ in the space l_2^{2s} is the linear transformation determined by Eq. (15) describing the law of transformation of the quantities ϕ_n^j, where $j = |s|, |s|+1, |s|+2, \cdots$ and $n = -j, -j+1, \cdots, j$. Here, $V_{nn'}^{jj'}(g; s, \rho)$ are functions of $g \in SL(2, C)$ and of ρ and s, where ρ is a real number and $2s$ is an integer.

[1] Throughout this paper, the term spinor is used to mean symmetrical spinor. For application of two component spinors in the theory of general relativity, see R. Penrose, Ann. Phys. (N.Y.) **10**, 171 (1960).

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$$\int T_n^j(u)\bar{T}_{n'}^{j'}(u)\,du = \frac{\delta^{jj'}\delta^{nn'}}{2j+1}.$$

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Instantaneous Interaction Relativistic Dynamics for Two Particles in One Dimension

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(Received 19 November 1968)

Differential conditions which guarantee the Lorentz invariance of instantaneous action-at-a-distance relativistic dynamics have been given by Currie and by Hill. The present paper obtains the general solution of these conditions for the special case of two particles in one dimension. The resulting equations of motion are integrated to obtain the world lines. World-line invariance is explicitly demonstrated. The equations of motion are cast into Hamiltonian form with the transformations of the inhomogeneous Lorentz group canonical. The Hamiltonian formulation is made unique up to canonical transformation for those forces which fall off faster than the inverse square of the interparticle separation by the demand of asymptotic reduction to free particle form. The special case of the inverse-square-law forces of electrodynamics is considered; the constant of the motion associated with Lorentz invariance is found to have an interaction piece which survives asymptotically as in the relativistic mechanics of Van Dam and Wigner. The Poisson bracket $[x_1, x_2]$ between the physical coordinates also has an interaction piece which survives asymptotically for electrodynamics.

I. INTRODUCTION

The relativity of simultaneity has as one consequence the fact that the differential statements of Lorentz invariance[1-3] of instantaneous interaction relativistic mechanics are nonlinear. The nonlinearity renders their integration difficult. This is in contrast to the corresponding statements of "manifest covariant" theories which are linear and can be readily integrated to obtain the specification of an arbitrary dynamics by arbitrary 4-vector functions of 4-vectors.

$L_2^{2s}(SU_2)$ can be written in the form (9), since the $T_n^j(u)$ provide a complete orthogonal set.[5,7] The two spaces $L_2^{2s}(SU_2)$ and l_2^{2s} are, in fact, isometric where the transition from one space to the other can be made by means of the generalized Fourier transform

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Similarly to spinors, which appear as coefficients in the polynomials of the space of representation, we see that the numbers ϕ_n^j appear as coefficients in the expansion given by Eq. (9) of the functions $\phi(u)$ of the space $L_2^{2s}(SU_2)$. By means of the mapping (10), the operator V_g of the representation (5) may also be regarded as an operator in the space l_2^{2s}, whose explicit expression we find below. This expression also defines another form of the principal series of representations.

Applying the operator V_g to the function $\phi(u)$ as given by Eq. (9), we obtain

$$V_g\phi(u) = \sum_j (2j+1) \sum_n \phi_n^j \frac{\alpha(ug)}{\alpha(u\bar{g})} T_n^j(u\bar{g}) \tag{11}$$

or

$$V_g\phi(u) = \sum_j (2j+1) \sum_n \phi_n^j \sum_{j'} (2j'+1) \times \sum_{n'} V_{nn'}^{jj'}(g; s, \rho) T_{n'}^{j'}(u), \tag{12}$$

where

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Accordingly, we obtain

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where, using Eq. (12), we have

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Thus, the operator V_g of the principal series of representations of $SL(2, C)$ in the space l_2^{2s} is the linear transformation determined by Eq. (15) describing the law of transformation of the quantities ϕ_n^j, where $j = |s|, |s|+1, |s|+2, \cdots$ and $n = -j, -j+1, \cdots, j$. Here, $V_{nn'}^{jj'}(g; s, \rho)$ are functions of $g \in SL(2, C)$ and of ρ and s, where ρ is a real number and $2s$ is an integer.

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I. INTRODUCTION

The relativity of simultaneity has as one consequence the fact that the differential statements of Lorentz invariance[1-3] of instantaneous interaction relativistic mechanics are nonlinear. The nonlinearity renders their integration difficult. This is in contrast to the corresponding statements of "manifest covariant" theories which are linear and can be readily integrated to obtain the specification of an arbitrary dynamics by arbitrary 4-vector functions of 4-vectors.

The present paper obtains the general solutions of the nonlinear Lorentz invariance conditions of instantaneous interaction relativistic dynamics for the special case of two particles in one dimension, thus making it possible to investigate an arbitrary 1-dimensional 2-particle dynamics in the instantaneous interaction format.

In Sec. II the differential statements of Lorentz invariance are integrated to obtain equations of motion. Section III is devoted to the integration of these equations of motion. Constants of the motion H, P, and K whose transformation properties are identical with the transformation properties of the generators of the inhomogeneous Lorentz group are found. These constants are not uniquely determined. The particle world lines are obtained and world-line invariance is explicitly demonstrated. In Sec. IV a Hamiltonian formulation of the dynamics is obtained for each of the possible choices of H, P, and K found in Sec. III. In Sec. V the constants H, P, K, and the Hamiltonian formulation are made unique (up to canonical transformation) by the demand of asymptotic reduction to free particle form. Section VI is devoted to examples, including electrodynamics.

The equations solved in Sec. II are derived in Ref. 1 and in Sec. III of Ref. 3. The work of Secs. III–VI is based on the paper "Canonical Formulation of Relativistic Mechanics,"[4] hereafter referred to as CF; it is recommended that the reader of the present paper be familiar with CF.

II. INTEGRATION OF THE DIFFERENTIAL STATEMENTS OF LORENTZ INVARIANCE

The differential statements of the Lorentz invariance of a 1-dimensional 2-particle instantaneous action-at-a-distance theory[1–3] are

$$\mathfrak{L}_1 e_1 = 0 \tag{1a}$$

and

$$\mathfrak{L}_2 e_2 = 0, \tag{1b}$$

where

$$\mathfrak{L}_1 \equiv -x_{12}v_2\frac{\partial}{\partial x_{12}} + (1-v_1^2)\frac{\partial}{\partial v_1} + [1 + x_{12}e_2(1-v_2^2)^{\frac{1}{2}}](1-v_2^2)\frac{\partial}{\partial v_2} \tag{2a}$$

and

$$\mathfrak{L}_2 \equiv -x_{12}v_1\frac{\partial}{\partial x_{12}} + [1 - x_{12}e_1(1-v_1^2)^{\frac{1}{2}}](1-v_1^2)\frac{\partial}{\partial v_1} + (1-v_2^2)\frac{\partial}{\partial v_2}. \tag{2b}$$

Here $x_{12} \equiv x_1(t) - x_2(t)$ is the (instantaneous) interparticle separation, and v_1 and v_2 are the particle velocities. The equations of motion are

$$a_1 = (1-v_1^2)^{\frac{3}{2}}e_1 \tag{3}$$

and

$$a_2 = (1-v_2^2)^{\frac{3}{2}}e_2, \tag{4}$$

where a_1 and a_2 are the particle accelerations.

We begin by remarking that, if e_2 were known, the differential operator $\mathfrak{L}_1$ would be known and Eq. (1a) could be solved by the usual method of characteristics.[5] Even with e_2 unknown, the characteristics of (1a) still exist and can be used as one set of coordinate lines in a system of "natural" coordinates for the system (1). The characteristics of Eq. (1b) can be used as a second set of coordinate lines in such a system of "natural" coordinates *if* $\mathfrak{L}_1$ and $\mathfrak{L}_2$ are not proportional (this exceptional case is considered in Appendix A). Thus we introduce a transformation from the coordinates x_{12}, v_1, v_2 to new coordinates s_1, s_2, ζ in such a way that

$$\frac{\partial x_{12}}{\partial s_1} = -x_{12}v_2\varphi_1, \tag{5a}$$

$$\frac{\partial x_{12}}{\partial s_2} = -x_{12}v_1\varphi_2, \tag{5b}$$

$$\frac{\partial v_1}{\partial s_1} = (1-v_1^2)\varphi_1, \tag{6a}$$

$$\frac{\partial v_1}{\partial s_2} = [1 - x_{12}e_1(1-v_1^2)^{\frac{1}{2}}](1-v_1^2)\varphi_2, \tag{6b}$$

$$\frac{\partial v_2}{\partial s_1} = [1 + x_{12}e_2(1-v_2^2)^{\frac{1}{2}}](1-v_2^2)\varphi_1, \tag{7a}$$

$$\frac{\partial v_2}{\partial s_2} = (1-v_2^2)\varphi_2. \tag{7b}$$

By comparing Eqs. (5), (6), and (7) with Eq. (2), we see that

$$\mathfrak{L}_1 = \varphi_1^{-1}\frac{\partial}{\partial s_1} \tag{8a}$$

and

$$\mathfrak{L}_2 = \varphi_2^{-1}\frac{\partial}{\partial s_2}. \tag{8b}$$

Thus the system (1) becomes, in the new coordinates, the system

$$\frac{\partial e_1}{\partial s_1} = 0, \tag{9a}$$

$$\frac{\partial e_2}{\partial s_2} = 0. \tag{9b}$$

We note that Eqs. (5a), (6a), and (7a), with some choice for φ_1 (usually $\varphi_1 = 1$), is just the equivalent system which is written down when the usual method of characteristics[5] is applied to (1a).

The introduction of equations for two sets of characteristics, with coordinates s_1 and s_2 along the characteristic lines, is not necessarily consistent, because each of the pairs (5), (6), and (7) must satisfy an integrability condition. The as yet unknown function φ_1 and μ_2 are integrating factors introduced to make possible the satisfaction of these integrability conditions, which are

$$\frac{\partial}{\partial s_2}(x_{12}v_2\varphi_1) = \frac{\partial}{\partial s_1}(x_{12}v_1\varphi_2), \tag{10a}$$

$$\frac{\partial}{\partial s_2}[(1-v_1^2)\varphi_1] = \frac{\partial}{\partial s_1}\{[1-x_{12}e_1(1-v_1^2)^{\frac{1}{2}}](1-v_1^2)\varphi_2\}, \tag{10b}$$

$$\frac{\partial}{\partial s_2}\{[1+x_{12}e_2(1-v_2^2)^{\frac{1}{2}}](1-v_2^2)\varphi_1\} = \frac{\partial}{\partial s_1}[(1-v_2^2)\varphi_2]. \tag{10c}$$

By carrying out the differentiation and introducing the derivatives from (5), (6), (7), and (9), the integrability conditions (10) can be reduced to

$$x_{12}\left(v_2\frac{\partial\varphi_1}{\partial s_2} - v_1\frac{\partial\varphi_2}{\partial s_1} + (v_1^2-v_2^2)\varphi_1\varphi_2\right) = 0, \tag{11a}$$

$$(1-v_1^2)\left(\frac{\partial\varphi_1}{\partial s_2} - [1-x_{12}e_1(1-v_1^2)^{\frac{1}{2}}]\frac{\partial\varphi_2}{\partial s_1} - x_{12}e_1(1-v_1^2)^{\frac{1}{2}}(v_1+v_2)\varphi_1\varphi_2\right) = 0, \tag{11b}$$

$$(1-v_2^2)\left([1+x_{12}e_2(1-v_2^2)^{\frac{1}{2}}]\frac{\partial\varphi_1}{\partial s_2} - \frac{\partial\varphi_2}{\partial s_1} - x_{12}e_2(1-v_2^2)^{\frac{1}{2}}(v_1+v_2)\varphi_1\varphi_2\right) = 0. \tag{11c}$$

Equations (11) comprise a homogeneous system of linear equations for the three unknowns $\partial\varphi_1/\partial s_2$, $\partial\varphi_2/\partial s_1$, and $\varphi_1\varphi_2$. The determinant of this system vanishes identically. Analysis of the system (11), with the assumptions $x_{12}\neq 0$, $v_1\neq 0$, $v_2\neq 0$, $1-v_1^2\neq 0$, and $1-v_2^2\neq 0$, shows that, unless both

$$e_1 = x_{12}^{-1}(1-v_1^2)^{-\frac{1}{2}}[1-(v_1/v_2)] \tag{12a}$$

and

$$e_2 = -x_{12}^{-1}(1-v_2^2)^{-\frac{1}{2}}[1-(v_2/v_1)] \tag{12b}$$

hold, necessarily

$$\frac{\partial\varphi_1}{\partial s_2} = \frac{\partial\varphi_2}{\partial s_1} = (v_1+v_2)\varphi_1\varphi_2. \tag{13}$$

If Eq. (12) holds, $\mathfrak{L}_2 = (v_1/v_2)\mathfrak{L}_1$ and our method fails (see Appendix A). We discard this case and note that the first equality of Eq. (13) implies that

$$\varphi_1 = \frac{\partial\varphi}{\partial s_1}, \tag{14a}$$

$$\varphi_2 = \frac{\partial\varphi}{\partial s_2}, \tag{14b}$$

for some φ. Reinserting this in Eq. (13), we see that φ is determined by

$$\frac{\partial^2\varphi}{\partial s_1\partial s_2} = (v_1+v_2)\frac{\partial\varphi}{\partial s_1}\frac{\partial\varphi}{\partial s_2}. \tag{15}$$

The use of (14) in (6a) and (7b) produces

$$(1-v_1^2)^{-1}\frac{\partial v_1}{\partial s_1} = \frac{\partial\varphi}{\partial s_1}, \tag{16a}$$

$$(1-v_2^2)^{-1}\frac{\partial v_2}{\partial s_2} = \frac{\partial\varphi}{\partial s_2}. \tag{16b}$$

Integration of (16) produces

$$v_1 = \tanh(\varphi+\psi_1), \tag{17a}$$

$$v_2 = \tanh(\varphi+\psi_2), \tag{17b}$$

where ψ_1 and ψ_2 are functions of integration and satisfy

$$\frac{\partial\psi_1}{\partial s_1} = \frac{\partial\psi_2}{\partial s_2} = 0. \tag{18}$$

The use of (17) in (15) produces

$$\frac{\partial^2\varphi}{\partial s_1\partial s_2} = [\tanh(\varphi+\psi_1)+\tanh(\varphi+\psi_2)]\frac{\partial\varphi}{\partial s_1}\frac{\partial\varphi}{\partial s_2}. \tag{19}$$

Before proceeding to integrate (19), we argue that, for a nontrivial dynamics, $\partial\psi_1/\partial s_2\neq 0$ and $\partial\psi_2/\partial s_1\neq 0$. The time-development operator D for the dynamical system is

$$D \equiv \frac{\partial}{\partial t} + \sum_{i=1}^{2}\left(v_i\frac{\partial}{\partial x_i} + a_i\frac{\partial}{\partial v_i}\right). \tag{20}$$

Define X by

$$X \equiv \tfrac{1}{2}(x_1+x_2). \tag{21}$$

The use of (2), (3), (4), and (21) in (20) yields

$$D = \frac{\partial}{\partial t} + \tfrac{1}{2}(v_1+v_2)\frac{\partial}{\partial X} + x_{12}^{-1}(\mathfrak{L}_1-\mathfrak{L}_2). \tag{22}$$

The use of (8) and (14) in (22) yields

$$D = \frac{\partial}{\partial t} + \tfrac{1}{2}(v_1+v_2)\frac{\partial}{\partial X} + x_{12}^{-1}\left[\left(\frac{\partial\varphi}{\partial s_1}\right)^{-1}\frac{\partial}{\partial s_1} - \left(\frac{\partial\varphi}{\partial s_2}\right)^{-1}\frac{\partial}{\partial s_2}\right]. \tag{23}$$

It follows immediately from (23) that φ and ζ are constants of the motion. The results (17) and (18) now yield

$$a_1 = Dv_1 = -x_{12}^{-1}\left(\frac{\partial\varphi}{\partial s_2}\right)^{-1}\operatorname{sech}^2(\varphi+\psi_1)\frac{\partial\psi_1}{\partial s_2}, \quad (24a)$$

$$a_2 = Dv_2 = x_{12}^{-1}\left(\frac{\partial\varphi}{\partial s_1}\right)^{-1}\operatorname{sech}^2(\varphi+\psi_2)\frac{\partial\psi_2}{\partial s_1}. \quad (24b)$$

Hence, for a nontrivial dynamics, $\partial\psi_1/\partial s_2 \neq 0$ and $\partial\psi_2/\partial s_1 \neq 0$. Thus we can take ξ and η as new variables where

$$\xi \equiv \exp(-2\psi_1), \quad (25a)$$

$$\eta \equiv \exp(-2\psi_2). \quad (25b)$$

If we also introduce

$$\Phi \equiv \exp(2\varphi), \quad (26)$$

Eq. (19) takes the somewhat simpler form

$$\frac{\partial^2\Phi}{\partial\xi\partial\eta} = \left(\frac{1}{\Phi+\xi}+\frac{1}{\Phi+\eta}\right)\frac{\partial\Phi}{\partial\xi}\frac{\partial\Phi}{\partial\eta}. \quad (27)$$

We now proceed to integrate (27) by showing that it is equivalent to the following system:

$$\alpha/\beta = \Phi, \quad (28a)$$

$$\frac{\partial\alpha}{\partial\xi}+\xi\frac{\partial\beta}{\partial\xi} = 0, \quad (28b)$$

$$\frac{\partial\alpha}{\partial\eta}+\eta\frac{\partial\beta}{\partial\eta} = 0. \quad (28c)$$

To demonstrate the equivalence, suppose α and β are given, satisfying Eqs. (28b) and (28c). Then we define Φ by (28a); by using (28a) to eliminate α from (28b) and (28c), we obtain

$$\frac{\partial}{\partial\xi}(\ln\beta) = -\frac{1}{\Phi+\xi}\frac{\partial\Phi}{\partial\xi} \quad (29a)$$

and

$$\frac{\partial}{\partial\eta}(\ln\beta) = -\frac{1}{\Phi+\eta}\frac{\partial\Phi}{\partial\eta}. \quad (29b)$$

Equations (29a) and (29b) are compatible if and only if

$$\frac{\partial}{\partial\eta}\left[\frac{1}{\Phi+\xi}\frac{\partial\Phi}{\partial\xi}\right] = \frac{\partial}{\partial\xi}\left[\frac{1}{\Phi+\eta}\frac{\partial\Phi}{\partial\eta}\right]. \quad (30)$$

The relation (30) is easily shown (for $\xi \neq \eta$) to be equivalent to (27). Conversely, suppose Φ is any solution of (27). Then the integrability condition (30) for the system (29) is satisfied and β is determined to within a multiplicative constant. If (28a) is now used to define α, we can eliminate Φ from (29) to obtain (28b) and (28c).

We now proceed to integrate (28b) and (28c). Their compatibility requires

$$\frac{\partial}{\partial\eta}\left(\xi\frac{\partial\beta}{\partial\xi}\right) = \frac{\partial}{\partial\xi}\left(\eta\frac{\partial\beta}{\partial\eta}\right),$$

which implies

$$\frac{\partial^2\beta}{\partial\xi\partial\eta} = 0. \quad (31)$$

Hence

$$\beta = \frac{\partial}{\partial\xi}f(\xi,\zeta)+\frac{\partial}{\partial\eta}g(\eta,\zeta), \quad (32)$$

where f and g are arbitrary functions of the two indicated variables. Insertion of (32) into (28) now gives

$$\frac{\partial\alpha}{\partial\xi} = -\xi\frac{\partial^2 f}{\partial\xi^2}, \quad (33a)$$

$$\frac{\partial\alpha}{\partial\eta} = -\eta\frac{\partial^2 g}{\partial\eta^2}. \quad (33b)$$

Integration yields

$$\alpha = f(\xi,\zeta)-\xi\frac{\partial f(\xi,\zeta)}{\partial\xi}+g(\eta,\zeta)-\eta\frac{\partial g(\eta,\zeta)}{\partial\eta}. \quad (34)$$

Here the integration constant has been absorbed into the arbitrary functions f and g.

The use of (25), (26), and (28a) in (17) yields

$$v_1 = \frac{\Phi-\xi}{\Phi+\xi} = \frac{\alpha-\beta\xi}{\alpha+\beta\xi}, \quad (35a)$$

$$v_2 = \frac{\Phi-\eta}{\Phi+\eta} = \frac{\alpha-\beta\eta}{\alpha+\beta\eta}. \quad (35b)$$

The use of (14), (25), (26), and (35) in (5) yields

$$\frac{\partial}{\partial\eta}(\ln x_{12}) = \left(\frac{1}{2\Phi}-\frac{1}{\Phi+\eta}\right)\frac{\partial\Phi}{\partial\eta}, \quad (36a)$$

$$\frac{\partial}{\partial\xi}(\ln x_{12}) = \left(\frac{1}{2\Phi}-\frac{1}{\Phi+\xi}\right)\frac{\partial\Phi}{\partial\xi}. \quad (36b)$$

The integration of (36) is carried out by using (29); one obtains

$$\ln x_{12} = \tfrac{1}{2}\ln\Phi+\ln\beta+\text{const} = \tfrac{1}{2}\ln(\alpha\beta)+\text{const}.$$

Inasmuch as Φ, v_1, and v_2 are left unchanged when α and β are multiplied by the same constant, this integration constant can be absorbed into f and g. Thus we have

$$x_{12} = (\alpha\beta)^{\frac{1}{2}}. \quad (37)$$

The quantities e_1 and e_2 can now be calculated from (6b) and (7a). By using (25), (26), (28a), (35), and (37), we obtain

$$e_1 = -\tfrac{1}{2}\xi^{-\frac{3}{2}}\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1}, \quad (38a)$$

$$e_2 = \tfrac{1}{2}\eta^{-\frac{3}{2}}\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1}. \quad (38b)$$

The fact that (38) is consistent with (9) is an obvious consequence of (18) and (25) and the fact that $\partial f/\partial\eta = \partial g/\partial\xi = 0$. The fact that (38) and (24) are consistent can be shown with the aid of (25), (26), (28a), (32), (34), and (37).

We have now succeeded in obtaining the solution to Eqs. (1) in parametric form. We can summarize this solution as follows: We make some choice of the arbitrary functions f and g. Equations (35) and (37) then define a transformation from the physical variables x_{12}, v_1, v_2 to new variables ξ, η, ζ [with α and β given by Eqs. (32) and (34)]. The unknowns e_1 and e_2 are then given in terms of these new variables by Eqs. (38). The only conditions on f and g is that they be so chosen that the Jacobian J of the transformation from the physical variables x_{12}, v_1, and v_2 to the new variables ξ, η, and ζ does not vanish. This Jacobian is

$$J \equiv \frac{\partial(x_{12}, v_1, v_2)}{\partial(\xi, \eta, \zeta)}. \tag{39}$$

The use of (32), (34), (35), and (37) shows that

$$J = 4(\alpha\beta)^{\frac{3}{2}}(\alpha + \beta\xi)^{-2}(\alpha + \beta\eta)^{-2}J_1, \tag{40}$$

where

$$J_1 \equiv \left[\xi\frac{\partial^2 f}{\partial\xi^2} + \eta\frac{\partial^2 g}{\partial\eta^2} + \tfrac{1}{2}\beta\right]\frac{\partial\alpha}{\partial\zeta} + \left[\xi^2\frac{\partial^2 f}{\partial\xi^2} + \eta^2\frac{\partial^2 g}{\partial\eta^2} + \tfrac{1}{2}\alpha\right]\frac{\partial\beta}{\partial\zeta}. \tag{41}$$

The cases for which J is identically zero or infinite are explored in Appendix B. The result is that the transformation from x_{12}, v_1, v_2 to ξ, η, ζ is everywhere singular if and only if

$$f = \xi^{\frac{1}{2}}h_1[\xi h_2(\zeta)] + \xi h_3(\zeta) + h_4(\zeta), \tag{42a}$$
$$g = \eta^{\frac{1}{2}}h_5[\eta h_2(\zeta)] + \eta h_6(\zeta) + h_7(\zeta), \tag{42b}$$

where the arbitrary functions h_i are restricted either by

$$h_2(h_4 + h_7)^2 = \text{const}, \tag{43a}$$
$$h_2^{-1}(h_3 + h_6)^2 = \text{const} \quad \text{for} \quad h_2 \neq 0, \tag{43b}$$
$$(h_3 + h_6)(h_4 + h_7) = \text{const}, \tag{43c}$$

or by

$$h_1(\xi h_2) = C_1(\xi h_2)^{\frac{1}{2}} + C_2(\xi h_2)^{-\frac{1}{2}} + C_3, \tag{44a}$$
$$h_5(\eta h_2) = C_4(\eta h_2)^{\frac{1}{2}} + C_5(\eta h_2)^{-\frac{1}{2}} + C_6, \tag{44b}$$
$$(C_1 + C_4)(h_4 + h_7)h_2^{\frac{1}{2}} + (C_2 + C_5)(h_3 + h_6)h_2^{-\frac{1}{2}} + (h_3 + h_6)(h_4 + h_7) = \text{const}, \tag{44c}$$

where the C_i are constants.

Redundancy in the General Solution

Because the arbitrary functions f and g which appear in the general solution of Eq. (1) enter both in the transformation from x_{12}, v_1, v_2 to ξ, η, ζ [Eqs. (32), (34), (35), (37)] and in the expressions for the solutions [Eq. (38)], it is possible that two different choices of f and g correspond to the same dynamics—i.e., imply the same dependence of e_1 and e_2 on x_{12}, v_1, and v_2. Thus, for example, any mapping of the domain of ζ in 1-to-1 fashion onto itself will leave the dynamics the same, since neither differentiation nor integration with respect to ζ appears in the general solution.

We now proceed to find those transformations on f and g which leave the dynamics the same and are continuously developable from the identity. To this end we consider the infinitesimal transformation

$$f(\xi, \zeta) \to f'(\xi', \zeta') = f(\xi', \zeta') + \epsilon F(\xi', \zeta'), \tag{45a}$$
$$g(\eta, \zeta) \to g'(\eta', \zeta') = g(\eta', \zeta') + \epsilon G(\eta', \zeta'), \tag{45b}$$

and ask if there is a corresponding infinitesimal transformation

$$\xi \to \xi' = \xi + \epsilon\Xi(\xi, \eta, \zeta), \tag{46a}$$
$$\eta \to \eta' = \eta + \epsilon\mathrm{H}(\xi, \eta, \zeta), \tag{46b}$$
$$\zeta \to \zeta' = \zeta + \epsilon\mathrm{Z}(\xi, \eta, \zeta), \tag{46c}$$

on the independent variables such that the numerical values of x_{12}, v_1, v_2, e_1, and e_2 are left unchanged. Under the transformations (45) and (46),

$$\frac{\partial f}{\partial\xi} \to \frac{\partial f'}{\partial\xi'} = \frac{\partial f}{\partial\xi} + \epsilon\left(\frac{\partial F}{\partial\xi} + \Xi\frac{\partial^2 f}{\partial\xi^2} + \mathrm{Z}\frac{\partial^2 f}{\partial\xi\partial\zeta}\right),$$
$$\frac{\partial^2 f}{\partial\xi^2} \to \frac{\partial^2 f'}{\partial\xi'^2} = \frac{\partial^2 f}{\partial\xi^2} + \epsilon\left(\frac{\partial^2 F}{\partial\xi^2} + \Xi\frac{\partial^3 f}{\partial\xi^3} + \mathrm{Z}\frac{\partial^3 f}{\partial\xi^2\partial\zeta}\right)$$

with similar expressions for the changes in $\partial g/\partial\eta$ and $\partial^2 g/\partial\eta^2$. Using these, we obtain

$$e_1 \to e_1' = e_1 + \epsilon e_1^2\xi^{\frac{1}{2}}\left[\xi\frac{\partial^2 F}{\partial\xi^2} + \Xi\left(\frac{3}{2}\frac{\partial^2 f}{\xi^2} + \xi\frac{\partial^3 f}{\partial\xi^3}\right) + \mathrm{Z}\xi\frac{\partial^3 f}{\partial\xi^2\partial\zeta}\right].$$

The demand that the numerical value of e_1 be left unchanged is thus equivalent to the condition

$$\xi\frac{\partial^2 F}{\partial\xi^2} + \Xi\left(\frac{3}{2}\frac{\partial^2 f}{\partial\xi^2} + \xi\frac{\partial^3 f}{\partial\xi^3}\right) + \mathrm{Z}\xi\frac{\partial^3 f}{\partial\xi^2\partial\zeta} = 0. \tag{47}$$

Similar considerations applied to e_2 yield

$$\eta\frac{\partial^2 G}{\partial\eta^2} + \mathrm{H}\left(\frac{3}{2}\frac{\partial^2 g}{\partial\eta^2} + \eta\frac{\partial^3 g}{\partial\eta^3}\right) + \mathrm{Z}\eta\frac{\partial^3 g}{\partial\eta^2\partial\zeta} = 0. \tag{48}$$

Under the transformation (45) and (46),

$$\alpha \to \alpha' = \alpha + \epsilon a, \tag{49a}$$
$$\beta \to \beta' = \beta + \epsilon b, \tag{49b}$$

where

$$a \equiv F - \xi\frac{\partial F}{\partial \xi} + G - \eta\frac{\partial G}{\partial \eta} - \Xi\xi\frac{\partial^2 f}{\partial \xi^2} - \mathrm{H}\eta\frac{\partial^2 g}{\partial \eta^2} + \mathrm{Z}\frac{\partial \alpha}{\partial \zeta} \quad (50a)$$

and

$$b = \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} + \Xi\frac{\partial^2 f}{\partial \xi^2} + \mathrm{H}\frac{\partial^2 g}{\partial \eta^2} + \mathrm{Z}\frac{\partial \beta}{\partial \zeta}. \quad (50b)$$

Using this, we see that $x \to x' = x + \epsilon(2x)^{-1} \times (\alpha b + \beta a)$. Hence, the demand that the numerical value of x be left unchanged yields the condition

$$(a/\alpha) + (b/\beta) = 0. \quad (51)$$

Similarly, the demands that v_1 and v_2 be left unchanged yield

$$\frac{a}{\alpha} - \frac{b}{\beta} - \frac{\Xi}{\xi} = 0, \quad (52)$$

$$\frac{a}{\alpha} - \frac{b}{\beta} - \frac{\mathrm{H}}{\eta} = 0. \quad (53)$$

Equations (52) and (53) imply $(\Xi/\xi) = (\mathrm{H}/\eta)$; we now define

$$\lambda \equiv \Xi/\xi = \mathrm{H}/\eta. \quad (54)$$

It now follows from Eqs. (51)–(54) that $-a + \frac{1}{2}\alpha\lambda = 0$ and $b + \frac{1}{2}\beta\lambda = 0$. By using (50) and (54), these become

$$\lambda\left(\xi^2\frac{\partial^2 f}{\partial \xi^2} + \eta^2\frac{\partial^2 g}{\partial \eta^2} + \tfrac{1}{2}\alpha\right) - \mathrm{Z}\frac{\partial \alpha}{\partial \zeta} + \xi\frac{\partial F}{\partial \xi} - F + \eta\frac{\partial G}{\partial \eta} - G = 0; \quad (55)$$

$$\lambda\left(\xi\frac{\partial^2 f}{\partial \xi^2} + \eta\frac{\partial^2 g}{\partial \eta^2} + \tfrac{1}{2}\beta\right) + \mathrm{Z}\frac{\partial \beta}{\partial \zeta} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} = 0. \quad (56)$$

By operating on (55) and (56) with $\partial/\partial\xi$ and using (32), (34), (47), and (54), it follows that

$$\frac{\partial \lambda}{\partial \xi}\left(\xi^2\frac{\partial^2 f}{\partial \xi^2} + \eta^2\frac{\partial^2 g}{\partial \eta^2} + \tfrac{1}{2}\alpha\right) - \frac{\partial \mathrm{Z}}{\partial \xi}\frac{\partial \alpha}{\partial \zeta} = 0, \quad (57a)$$

$$\frac{\partial \lambda}{\partial \xi}\left(\xi\frac{\partial^2 f}{\partial \xi^2} + \eta\frac{\partial^2 g}{\partial \eta^2} + \tfrac{1}{2}\beta\right) + \frac{\partial \mathrm{Z}}{\partial \xi}\frac{\partial \beta}{\partial \zeta} = 0. \quad (57b)$$

The pair (57) can be viewed as a homogeneous linear system for the determination of $\partial\lambda/\partial\xi$ and $\partial \mathrm{Z}/\partial\xi$. Its determinant is the J_1 defined in (41); J_1 is nonzero where the transformation from x_{12}, v_1, v_2 is nonsingular. Hence

$$\frac{\partial \lambda}{\partial \xi} = \frac{\partial \mathrm{Z}}{\partial \xi} = 0. \quad (58)$$

A similar analysis which begins by operating on (55) and (56) with $\partial/\partial\eta$ and uses (48) in place of (47) yields

$$\frac{\partial \lambda}{\partial \eta} = \frac{\partial \mathrm{Z}}{\partial \eta} = 0. \quad (59)$$

Equations (58) and (59) imply that λ and Z depend only on ζ. Employing this fact together with (54), we integrate (47) twice with respect to ξ and (48) twice with respect to η to obtain

$$F = \lambda\left(\tfrac{1}{2}f - \xi\frac{\partial f}{\partial \xi}\right) - \mathrm{Z}\frac{\partial f}{\partial \zeta} + \xi F_1(\zeta) + F_2(\zeta), \quad (60a)$$

$$G = \lambda\left(\tfrac{1}{2}g - \eta\frac{\partial g}{\partial \eta}\right) - \mathrm{Z}\frac{\partial g}{\partial \zeta} + \eta G_1(\zeta) + G_2(\zeta). \quad (60b)$$

Here the functions of integration F_i and G_i depend only on ζ because $\partial F/\partial\eta = \partial G/\partial\xi = 0$. The use of (60) in (55) and (56) shows that

$$F_i = -G_i. \quad (61)$$

Equations (45), (46), (54), and (58)–(61) specify the most general infinitesimal transformation which leaves the dynamics unchanged. The corresponding finite transformation is

$$f'(\xi', \zeta') = \Lambda(\zeta)f(\xi, \zeta) + \xi f_1(\zeta) + f_2(\zeta), \quad (62a)$$

$$g'(\eta', \zeta') = \Lambda(\zeta)g(\eta, \zeta) - \eta f_1(\zeta) - f_2(\zeta), \quad (62b)$$

$$\xi' = \Lambda^2(\zeta)\xi, \quad (62c)$$

$$\eta' = \Lambda^2(\zeta)\eta, \quad (62d)$$

$$\zeta' = \mathrm{Z}(\zeta). \quad (62e)$$

Here Λ, f_1, f_2, and Z are arbitrary functions of the indicated variables subject only to the restrictions that $\Lambda \neq 0$ and that Z map the domain of ζ in 1-to-1 fashion onto itself. Equations (62) comprise the most general transformation which leaves the dynamics unchanged and is continuously developable from the identity.

III. INVARIANCE TRANSFORMATIONS, INTEGRALS OF THE MOTION, AND WORLD LINES

Integrals of the motion in classical dynamics can be conveniently classified by their transformation properties under the invariance transformations of the dynamics. Thus, for example, in a relativistic 1-dimensional system the total momentum P is an integral of the motion which is invariant under space and time translations and transforms as a 2-vector (the other component, of course, being the energy) under Lorentz transformation. We begin this section by looking for a set of three integrals of the motion H, P, and K which satisfy the Poisson bracket algebra

of the inhomogeneous Lorentz group in one dimension[6]:

$$[H, P] = 0, \quad [H, K] = -P, \quad [P, K] = -H. \tag{63}$$

We do not yet have a Hamiltonian formulation with respect to which the Poisson brackets in (63) are to be computed. However, the statements of transformation properties contained in (63) can be rewritten by using the differential operators L_{CTT}, L_{ST}, and L_{LT} which effect, respectively, infinitesimal time translation, space translation, and Lorentz transformation. Expressed in physical variables,[7]

$$L_{\mathrm{CTT}} = \sum_{i=1}^{2} \left(v_i \frac{\partial}{\partial x_i} + a_i \frac{\partial}{\partial v_i} \right), \tag{64a}$$

$$L_{\mathrm{ST}} = \sum_{i=1}^{2} \frac{\partial}{\partial x_i}, \tag{64b}$$

$$L_{\mathrm{LT}} = \sum_{i=1}^{2} \left((v_i x_i - t) \frac{\partial}{\partial x_i} + (a_i x_i - 1 + v_i^2) \frac{\partial}{\partial v_i} \right). \tag{64c}$$

Now H, P, and K are, respectively, the generators of time translation, space translation, and Lorentz transformation. Each of the brackets in (63) can be interpreted in two ways by regarding one of the elements as the object being transformed and the other as the generator of the transformation. By using (63), the differential operator L_{CTT}, L_{ST}, L_{LT}, and the fact that the Poisson bracket of a quantity with itself vanishes, we obtain

$$L_{\mathrm{CTT}} H = 0, \tag{65a}$$
$$L_{\mathrm{ST}} H = 0, \tag{65b}$$
$$L_{\mathrm{LT}} H = -P, \tag{65c}$$
$$L_{\mathrm{CTT}} P = 0, \tag{65d}$$
$$L_{\mathrm{ST}} P = 0, \tag{65e}$$
$$L_{\mathrm{LT}} P = -H, \tag{65f}$$
$$L_{\mathrm{CTT}} K = P, \tag{65g}$$
$$L_{\mathrm{ST}} K = H, \tag{65h}$$
$$L_{\mathrm{LT}} K = 0. \tag{65i}$$

The statement that H, P, and K are constants of the motion reads

$$DH = 0, \tag{66a}$$
$$DP = 0, \tag{66b}$$
$$DK = 0. \tag{66c}$$

Equations (65) and (66) are a set of partial differential equations for H, P, and K. In order to solve them, we first rewrite the operators L_{CTT}, L_{ST}, and L_{LT} in terms of the variables X, t, ξ, η, and ζ introduced in Sec. II [Eqs. (21), (32), (34), (35), and (37)]. From Eqs. (8), (14), (18), (25), and (26) it follows that

$$\mathfrak{L}_1 = \left(\frac{\partial \varphi}{\partial \eta} \right)^{-1} \frac{\partial}{\partial \eta} = 2\Phi \left(\frac{\partial \Phi}{\partial \eta} \right)^{-1} \frac{\partial}{\partial \eta}, \tag{67a}$$

$$\mathfrak{L}_2 = \left(\frac{\partial \varphi}{\partial \xi} \right)^{-1} \frac{\partial}{\partial \xi} = 2\Phi \left(\frac{\partial \Phi}{\partial \xi} \right)^{-1} \frac{\partial}{\partial \xi}. \tag{67b}$$

The use of (22), (35), and (37) shows that

$$D = \frac{\partial}{\partial t} + \frac{(\Phi^2 - \xi\eta)}{(\Phi + \xi)(\Phi + \eta)} \frac{\partial}{\partial X} + (\alpha\beta)^{-\frac{1}{2}} (\mathfrak{L}_1 - \mathfrak{L}_2). \tag{68}$$

It follows from (20), (21), (64a), and (64b) that

$$L_{\mathrm{CTT}} = D - \frac{\partial}{\partial t}, \tag{69a}$$

$$L_{\mathrm{ST}} = \frac{\partial}{\partial X}. \tag{69b}$$

The use of (2), (20), (21), (35), (37), and (64c) yields

$$L_{\mathrm{LT}} = X \left(D - \frac{\partial}{\partial t} \right) + \left(\frac{\Phi(\eta - \xi)(\alpha\beta)^{\frac{1}{2}}}{2(\Phi + \xi)(\Phi + \eta)} - t \right) \frac{\partial}{\partial X} - \tfrac{1}{2}(\mathfrak{L}_1 + \mathfrak{L}_2). \tag{70}$$

It now follows from (65a), (65b), (65d), (65e), (66a), (66b), and (69) that

$$\frac{\partial H}{\partial t} = 0, \quad \frac{\partial H}{\partial X} = 0, \quad \frac{\partial P}{\partial t} = 0, \quad \frac{\partial P}{\partial X} = 0. \tag{71}$$

Equations (65c), (65f), (66a), and (66b) can now be reduced with the aid of (68), (70), and (71) to the form

$$\mathfrak{L}_1 H = \mathfrak{L}_2 H = P, \quad \mathfrak{L}_1 P = \mathfrak{L}_2 P = H. \tag{72}$$

The solution of (71) and (72) is easily found by using (67); it is

$$H = A(\zeta)\Phi^{-\frac{1}{2}} + B(\zeta)\Phi^{\frac{1}{2}}, \tag{73a}$$
$$P = -A(\zeta)\Phi^{-\frac{1}{2}} + B(\zeta)\Phi^{\frac{1}{2}}, \tag{73b}$$

where A and B, which depend only on ζ, are arbitrary functions of integration. Having found H and P, we now proceed to find K. It follows from (65g), (65h), (66c), and (69) that

$$\frac{\partial K}{\partial t} = -P, \tag{74a}$$

$$\frac{\partial K}{\partial X} = H. \tag{74b}$$

Hence

$$K = HX - Pt + k(\xi, \eta, \zeta). \tag{75}$$

We now insert (75) into (65i) and (66c) and use (65c), (65f), (66a), (66b), (68), and (70) to obtain

$$\mathfrak{L}_1 k = \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}[P - H(\Phi - n)/(\Phi + \eta)], \tag{76a}$$

$$\mathfrak{L}_2 k = \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}[-P + H(\Phi - \xi)/(\Phi + \xi)]. \tag{76b}$$

The use of (28), (32), (34), (67), and (73) reduces (76) to

$$\frac{\partial k}{\partial \xi} = \tfrac{1}{2}(-A + B\xi)\frac{\partial^2 f}{\partial \xi^2}, \tag{77a}$$

$$\frac{\partial k}{\partial \eta} = \tfrac{1}{2}(A - B\eta)\frac{\partial^2 g}{\partial \eta^2}. \tag{77b}$$

Integrating, we obtain

$$k = \tfrac{1}{2}A(\zeta)\left(-\frac{\partial f}{\partial \xi} + \frac{\partial g}{\partial \eta}\right) + \tfrac{1}{2}B(\zeta)\left(-f + \xi\frac{\partial f}{\partial \xi} + g - \eta\frac{\partial g}{\partial \eta}\right) + C(\zeta). \tag{78}$$

Here C, which depends only on ζ, is an arbitrary function of integration. We have now succeeded in finding a set of integrals H, P, and K; the results are given by (73), (75), and (78).

World Lines

In order to completely integrate the equations of motion and find the world lines, we need a fourth integral of the motion independent of H, P, and K. We introduce this fourth integral, which we call Θ, by requiring that its Poisson brackets with the other integrals be given by

$$[H, \Theta] = -H, \quad [P, \Theta] = -P, \quad [K, \Theta] = 0. \tag{79}$$

The consistency of (79) with (63) can be verified by checking that the Jacobi identity holds for each of the four possible sets of three independent integrals of the motion. Equation (79) and the statement that Θ is conserved imply

$$L_{\mathrm{CTT}}\Theta = H, \tag{80a}$$

$$L_{\mathrm{ST}}\Theta = P, \tag{80b}$$

$$L_{\mathrm{LT}}\Theta = 0, \tag{80c}$$

$$D\Theta = 0. \tag{80d}$$

It follows from (80a), (80b), (80d), and (69) that

$$\frac{\partial \Theta}{\partial t} = -H, \tag{81a}$$

$$\frac{\partial \Theta}{\partial X} = P. \tag{81b}$$

Hence

$$\Theta = PX - Ht + \theta(\xi, \eta, \zeta). \tag{82}$$

We now insert (82) in (80c) and (80d), and use (65c), (65f), (66a), (66b), (68), and (70) to obtain

$$\mathfrak{L}_1 \theta = \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}[H - P(\Phi - \eta)/(\Phi + \eta)], \tag{82a}$$

$$\mathfrak{L}_2 \theta = \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}[-H + P(\Phi - \xi)/(\Phi + \xi)]. \tag{82b}$$

The use of (28), (32), (34), (67), and (73) reduces (82) to

$$\frac{\partial \theta}{\partial \xi} = \tfrac{1}{2}(A + B\xi)\frac{\partial^2 f}{\partial \xi^2}, \tag{83a}$$

$$\frac{\partial \theta}{\partial \eta} = \tfrac{1}{2}(-A - \eta B)\frac{\partial^2 g}{\partial \eta^2}. \tag{83b}$$

Integrating, we obtain

$$\theta = \tfrac{1}{2}A(\zeta)\left(\frac{\partial f}{\partial \xi} - \frac{\partial g}{\partial \eta}\right) + \tfrac{1}{2}B(\zeta)\left(-f + \xi\frac{\partial f}{\partial \xi} + g - \eta\frac{\partial g}{\partial \eta}\right) + \gamma(\zeta), \tag{84}$$

where γ, which depends only on ζ, is an arbitrary function of integration.

We now form the quantities

$$c_1 = (K - C - \Theta + \gamma)/(H - P), \tag{85a}$$

$$c_2 = (K - C + \Theta - \gamma)/(H + P). \tag{85b}$$

Inasmuch as K, C, Θ, γ, H, and P are all constants of the motion, c_1 and c_2 are constants of the motion. It now follows from (73), (75), (78), (82), (84), and (85) that

$$c_1 = X + t - \tfrac{1}{2}\Phi^{\frac{1}{2}}\left(\frac{\partial f}{\partial \xi} - \frac{\partial g}{\partial \eta}\right), \tag{86a}$$

$$c_2 = X - t - \tfrac{1}{2}\Phi^{-\frac{1}{2}}\left(f - \xi\frac{\partial f}{\partial \xi} - g + \eta\frac{\partial g}{\partial \eta}\right). \tag{86b}$$

If we now add and subtract zero in the form

$$0 = \tfrac{1}{2}x_{12} - \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}$$

[see Eq. (37)] from (86a) and (86b), we obtain, with the aid of (28a), (32), and (34),

$$c_1 = x_1 + t - \Phi^{\frac{1}{2}}\frac{\partial f}{\partial \xi}, \tag{87a}$$

$$c_2 = x_1 - t - \Phi^{-\frac{1}{2}}\left(f - \xi\frac{\partial f}{\partial \xi}\right), \tag{87b}$$

$$c_1 = x_2 + t + \Phi^{\frac{1}{2}}\frac{\partial g}{\partial \eta}, \tag{88a}$$

$$c_2 = x_2 - t + \Phi^{-\frac{1}{2}}\left(g - \eta\frac{\partial g}{\partial \eta}\right). \tag{88b}$$

The world lines can be obtained in parametric form from (87) and (88) by solving for x_i and t. From (87) we obtain

$$x_1 = \tfrac{1}{2}\left[c_1 + c_2 + \Phi^{\frac{1}{2}}\frac{\partial f}{\partial \xi} + \Phi^{-\frac{1}{2}}\left(f - \xi\frac{\partial f}{\partial \xi}\right)\right], \quad (89a)$$

$$t = \tfrac{1}{2}\left[c_1 - c_2 + \Phi^{\frac{1}{2}}\frac{\partial f}{\partial \xi} - \Phi^{-\frac{1}{2}}\left(f - \xi\frac{\partial f}{\partial \xi}\right)\right]. \quad (89b)$$

From (88) we obtain

$$x_2 = \tfrac{1}{2}\left[c_1 + c_2 - \Phi^{\frac{1}{2}}\frac{\partial g}{\partial \eta} - \Phi^{-\frac{1}{2}}\left(g - \eta\frac{\partial g}{\partial \eta}\right)\right], \quad (90a)$$

$$t = \tfrac{1}{2}\left[c_1 - c_2 - \Phi^{\frac{1}{2}}\frac{\partial g}{\partial \eta} + \Phi^{-\frac{1}{2}}\left(g - \eta\frac{\partial g}{\partial \eta}\right)\right]. \quad (90b)$$

The result (89) gives the world line of particle one in parametric form with ξ as parameter; similarly, (90) gives the world line of particle two in parametric form with η as parameter. The world lines depend on the four constants of the motion c_1, c_2, Φ, and ζ; thus, specification of initial position and velocities specifies the world lines just as in nonrelativistic Newtonian mechanics. The results (35) and (38) give the velocities and accelerations in parametric form with the same parameters. The fact that it has been possible to integrate the equations of motion completely rather then just reduce them to quadratures is a consequence of the fact that the solutions to the differential statements of Lorentz invariance were specified in terms of derivatives of arbitrary functions rather than in terms of arbitrary functions.

World-line invariance under the transformations of the inhomogeneous Lorentz group is easily demonstrated from (89) and (90) by conducting the transformation and discovering that the transformed world lines can be rewritten in the forms (89) and (90) with different numerical values of c_1, c_2, and Φ. Thus, under the time translation $t \to t' = t + t_0$, we find that $c_1 \to c_1' = c_1 + t_0$ and $c_2 \to c_2' = c_2 - t_0$, with Φ and ζ left unchanged. Under the space translation $x_i \to x_i' = x_i + x_0$, we find that $c_1 \to c_1' = c_1 + x_0$ and $c_2 \to c_2' = c_2 + x_0$, with Φ and ζ left unchanged. Under the pure Lorentz transformation

$$x_i \to x_i' = (x_i - \beta t)(1 - \beta^2)^{-\frac{1}{2}}$$

and

$$t \to t' = (t - \beta x_i)(1 - \beta^2)^{-\frac{1}{2}}$$

[where each of the two orbits must be transformed *separately* and rewritten in the forms (89) and (90)], we find that

$$c_1 \to c_1' = c_1(1 - \beta)^{\frac{1}{2}}(1 + \beta)^{-\frac{1}{2}},$$
$$c_2 \to c_2' = c_2(1 - \beta)^{-\frac{1}{2}}(1 + \beta)^{\frac{1}{2}},$$

and

$$\Phi \to \Phi' = (1 - \beta)(1 + \beta)^{-1}\Phi,$$

with ζ left unchanged. This transformation property of Φ under Lorentz transformation is consistent with that obtained by iterating the infinitesimal transformation: from (67) and (70), $L_{\mathrm{LT}}\Phi = -2\Phi$ whence

$$\begin{aligned}\Phi' &= [\exp(sL_{\mathrm{LT}})]\Phi \\ &= [1 - sL_{\mathrm{LT}} + (2!)^{-1}s^2L_{\mathrm{LT}}^2 - \cdots]\Phi \\ &= \exp(-2s)\Phi = (1 - \beta)(1 + \beta)^{-1}\Phi\end{aligned}$$

by using $\beta = \tanh s$.

IV. A CANONICAL FORMULATION

This section is devoted to the construction of the Hamiltonian formulation whose existence for every even-order differential system is guaranteed by the Lie–Königs theorem. We will find those Hamiltonian formulations for which the transformations of the inhomogeneous Lorentz group are canonical transformations, restricting ourselves to the case of no neutral elements.[6]

The center-of-mass coordinate Q for a 1-dimensional relativistic system is introduced via

$$K = HQ - Pt. \quad (91)$$

It follows from (63) and (91) that

$$[Q, P] = 1. \quad (92)$$

Hence, Q can be taken as the canonical mate to P. Because we already have the canonical pair P and Q, we can save considerable labor by applying the Lie–Königs Hamiltonization procedure to the dynamics expressed in the variables ξ, η, ζ, Q, and t, rather than the variables ξ, η, ζ, X, and t.

It follows from (75), (78), and (91) that

$$Q = X + H^{-1}\left[-\tfrac{1}{2}A\left(\frac{\partial f}{\partial \xi} - \frac{\partial g}{\partial \eta}\right) - \tfrac{1}{2}B\left(f - \xi\frac{\partial f}{\partial \xi} - g + \eta\frac{\partial g}{\partial \eta}\right) + C\right]. \quad (93)$$

It can be shown with the aid of (28), (32), (34), (67), (73), and (91) that, in the new variables,

$$\mathfrak{L}_1 = 2\Phi\left(\frac{\partial \Phi}{\partial \eta}\right)^{-1}\frac{\partial}{\partial \eta} + \left[[X - Q + \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}]\left(\frac{P}{H}\right) - \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}(\Phi - \eta)(\Phi + \eta)^{-1}\right]\frac{\partial}{\partial Q}, \quad (94a)$$

$$\mathfrak{L}_2 = 2\Phi\left(\frac{\partial \Phi}{\partial \xi}\right)^{-1}\frac{\partial}{\partial \xi} + \left[[X - Q - \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}]\left(\frac{P}{H}\right) + \tfrac{1}{2}(\alpha\beta)^{\frac{1}{2}}(\Phi - \xi)(\Phi + \xi)^{-1}\right]\frac{\partial}{\partial Q}. \quad (94b)$$

The use of (93) and (94) in (68), (69), and (70) now produces

$$L_{\mathrm{CTT}} = \frac{P}{H}\frac{\partial}{\partial Q} + 2\Phi(\alpha\beta)^{-\frac{1}{2}}\left[\left(\frac{\partial\Phi}{\partial\eta}\right)^{-1}\frac{\partial}{\partial\eta} - \left(\frac{\partial\Phi}{\partial\xi}\right)^{-1}\frac{\partial}{\partial\xi}\right], \quad (95a)$$

$$L_{\mathrm{ST}} = \frac{\partial}{\partial Q}, \quad (95b)$$

$$L_{\mathrm{LT}} = \left[Q\left(\frac{P}{H}\right) - t\right]\frac{\partial}{\partial Q} + 2(\alpha\beta)^{-\frac{1}{2}}H^{-1}\Phi\left\{\left[-HQ - A\frac{\partial f}{\partial\xi} - B\left(f - \xi\frac{\partial f}{\partial\xi}\right) + C\right]\left(\frac{\partial\Phi}{\partial\xi}\right)^{-1}\frac{\partial}{\partial\xi} + \left[HQ - A\frac{\partial g}{\partial\eta} - B\left(g - \eta\frac{\partial g}{\partial\eta}\right) - C\right] \times \left(\frac{\partial\Phi}{\partial\eta}\right)^{-1}\frac{\partial}{\partial\eta}\right\}, \quad (95c)$$

$$D = L_{\mathrm{CTT}} + \frac{\partial}{\partial t}. \quad (95d)$$

In order to avoid writing out explicitly the sums which appear in the Hamiltonian procedure given in CF, we relabel the independent variables:

$$y_0 = t, \quad y_1 = Q, \quad y_2 = \xi, \quad y_3 = \eta, \quad y_4 = \zeta. \quad (96)$$

By comparing $L_\alpha \equiv \sum_{i=0}^{2n} g_i^\alpha \partial/\partial y_i$ and $D \equiv \sum_{i=0}^{2n} h_i \partial/\partial y_i$ [Eqs. (CF-14) and (CF-15)] with (95) and using (96), we see that

$$g_0^{\mathrm{CTT}} = 0, \quad h_0 = 1, \quad g_1^{\mathrm{CTT}} = h_1 = \frac{P}{H},$$

$$g_2^{\mathrm{CTT}} = h_2 = -2\Phi(\alpha\beta)^{-\frac{1}{2}}\left(\frac{\partial\Phi}{\partial y_2}\right)^{-1},$$

$$g_3^{\mathrm{CTT}} = h_3 = 2\Phi(\alpha\beta)^{-\frac{1}{2}}\left(\frac{\partial\Phi}{\partial y_3}\right)^{-1},$$

$$g_4^{\mathrm{CTT}} = h_4 = 0, \quad g_1^{\mathrm{ST}} = 1, \quad g_i^{\mathrm{ST}} = 0, \quad i \neq 1,$$

$$g_0^{\mathrm{LT}} = 0, \quad g_1^{\mathrm{LT}} = Q\left(\frac{P}{H}\right) - y_0, \quad (97)$$

$$g_2^{\mathrm{LT}} = 2(\alpha\beta)^{-\frac{1}{2}}H^{-1}\Phi\left\{-HQ - A\left(\frac{\partial f}{\partial y_2}\right) - B\left[f - y_2\left(\frac{\partial f}{\partial y_2}\right)\right] + C\right\}\left(\frac{\partial\Phi}{\partial y_2}\right)^{-1},$$

$$g_3^{\mathrm{LT}} = 2(\alpha\beta)^{-\frac{1}{2}}H^{-1}\Phi\left\{HQ - A\left(\frac{\partial g}{\partial y_3}\right) - B\left[g - y_3\left(\frac{\partial g}{\partial y_3}\right)\right] - C\right\}\left(\frac{\partial\Phi}{\partial y_3}\right)^{-1},$$

and

$$g_4^{\mathrm{LT}} = 0.$$

The generators H, P, and K are related to the U_i of the variational principle $\delta\int\sum_{i=0}^{2n} U_i\,dy_i = 0$ [Eq. (CF-2)] via the relation $G_\alpha = \sum_{i=0}^{2n} g_i^\alpha U_i - \Omega_\alpha$ [Eq. (CF-19)]. As was shown in Sec. IVC of CF, the Ω_α can be taken to be zero if for the g_i^α we use g_i^{TT}, g_i^{ST}, and g_i^{MLT}, where

$$g_i^{\mathrm{TT}} = g_i^{\mathrm{CTT}} - h_i,$$
$$g_i^{\mathrm{MLT}} = g_i^{\mathrm{LT}} - Qh_i. \quad (98)$$

By the use of (96), (97), (98), and (CF-19) with $\Omega_\alpha = 0$, we obtain

$$H = G_{\mathrm{TT}} = -U_0, \quad (99a)$$

$$P = G_{\mathrm{ST}} = U_1, \quad (99b)$$

$$K = G_{\mathrm{MLT}} = -y_1U_0 - y_0U_1 - 2(\alpha\beta)^{-\frac{1}{2}}H^{-1}\Phi \times \left\{\left[A\frac{\partial f}{\partial y_2} + B\left(f - y_2\frac{\partial f}{\partial y_2}\right) - C\right]\left(\frac{\partial\Phi}{\partial y_2}\right)^{-1}U_2 + \left[A\frac{\partial g}{\partial y_3} + B\left(g - y_3\frac{\partial g}{\partial y_3}\right) + C\right]\right\}\left(\frac{\partial\Phi}{\partial y_3}\right)^{-1}U_3. \quad (99c)$$

The manifest invariance implicit in taking $\Omega_\alpha = 0$ implies that (see Sec. IIIE of CF)

$$\frac{\partial U_i}{\partial y_0} = \frac{\partial U_i}{\partial y_1} = 0. \quad (100)$$

By the use of (99a), (99b), (100), and the definition

$$\Gamma_{ij} = \frac{\partial U_i}{\partial y_j} - \frac{\partial U_j}{\partial y_i}$$

[Eq. (CF-3)], we obtain

$$\Gamma_{0j} = -\Gamma_{j0} = -\frac{\partial H}{\partial y_j}, \quad (101a)$$

$$\Gamma_{1j} = -\Gamma_{j1} = \frac{\partial P}{\partial y_j}. \quad (101b)$$

By writing out $\sum_{j=0}^{4}\Gamma_{ij}h_j = 0$ [Eq. (CF-4)] for $i = 2$, we obtain

$$\Gamma_{20} + \Gamma_{21}\left(\frac{P}{H}\right) + 2\Phi(\alpha\beta)^{-\frac{1}{2}}\left(\frac{\partial\Phi}{\partial y_3}\right)^{-1}\Gamma_{23} = 0.$$

But the use of (73), (96), and (101) shows that $\Gamma_{20} + \Gamma_{21}(P/H) = 0$. Hence

$$\Gamma_{23} = -\Gamma_{32} = 0, \quad (102)$$

whence $\partial U_2/\partial y_3 = \partial U_3/\partial y_2$, which implies the existence of a function U such that

$$U_2 = \frac{\partial U}{\partial y_2}, \quad U_3 = \frac{\partial U}{\partial y_3}. \quad (103)$$

If now we use (91), (96), (99a), (99b), and (103) in (99c), we see that U satisfies

$$\left\{A\left(\frac{\partial f}{\partial y_2}\right)+B\left[f-y_2\left(\frac{\partial f}{\partial y_2}\right)\right]-C\right\}\left(\frac{\partial \Phi}{\partial y_2}\right)^{-1}\left(\frac{\partial U}{\partial y_2}\right)+\left\{A\left(\frac{\partial g}{\partial y_3}\right)+B\left[g-y_3\left(\frac{\partial g}{\partial y_3}\right)\right]+C\right\}\times\left(\frac{\partial \Phi}{\partial y_3}\right)^{-1}\left(\frac{\partial U}{\partial y_3}\right)=0. \quad (104)$$

Equation (104) can be solved by application of the method of characteristics; the general solution is

$$U = U(S, y_4), \quad (105)$$

where

$$S \equiv (A\beta + B\alpha)^{-1}\left\{\left(\frac{\partial f}{\partial y_2}\right)\left[g-y_3\left(\frac{\partial g}{\partial y_3}\right)\right]-\left(\frac{\partial g}{\partial y_3}\right)\left[f-y_2\left(\frac{\partial f}{\partial y_2}\right)\right]+B^{-1}C\beta\right\}. \quad (106)$$

We have now only U_4 left to find; toward this end, we write out

$$\sum_{j=0}^{4}\Gamma_{ij}h_j = 0 \quad \text{and} \quad \sum_{j=0}^{4}\Gamma_{ij}g_j^{\mathrm{MLT}} = -\frac{\partial K}{\partial y_i}$$

[see Eq. (CF-20)] for $i = 4$, with K given by (91), to obtain

$$\Gamma_{40}+\left(\frac{P}{H}\right)\Gamma_{41}+2\Phi(\alpha\beta)^{-\frac{1}{2}}\left[-\left(\frac{\partial \Phi}{\partial y_2}\right)^{-1}\Gamma_{42}+\left(\frac{\partial \Phi}{\partial y_3}\right)^{-1}\Gamma_{43}\right]=0,$$

$$-y_1\Gamma_{40}-y_0\Gamma_{41}-2\Phi(\alpha\beta)^{-\frac{1}{2}}H^{-1}\times\left\{\left[A\frac{\partial f}{\partial y_2}+B\left(f-y_2\frac{\partial f}{\partial y_2}\right)-C\right]\left(\frac{\partial \Phi}{\partial y_2}\right)^{-1}\Gamma_{42}+\left[A\frac{\partial g}{\partial y_3}+B\left(g-y_3\frac{\partial g}{\partial y_3}\right)+C\right]\left(\frac{\partial \Phi}{\partial y_3}\right)^{-1}\Gamma_{43}\right\}=-y_1\left(\frac{\partial H}{\partial y_4}\right)+y_0\left(\frac{\partial P}{\partial y_4}\right).$$

By using (101) for Γ_{40} and Γ_{41}, we can solve this pair for Γ_{42} and Γ_{43} to obtain, with the aid of (28a), (73), and (96),

$$\Gamma_{42} = -\Gamma_{24} = H^{-2}\Phi^{-1}\left\{A\left(\frac{\partial g}{\partial y_3}\right)+B\left[g-y_3\left(\frac{\partial g}{\partial y_3}\right)\right]+C\right\}\times\left(\frac{\partial \Phi}{\partial y_2}\right)\frac{\partial(AB)}{\partial y_4}, \quad (107a)$$

$$\Gamma_{43} = -\Gamma_{34} = -H^{-2}\Phi^{-1}\left\{A\left(\frac{\partial f}{\partial y_2}\right)+B\left[f-y_2\left(\frac{\partial f}{\partial y_2}\right)\right]-C\right\}\times\left(\frac{\partial \Phi}{\partial y_3}\right)\frac{\partial(AB)}{\partial y_4}. \quad (107b)$$

It follows from the definition of Γ_{ij} [Eq. (CF-3)] and Eq. (103) that

$$\frac{\partial U_4}{\partial y_2} = \Gamma_{42}+\frac{\partial^2 U}{\partial y_2 \partial y_4}, \quad (108a)$$

$$\frac{\partial U_4}{\partial y_3} = \Gamma_{43}+\frac{\partial^2 U}{\partial y_3 \partial y_4}. \quad (108b)$$

Equation (108) can be easily integrated after (107) has been inserted for Γ_{42} and Γ_{43}; the result is (where the constant of integration has been absorbed into the arbitrary function U)

$$U_4 = -S\frac{\partial(AB)}{\partial y_4}+\frac{\partial U}{\partial y_4}. \quad (109)$$

We now find, using (96), (99a), (99b), (103), and (109), that

$$\sum_{i=0}^{4}U_i\,dy_i = P\,dQ - S\,d(AB) + dU - H\,dt. \quad (110)$$

Clearly different choices of the arbitrary function U correspond to different canonical transformations on the internal variables. It is convenient to take $U = 2SAB$. Then

$$\sum_{i=0}^{4}U_i\,dy_i = P\,dQ + p\,dq - H\,dt, \quad (111)$$

where

$$p = 2(AB)^{\frac{1}{2}}, \quad (112a)$$

$$q = (AB)^{\frac{1}{2}}S. \quad (112b)$$

From (73) and (112a), it follows that

$$H = (P^2+p^2)^{\frac{1}{2}}. \quad (113)$$

The task of obtaining a Hamiltonian formulation is now complete. We have canonical variables P, Q, p, and q given by (73b), (93), and (112), where S is given by (96) and (106); the generators H and K are given in terms of these canonical variables by (91) and (113). It should be noted that we have completely avoided the labor of solving Pfaff's problem to reduce $\sum_{i=0}^{4}U_i\,dy_i$ to the form (111) by choosing Q as one of the variables for the application of the Hamiltonization procedure.

Poisson Brackets Among Physical Variables

Because the Currie–Jordan–Sudarshan zero-interaction theorem[8] follows from the assumptions of (a) world-line invariance, (b) invariance of the equations

of motion, and (c) vanishing of the Poisson brackets $[x_i, x_j]$ of the physical coordinates among themselves, it is of some interest to compute explicitly the Poisson brackets among the physical positions and velocities. The details of the computation, which is somewhat tedious, are sketched in Appendix C. The results are

$$[x_1, x_2] = (\Phi+\xi)^{-1}(\Phi+\eta)^{-1}\left(\frac{d(AB)}{d\zeta}\right)^{-1}\Phi \times \left\{\left[g - 2\eta\left(\frac{\partial g}{\partial \eta}\right)\right]\left(\frac{\partial(A+\xi B)}{\partial\zeta}\right) + \left[f - 2\xi\left(\frac{\partial f}{\partial\xi}\right)\right]\left(\frac{\partial(A+\eta B)}{\partial\zeta}\right) + (\xi-\eta)\left(\frac{dC}{d\zeta}\right) - (A-\xi B)\left(\frac{\partial g}{\partial\zeta}\right) - (A-\eta B)\left(\frac{\partial f}{\partial\zeta}\right)\right\}, \tag{114a}$$

$$[x_1, v_1] = 2\Phi^{\frac{3}{2}}(\Phi+\xi)^{-3}\left(\frac{d(AB)}{d\zeta}\right)^{-1} \times \left[\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1}\left(\frac{\partial k_1}{\partial\zeta}\right) + 2\xi\frac{\partial(A+\xi B)}{\partial\zeta}\right], \tag{114b}$$

$$[x_1, v_2] = 2\Phi^{\frac{3}{2}}(\Phi+\xi)^{-1}(\Phi+\eta)^{-3}\left(\frac{d(AB)}{d\zeta}\right)^{-1} \times \left\{2\eta\left(\Phi+\eta+\Phi^{\frac{1}{2}}\eta^{-1}(\alpha\beta)^{\frac{1}{2}}\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1}\right) \times \left(\frac{\partial(A+\xi B)}{\partial\zeta}\right) - (\Phi+\xi)\left(\frac{\partial k_1}{\partial\zeta}\right)\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1} - (A-\xi B)\Phi^{-\frac{1}{2}}\left(\frac{\partial\Phi}{\partial\zeta}\right)(\alpha\beta)^{\frac{1}{2}}\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1}\right\}, \tag{114c}$$

$$[x_2, v_1] = 2\Phi^{\frac{3}{2}}(\Phi+\xi)^{-3}(\Phi+\eta)^{-1}\left(\frac{d(AB)}{d\zeta}\right)^{-1} \times \left\{2\xi\left[\Phi+\xi+\Phi^{\frac{1}{2}}\xi^{-1}(\alpha\beta)^{\frac{1}{2}}\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1}\right] \times \left(\frac{\partial(A+\eta B)}{\partial\zeta}\right) + (\Phi+\eta)\left(\frac{\partial k_2}{\partial\zeta}\right)\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1} - (A-\eta B)\Phi^{-\frac{1}{2}}\left(\frac{\partial\Phi}{\partial\zeta}\right)(\alpha\beta)^{\frac{1}{2}}\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1}\right\}, \tag{114d}$$

$$[x_2, v_2] = 2\Phi^{\frac{3}{2}}(\Phi+\eta)^{-3}\left(\frac{d(AB)}{d\zeta}\right)^{-1} \times \left[-\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1}\left(\frac{\partial k_2}{\partial\zeta}\right) + 2\eta\frac{\partial(A+\eta B)}{\partial\zeta}\right], \tag{114e}$$

$$[v_1, v_2] = 4\Phi^2(\Phi+\xi)^{-3}(\Phi+\eta)^{-3}\left(\frac{d(AB)}{d\zeta}\right)^{-1} \times \left\{H(\alpha\beta)^{\frac{1}{2}}\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1}\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1}\frac{\partial\Phi}{\partial\zeta} - 2\left[\frac{dA}{d\zeta} - \Phi\left(\frac{dB}{d\zeta}\right)\right]\left[\xi(\Phi+\xi)\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1} + \eta(\Phi+\eta)\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1} + \Phi^{\frac{1}{2}}(\alpha\beta)^{\frac{1}{2}}\left(\frac{\partial^2 f}{\partial\xi^2}\right)^{-1}\left(\frac{\partial^2 g}{\partial\eta^2}\right)^{-1}\right]\right\}, \tag{114f}$$

where k_1, k_2 are defined by

$$k_1 \equiv A\left(\frac{\partial f}{\partial\xi}\right) + B\left[f - \xi\left(\frac{\partial f}{\partial\xi}\right)\right] - C, \tag{115a}$$

$$k_2 \equiv -A\left(\frac{\partial g}{\partial\eta}\right) - B\left[g - \eta\left(\frac{\partial g}{\partial\eta}\right)\right] - C. \tag{115b}$$

Clearly, these Poisson brackets do not, in general, have the values appropriate to the usual free-particle canonical formalism.

V. THE ASYMPTOTIC REGION AND THE UNIQUENESS OF THE HAMILTONIAN FORMULATION

It has been claimed previously[9] that the demand that the Hamiltonian formulation reduce asymptotically to the usual free-particle Hamiltonian formulation fixes the Hamiltonian formulation up to canonical transformation. The present section discusses this in detail for the particular case of two particles in one dimension.

As is clear from the fact that H, P, and K are canonical invariants (Sec. IVC of CF), different choices of the arbitrary functions $A(\zeta)$, $B(\zeta)$, and $C(\zeta)$ yield canonically inequivalent Hamiltonizations. The determination of A, B, and C fixes the canonical formulation.

We demand that the interaction fall off fast enough for the particle velocities to possess limits $v_1, v_2 \to v_{1b}, v_{2b}$ as $t \to -\infty$ before the collision and limits $v_1, v_2 \to v_{1a}, v_{2a}$ as $t \to +\infty$ after the collision. It then follows, from (35) and the fact that Φ is a constant of the motion, that corresponding to these limiting values of the velocities are limiting values ξ_b, η_b and ξ_a, η_a of ξ and η such that

$$v_{1b} = (\Phi-\xi_b)/(\Phi+\xi_b), \quad v_{1a} = (\Phi-\xi_a)/(\Phi+\xi_a), \quad v_{2b} = (\Phi-\eta_b)/(\Phi+\eta_b), \quad v_{2a} = (\Phi-\eta_a)/(\Phi+\eta_a). \tag{116}$$

Under Lorentz transformation, a limiting velocity v transforms according to $v \to v' = (v - \beta)/(1 - v\beta)$, while Φ transforms according to $\Phi \to \Phi' = (1 - \beta) \times (1 + \beta)^{-1}\Phi$. If we now use (116), it follows that ξ_b, η_b, ξ_a, and η_a are invariant under Lorentz transformation. Since Φ and the limiting velocities are invariant under space and time translation, the same is true of ξ_b, η_b, ξ_a, and η_a. Hence ξ_b, η_b, ξ_a, and η_a depend only on ζ.

For free particles, H and P are

$$H_{\text{free}} = \sum_{i=1}^{2} m_i(1 - v_i^2)^{-\frac{1}{2}}, \tag{117a}$$

$$P_{\text{free}} = \sum_{i=1}^{2} m_i v_i(1 - v_i^2)^{-\frac{1}{2}}. \tag{117b}$$

If we insert the limiting values (116) into (117), we find that the demand of asymptotic reduction to free particle form before the collision means that $H, P \to H_b, P_b$ as $t \to -\infty$, where

$$H_b = \tfrac{1}{2}(m_1\xi_b^{\frac{1}{2}} + m_2\eta_b^{\frac{1}{2}})\Phi^{-\frac{1}{2}} + \tfrac{1}{2}(m_1\xi_b^{-\frac{1}{2}} + m_2\eta_b^{-\frac{1}{2}})\Phi^{\frac{1}{2}}, \tag{118a}$$

$$P_b = -\tfrac{1}{2}(m_1\xi_b^{\frac{1}{2}} + m_2\eta_b^{\frac{1}{2}})\Phi^{-\frac{1}{2}} + \tfrac{1}{2}(m_1\xi_b^{-\frac{1}{2}} + m_2\eta_b^{-\frac{1}{2}})\Phi^{\frac{1}{2}}. \tag{118b}$$

Comparison of (118) with (73) yields

$$A(\zeta) = \tfrac{1}{2}\{m_1[\xi_b(\zeta)]^{\frac{1}{2}} + m_2[\eta_b(\zeta)]^{\frac{1}{2}}\}, \tag{119a}$$

$$B(\zeta) = \tfrac{1}{2}\{m_1[\xi_b(\zeta)]^{-\frac{1}{2}} + m_2[\eta_b(\zeta)]^{-\frac{1}{2}}\}. \tag{119b}$$

A corresponding demand of asymptotic reduction to free particle form, as $t \to +\infty$, yields

$$A(\zeta) = \tfrac{1}{2}\{m_1[\xi_a(\zeta)]^{\frac{1}{2}} + m_2[\eta_a(\zeta)]^{\frac{1}{2}}\}, \tag{120a}$$

$$B(\zeta) = \tfrac{1}{2}\{m_1[\xi_a(\zeta)]^{-\frac{1}{2}} + m_2[\eta_a(\zeta)]^{-\frac{1}{2}}\}. \tag{120b}$$

Clearly, (119) and (120) are compatible only if the interactions are such that the total free-particle energy (and momentum) at $t = -\infty$ equals the total free-particle energy (and momentum) at $t = +\infty$. Demanding their compatibility yields

$$\xi_a\xi_b = \eta_a\eta_b \tag{121}$$

and

$$m_1/m_2 = -(\xi_a^{\frac{1}{2}} - \xi_b^{\frac{1}{2}})/(\eta_a^{\frac{1}{2}} - \eta_b^{\frac{1}{2}}). \tag{122}$$

If (121) is satisfied, (122) can be adopted as a definition of the mass ratio of the particles.

For free particles, K is

$$K_{\text{free}} = \sum_{i=1}^{2} m_i(1 - v_i^2)^{-\frac{1}{2}}(x_i - v_i t). \tag{123}$$

The use of (35), (89), (90), and (117) in (123) shows that

$$K_{\text{free}} = \tfrac{1}{2}[H_{\text{free}}(c_1 + c_2) - P_{\text{free}}(c_1 - c_2) + m_1\xi^{-\frac{1}{2}}f(\xi, \zeta) - m_2\eta^{-\frac{1}{2}}g(\eta, \zeta)]. \tag{124}$$

It now follows from (85) and (124) that

$$K - K_{\text{free}} = \tfrac{1}{2}[(H - H_{\text{free}})(c_1 + c_2) - (P - P_{\text{free}})(c_1 - c_2) - (m_1\xi^{-\frac{1}{2}}f - m_2\eta^{-\frac{1}{2}}g)] + C(\zeta). \tag{125}$$

Inasmuch as $|x_i| \to \infty$ and $t \to -\infty$ as $\xi, \eta \to \xi_b, \eta_b$, it is clear from (89) and (90) that $\partial f/\partial\xi$ and $\partial g/\partial\eta$ both become infinite as $\xi, \eta \to \xi_b, \eta_b$. It is then not clear that the quantity $(m_1\xi^{-\frac{1}{2}}f - m_2\eta^{-\frac{1}{2}}g)$ which appears on the right-hand side of (125) has a finite Lorentz-invariant limit as $t \to -\infty$. The behavior of this limit is not determined by the assumption that the particle velocities have finite limits as $t \to -\infty$. A similar problem will arise when we come to consider $\lim [x_1, x_2]$ as $t \to -\infty$. We will first consider these limits under certain additional assumptions which, as will be seen in Sec. VIB, imply that the forces fall off more rapidly than x_{12}^{-2} as $|x_{12}| \to \infty$. To state these additional assumptions, we put

$$f(\xi, \zeta) = F(\xi_0, \zeta), \qquad g(\eta, \zeta) = G(\eta_0, \zeta), \tag{126}$$

where

$$\xi_0 = \xi - \xi_b(\zeta) \quad \text{and} \quad \eta_0 = \eta - \eta_b(\zeta). \tag{127}$$

The assumptions then are

$$\lim_{\xi_0 \to 0} \xi_0 \frac{\partial F}{\partial \xi_0} = 0, \tag{128a}$$

$$\lim_{\eta_0 \to 0} \eta_0 \frac{\partial G}{\partial \eta_0} = 0, \tag{128b}$$

$$\lim_{\xi_0 \to 0} \frac{\partial F}{\partial \zeta} \text{ exists}, \tag{128c}$$

$$\lim_{\eta_0 \to 0} \frac{\partial G}{\partial \zeta} \text{ exists}. \tag{128d}$$

Under the assumptions (128), which exclude the interaction contributions to K which persist in the asymptotic region for long range forces,[10] the demand that $K \to K_{\text{free}}$ as $t \to -\infty$ yields

$$C(\zeta) = \tfrac{1}{2}[m_1\xi_b^{-\frac{1}{2}}F(0, \zeta) - m_2\eta_b^{-\frac{1}{2}}G(0, \zeta)]. \tag{129}$$

The demand $K \to K_{\text{free}}$ as $t \to +\infty$, with restrictions analogous to (128), yields

$$C(\zeta) = \tfrac{1}{2}[m_1\xi_a^{-\frac{1}{2}}f(\xi_a, \zeta) - m_2\eta_a^{-\frac{1}{2}}g(\eta_a, \zeta)]. \tag{130}$$

Clearly, the demand that (129) and (130) be compatible places an additional requirement on f and g.

We turn now to the computation of the asymptotic values of the Poisson brackets among physical

variables. We compute these under the following assumptions:

$$\lim_{\xi_0\to 0}\left(\frac{\partial F}{\partial \xi_0}\right)^{-1}F = 0, \tag{131a}$$

$$\lim_{\xi_0\to 0}\left(\frac{\partial F}{\partial \xi_0}\right)^{-1}\left(\frac{\partial F}{\partial \zeta}\right) = 0, \tag{131b}$$

$$\lim_{\xi_0\to 0}\left(\frac{\partial^2 F}{\partial \xi_0^2}\right)^{-1}\left(\frac{\partial F}{\partial \xi_0}\right) = 0, \tag{131c}$$

$$\lim_{\xi_0\to 0}\left(\frac{\partial^2 F}{\partial \xi_0^2}\right)^{-1}\left(\frac{\partial^2 F}{\partial \xi_0\partial \zeta}\right) = 0, \tag{131d}$$

$$\lim_{\eta_0\to 0}\left(\frac{\partial G}{\partial \eta_0}\right)^{-1}G = 0, \tag{131e}$$

$$\lim_{\eta_0\to 0}\left(\frac{\partial G}{\partial \eta_0}\right)^{-1}\left(\frac{\partial G}{\partial \zeta}\right) = 0, \tag{131f}$$

$$\lim_{\eta_0\to 0}\left(\frac{\partial^2 G}{\partial \eta_0^2}\right)^{-1}\left(\frac{\partial G}{\partial \eta_0}\right) = 0, \tag{131g}$$

$$\lim_{\eta_0\to 0}\left(\frac{\partial^2 G}{\partial \eta_0^2}\right)^{-1}\left(\frac{\partial^2 G}{\partial \eta_0\partial \zeta}\right) = 0, \tag{131h}$$

$$\frac{d\xi_b}{d\zeta},\quad \frac{d\eta_b}{d\zeta},\quad \text{and}\quad \frac{dC}{d\zeta}\quad \text{are finite,} \tag{131i}$$

the second partial derivatives of F (of G) exist in a

deleted neighborhood of $\xi_0 = 0$ (of $\eta_0 = 0$). (131j)

It follows from (115), with the aid of (119), (126), (127), and (131), that

$$\lim_{\xi\to\xi_b}\left(\frac{\partial^2 f}{\partial \xi^2}\right)^{-1}\left(\frac{\partial k_1}{\partial \zeta}\right) = -\tfrac{1}{2}m_2\eta_b^{-\frac{1}{2}}(\eta_b - \xi_b)\left(\frac{d\xi_b}{d\zeta}\right), \tag{132a}$$

$$\lim_{\eta\to\eta_b}\left(\frac{\partial^2 g}{\partial \eta^2}\right)^{-1}\left(\frac{\partial k_2}{\partial \zeta}\right) = -\tfrac{1}{2}m_1\xi_b^{-\frac{1}{2}}(\eta_b - \xi_b)\left(\frac{d\eta_b}{d\zeta}\right). \tag{132b}$$

It follows, from (28a), (32), (34), (126), (127), (131a), (131e), and the fact that Φ is a constant of the motion, that

$$\lim_{t\to-\infty}\frac{(\partial f/\partial \xi)}{(\partial g/\partial \eta)} = -\frac{(\Phi + \eta_b)}{(\Phi + \xi_b)}, \tag{133a}$$

$$\lim_{t\to-\infty}\frac{(\Phi + \eta)(\alpha\beta)^{\frac{1}{2}}}{(\partial f/\partial \xi)} = -\lim_{t\to-\infty}\frac{(\Phi + \xi)(\alpha\beta)^{\frac{1}{2}}}{(\partial g/\partial \eta)} = (\eta_b - \xi_b)\Phi^{\frac{1}{2}}. \tag{133b}$$

The fact that Φ and ζ are constants of the motion implies that $\partial\Phi/\partial\zeta$ [guaranteed to be finite by (131j)] is a constant of the motion. Explicit computation using (28a), (32), (34), (126), (127), and (131) shows that

$$\lim_{t\to-\infty}\frac{(\alpha\beta)^{\frac{1}{2}}(\partial\Phi/\partial\zeta)}{\Phi^{\frac{1}{2}}(\Phi + \xi)(\partial^2 f/\partial\xi^2)(d\xi_b/d\zeta)} = 1 + \lim_{t\to-\infty}\frac{(\Phi + \eta_b)(\partial^2 g/\partial\eta^2)(d\eta_b/d\zeta)}{(\Phi + \xi_b)(\partial^2 f/\partial\xi^2)(d\xi_b/d\zeta)}. \tag{134}$$

But the left-hand side of (134) is zero as a consequence of (131c) and (133b). Hence,

$$\lim_{t\to-\infty}\frac{(\partial^2 g/\partial\eta^2)}{(\partial^2 f/\partial\xi^2)} = -\frac{(\Phi + \xi_b)(d\xi_b/d\zeta)}{(\Phi + \eta_b)(d\eta_b/d\zeta)}. \tag{135}$$

It now follows from (35), (114), (120), (131), (132), (133), and (135) that

$$\lim_{t\to-\infty}[x_1, v_1] = m_1^{-1}(1 - v_1^2)^{\frac{3}{2}}, \tag{136a}$$

$$\lim_{t\to-\infty}[x_1, v_2] = 0, \tag{136b}$$

$$\lim_{t\to-\infty}[x_2, v_1] = 0, \tag{136c}$$

$$\lim_{t\to-\infty}[x_2, v_2] = m_2^{-1}(1 - v_2^2)^{\frac{3}{2}}, \tag{136d}$$

$$\lim_{t\to-\infty}[v_1, v_2] = 0. \tag{136e}$$

Nowhere in the derivation of the result (136) has the assumption (128) been used. If, however, we adopt (128) and hence (129), it can be easily shown that

$$\lim_{t\to-\infty}[x_1, x_2] = 0. \tag{137}$$

The limiting values (136) and (137) of the Poisson brackets are just the values which these brackets have in the usual free-particle canonical formulation of relativistic mechanics. Thus, with the added assumption (128), our canonical formulation goes over completely into the usual free-particle canonical formulation as $t\to-\infty$; in particular, physical coordinates can be canonical asymptotically. A similar analysis can be given for $t\to+\infty$. The important special case of electrodynamics, which violates (128), is considered in Sec. VIC.

VI. EXAMPLES

A. Kerner's Example

A simple example, given by Kerner,[11] was considered in Sec. VB of CF. We obtain here the particular $f(\xi, \zeta)$ and $g(\eta, \zeta)$ which correspond to this example, thus exhibiting concretely the relation between the present work and that of CF. The equations of motion of Kerner's example are

$$-a_1 = a_2 = (v_1 - v_2)^2/(2x_{12}). \tag{138}$$

The use of (3), (4), (35), (37), and (38) to transform (138) into the variables ξ, η, and ζ yields

$$\frac{\partial^2 f}{\partial\xi^2} = 2(\alpha + \eta\beta)^2(\alpha + \beta\xi)^{-1}(\eta - \xi)^{-2}, \tag{139a}$$

$$\frac{\partial^2 g}{\partial\eta^2} = 2(\alpha + \beta\xi)^2(\alpha + \beta\eta)^{-1}(\eta - \xi)^{-2}, \tag{139b}$$

where α and β are given by (32) and (34). The result (139) is a pair of partial differential equations for the particular f and g which yield the dynamics (138). This pair is solved in Appendix C; the result is

$$f(\xi, \zeta) = \xi f_1(\zeta) + f_2(\zeta) + f_3(\zeta)[\xi - w(\zeta)]^{-1}, \quad (140a)$$

$$g(\eta, \zeta) = -\eta f_1(\zeta) - f_2(\zeta) - f_3(\zeta)[\eta - w(\zeta)]^{-1}. \quad (140b)$$

Clearly, the result (140) exhibits the redundancy discussed at the end of Sec. II: the form of (140) is invariant under the transformation (62). All of the results of Sec. VB of CF can be deduced by inserting (140) in the general results of the present paper.

B. Asymptotic Force Laws

By setting $e_2 = 0$ in $\mathfrak{L}_1$ and solving Eq. (1a), it can be shown that, for forces which fall off faster than x_{12}^{-1} asymptotically,

$$e_1 \xrightarrow[|x_{12}|\to\infty]{} e_{10}[x_{12}(1 - v_{2b}^2)^{-\frac{1}{2}}, \zeta_0], \quad (141)$$

where

$$\zeta_0 \equiv (1 - v_{1b}v_{2b})(1 - v_{1b}^2)^{-\frac{1}{2}}(1 - v_{2b}^2)^{-\frac{1}{2}}. \quad (142)$$

By using (35), (38a), and (133b) in (141) and (142), we can relate e_{10} to the behavior of f as $\xi \to \xi_b$:

$$\lim_{\xi\to\xi_b} 2\xi_b^{\frac{3}{2}} e_{10}\left(\left|\frac{(\xi_b - \eta_b)}{2\eta_b^{\frac{1}{2}}}\frac{\partial f}{\partial \xi}\right|, \zeta_0\right)\frac{\partial^2 f}{\partial \xi^2} = -1, \quad (143)$$

$$\zeta_0 = \tfrac{1}{2}(\xi_b^{\frac{1}{2}}\eta_b^{-\frac{1}{2}} + \xi_b^{-\frac{1}{2}}\eta_b^{\frac{1}{2}}). \quad (144)$$

If e_{10} is known, (143) can be used to deduce the dominant part of the singularity of $\partial f/\partial \xi$ as $\xi \to \xi_b$; with f known, (143) can be used to deduce the asymptotic force law. A similar analysis for e_2 shows that

$$e_2 \xrightarrow[|x_{12}|\to\infty]{} e_{20}[x_{12}(1 - v_{1b}^2)^{-\frac{1}{2}}, \zeta_0] \quad (145)$$

and

$$\lim_{\eta\to\eta_b} 2\eta_b^{\frac{3}{2}} e_{20}\left[\left|\frac{(\xi_b - \eta_b)}{2\xi_b^{\frac{1}{2}}}\frac{\partial g}{\partial \eta}\right|, \zeta_0\right]\frac{\partial^2 g}{\partial \eta^2} = 1. \quad (146)$$

We now consider the special case of power-law forces. Suppose

$$e_{10} = x_{12}^{-n}(1 - v_2^2)^{\frac{1}{2}n}\mu(\zeta_0), \quad (147)$$

Eq. (147) can then be used in (143) to show that

$$\lim_{\xi\to\xi_b}(\xi - \xi_b)^{1/(n-1)}\frac{\partial f}{\partial \xi} = \left(\frac{\eta - 1}{2\xi_b^{\frac{3}{2}}\mu(\zeta_0)}\right)^{-1/(n-1)}\left|\frac{2\eta_b^{\frac{1}{2}}}{\xi_b - \eta_b}\right|^{n/(n-1)} \quad (148)$$

We see from (148) that for $\eta \leq 2$, which includes the physically important case of electrodynamics, the condition (128) does not hold, so that $C(\zeta)$ cannot be evaluated from (129).

C. Electrodynamics

In the electrodynamic problem of two 3-dimensional point particles whose motion is confined to one dimension as a consequence of the initial data,[12]

$$e_{10} = (e_1e_2/m_1)(1 - v_2^2)x_{12}^{-2}, \quad (149a)$$

$$e_{20} = -(e_1e_2/m_2)(1 - v_1^2)x_{12}^{-2}. \quad (149b)$$

The use of Eqs. (141)–(149) then shows that, for this electrodynamic problem,

$$\lim_{\xi\to\xi_b}(\xi - \xi_b)\frac{\partial f}{\partial \xi} = \frac{8e_1e_2\xi_b^{\frac{3}{2}}\eta_b}{m_1(\xi_b - \eta_b)^2}, \quad (150a)$$

$$\lim_{\eta\to\eta_b}(\eta - \eta_b)\frac{\partial g}{\partial \eta} = \frac{8e_1e_2\xi_b\eta_b^{\frac{3}{2}}}{m_2(\xi_b - \eta_b)^2}. \quad (150b)$$

From (150) it follows that

$$f(\xi, \zeta) = \frac{8e_1e_2\xi_b^{\frac{3}{2}}\eta_b}{m_1(\xi_b - \eta_b)^2}\ln|\xi - \xi_b| + F_0(\xi - \xi_b, \zeta), \quad (151a)$$

$$g(\eta, \zeta) = \frac{8e_1e_2\xi_b\eta_b^{\frac{3}{2}}}{m_2(\xi_b - \eta_b)^2}\ln|\eta - \eta_b| + G_0(\eta - \eta_b, \zeta), \quad (151b)$$

where F_0 and G_0 satisfy the conditions (128). We are now in a position to see the existence of an asymptotic interaction contribution to K. From (151) it follows that

$$\tfrac{1}{2}(m_1\xi^{-\frac{1}{2}}f - m_2\eta^{-\frac{1}{2}}g) = 4e_1e_2\frac{\xi_b\eta_b}{(\xi_b - \eta_b)^2}\ln\left|\frac{(\xi - \xi_b)}{(\eta - \eta_b)}\right| + F_1(\xi, \eta, \zeta), \quad (152)$$

where

$$\lim_{t\to-\infty} F_1 = \tfrac{1}{2}[m_1\xi_b^{-\frac{1}{2}}F_0(0, \zeta) - m_2\eta_b^{-\frac{1}{2}}G_0(0, \zeta)]. \quad (153)$$

The use of (133a) and (151)–(153) in (125) yields

$$\lim_{\to-\infty}(K - K_{\text{free}}) = \frac{4e_1e_2\xi_b\eta_b}{(\xi_b - \eta_b)^2}\ln\left|\frac{m_1\eta_b^{\frac{1}{2}}(\Phi + \eta_b)}{m_2\xi_b^{\frac{1}{2}}(\Phi + \xi_b)}\right| - \tfrac{1}{2}[m_1\xi_b^{-\frac{1}{2}}F_0(0, \zeta) - m_2\eta_b^{-\frac{1}{2}}G_0(0, \zeta)] + C(\zeta). \quad (154)$$

Inasmuch as the right-hand side of (154) depends on the non-Lorentz-invariant quantity Φ, this limit cannot be made to vanish in every reference frame.

There is one distinguished frame, namely the center-of-momentum frame. By setting $P_b = 0$ in (118b), we see that, in the center-of-momentum frame, $\Phi = \Phi_{cp}$, where

$$\Phi_{cp} \equiv (m_1\xi_b^{\frac{1}{2}} + m_2\eta_b^{\frac{1}{2}})/(m_1\xi_b^{-\frac{1}{2}} + m_2\eta_b^{-\frac{1}{2}}). \quad (155)$$

We choose to write $C(\zeta)$ in the form

$$C(\zeta) = \frac{4e_1e_2\xi_b\eta_b}{(\xi_b - \eta_b)^2} \ln\left|\frac{m_2\xi_b^{\frac{1}{2}}(\Phi_{cp} + \xi_b)}{m_1\eta_b^{\frac{1}{2}}(\Phi_{cp} + \eta_b)}\right| + \tfrac{1}{2}[m_1\xi_b^{-\frac{1}{2}}F_0(0, \zeta) - m_2\eta_b^{-\frac{1}{2}}G_0(0, \zeta)] + C_0(\zeta). \quad (156)$$

By the use of (35), (144), and (156) in (154), we obtain

$$\begin{aligned}\lim_{t\to-\infty}(K - K_{free}) &= \frac{4e_1e_2\xi_b\eta_b}{(\xi_b - \eta_b)^2} \ln\left|\frac{(\Phi + \eta_b)(\Phi_{cp} + \xi_b)}{(\Phi + \xi_b)(\Phi_{cp} + \eta_b)}\right| + C_0(\zeta) \\ &= \frac{e_1e_2(1 - v_{1b}^2)(1 - v_{2b}^2)}{(v_{1b} - v_{2b})^2} \ln\left|\frac{(1 - v_{1b}^2)^{\frac{1}{2}}(m_1 + m_2\zeta_0)}{(1 - v_{2b}^2)^{\frac{1}{2}}(m_1\zeta_0 + m_2)}\right| + C_0(\zeta). \quad (157)\end{aligned}$$

Clearly, the choice $C_0(\zeta) = 0$ corresponds to the vanishing of this limit in the center-of-momentum frame.[13] The long range of electrodynamic forces also gives rise to an asymptotic interaction contribution to $[x_1, x_2]$. The use of (116), (119), (133a), (144), (151), (155), and (156) in (114a) shows that

$$\begin{aligned}\lim_{t\to-\infty}[x_1, x_2] &= \frac{32\Phi e_1e_2\xi_b^{\frac{3}{2}}\eta_b^{\frac{3}{2}}}{(\Phi + \xi_b)(\Phi + \eta_b)m_1m_2(\xi_b - \eta_b)^2} \\ &\times \left[-\left(\frac{\xi_b + \eta_b}{\xi_b - \eta_b}\right) \ln\left|\frac{(\Phi_{cp} + \xi_b)(\Phi + \eta_b)}{(\Phi + \xi_b)(\Phi_{cp} + \eta_b)}\right| + (\Phi - \Phi_{cp})\left(\frac{\xi_b}{(\Phi + \xi_b)(\Phi_{cp} + \xi_b)} + \frac{\eta_b}{(\Phi + \eta_b)(\Phi_{cp} + \eta_b)}\right)\right] \\ &+ \frac{\Phi(\xi_b - \eta_b)(dC_0/d\zeta)}{(\Phi + \xi_b)(\Phi + \eta_b)[d(AB)/d\zeta]} \\ &= \frac{2e_1e_2(1 - v_{1b}^2)^{\frac{3}{2}}(1 - v_{2b}^2)^{\frac{3}{2}}}{m_1m_2(v_{1b} - v_{2b})^2} \\ &\times \left[\left(\frac{1 - v_{1b}v_{2b}}{v_{1b} - v_{2b}}\right) \ln\left|\frac{(1 - v_{1b}^2)^{\frac{1}{2}}(m_1 + m_2\zeta_0)}{(1 - v_{2b}^2)^{\frac{1}{2}}(m_1\zeta_0 + m_2)}\right| + \tfrac{1}{2}(v_{1b} + v_{2b}) + \frac{(v_{1b} - v_{2b})}{2(1 - v_{1b}^2)^{\frac{1}{2}}(1 - v_{2b}^2)^{\frac{1}{2}}} \times \left(\frac{m_2}{m_1 + m_2\zeta_0} - \frac{m_1}{m_1\zeta_0 + m_2}\right)\right] \\ &- \tfrac{1}{2}(v_{1b} - v_{2b})[dC_0/d\zeta][d(AB)/d\zeta]^{-1}. \quad (158)\end{aligned}$$

The fact that the right-hand side of (158) depends on Φ makes it clear that $\lim [x_1, x_2]$ as $t \to -\infty$ cannot vanish in every Lorentz frame. The choice $C_0(\zeta) =$ const, however, will make it vanish in the center-of-momentum frame. All of the other Poisson brackets among physical variables do approach their free-particle values asymptotically: the results (136) were obtained without the assumption (128) which is violated for electrodynamics. What significance, if any, is to be attached to the survival of an asymptotic interaction contribution to $[x_1, x_2]$ is not clear at present.

VII. SUMMARY

The differential conditions which guarantee world-line invariance and form invariance of the equations of motion for a Lorentz-invariant instantaneous action-at-a-distance theory form a set of coupled nonlinear partial differential equations. The general solution of these equations has been obtained for the special case of two particles in one dimension. The result is given by Eqs. (3), (4), (32), (34), (35), (37), and (38); it has been summarized following equation (38). The solution is expressed in variables ξ, η, and ζ. Because the arbitrary functions defining the solution appear both in the solution and in the transformation between ξ, η, and ζ and the physical variables x_{12}, v_1, and v_2, there is a possible redundancy. The result of analyzing this redundancy is given in Eq. (62) and in the discussion immediately preceding (62).

The equations of motion for the general 2-particle 1-dimensional case have been integrated to obtain the particle world lines in parametric form [Eqs. (89) and (90)]. World-line invariance has been explicitly demonstrated.

In Sec. IV the general dynamics is cast into a Hamiltonian form wherein the transformations of the inhomogeneous Lorentz group are canonical. The canonical variables are given as functions of ξ, η, ζ, and $X = \frac{1}{2}(x_1 + x_2)$ by Eqs. (73), (93), (96), (106), and (112). The generators H, P, and K are given as functions of ξ, η, ζ, X, and t by Eqs. (73), (75), and (78) and as functions of the canonical variables by (91) and (113). The Poisson brackets among the physical variables x_i and v_i have been calculated as functions of ξ, η, and ζ; the results are given by Eqs. (114) and (115).

The Hamiltonian formulation obtained is not unique up to canonical transformation; it depends on arbitrary functions $A(\zeta)$, $B(\zeta)$, and $C(\zeta)$. Different choices of A, B, and C yield canonically inequivalent Hamiltonian formulations. In Sec. V the functions A, B, and C have been determined by the demand that the Hamiltonian formulation go over into the

usual free-particle one asymptotically for the case of interactions which fall off faster than x_{12}^{-2}. The result is given by Eqs. (116), (119), (120), (129), and (130). The Poisson brackets among physical variables have been shown to go over into their free-particle values asymptotically.

The analysis of asymptotic behavior for the electrodynamic case, where the interaction falls off as x_{12}^{-2}, revealed that the generator K and the Poisson bracket $[x_1, x_2]$ have interaction pieces which survive asymptotically [Eqs. (157) and (158)]. These surviving pieces are not Lorentz invariant; this makes it impossible to fix $C(\zeta)$ by the demand of asymptotic reduction to free-particle form in every Lorentz frame. $C(\zeta)$ can be determined for this case by the demand of asymptotic reduction to free particle form in the center-of-momentum frame; there are then surviving interaction pieces in all other frames. The surviving interaction piece of K then agrees (after correction of an error) with that found by Van Dam and Wigner.[10,13]

VIII. ACKNOWLEDGMENTS

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APPENDIX A: THE CASE $\mathfrak{L}_1$ PROPORTIONAL TO $\mathfrak{L}_2$

The analysis of Sec. II excluded the case $\mathfrak{L}_1$ proportional to $\mathfrak{L}_2$, which is considered here. We assume

$$\mathfrak{L}_1 = \lambda(x_{12}, v_1, v_2)\mathfrak{L}_2. \tag{A1}$$

It follows from (A1) by using (2) that

$$v_2 = \lambda v_1, \tag{A2}$$

$$1 = \lambda[1 - x_{12}e_1(1 - v_1^2)^{\frac{1}{2}}], \tag{A3}$$

$$[1 + x_{12}e_2(1 - v_2^2)^{\frac{1}{2}}] = \lambda. \tag{A4}$$

Solving for e_1 and e_2, we obtain

$$\begin{aligned} e_1 &= x_{12}^{-1}(1 - v_1^2)^{-\frac{1}{2}}[1 - (v_1/v_2)], \\ e_2 &= -x_{12}^{-1}(1 - v_2^2)^{-\frac{1}{2}}[1 - (v_2/v_1)]. \end{aligned} \tag{A5}$$

It can be easily verified that the pair (A5) are solutions of (1); in fact, they specify the dynamics considered in Sec. VC of CF.

In CF it was claimed that the dynamics of (A5) could not be cast into Hamiltonian form with all of the transformations of the inhomogeneous Lorentz group canonical. The argument advanced for this claim excluded only those canonical representations with vanishing neutral elements; it is, in fact, possible to have a canonical formulation of this dynamics wherein the inhomogeneous Lorentz group is canonically represented with a nonvanishing neutral element as will now be shown. To show this, we begin by replacing (63) with

$$[H, P] = \mu, \quad [H, K] = -P, \quad [P, K] = -H. \tag{A6}$$

The ensuing generalizations of (65) and (66) can then be written out and easily solved; the result is

$$\begin{aligned} H &= \mu(x_1v_1 - x_2v_2)(v_1 - v_2)^{-1}, \\ P &= \mu[t + v_1v_2x_{12}(v_1 - v_2)^{-1}], \\ K &= \tfrac{1}{2}\mu(H^2 - P^2) + k, \end{aligned} \tag{A7}$$

where k is any constant of the motion invariant under time translation, space translation, and Lorentz transformation. By writing out Eqs. (CF-4), and (CF-20) for each of these three transformations, it can be shown that k must be independent of all of the dynamical variables. Hence, we set $k = 0$.

In order to find the canonical formulation, we use variables $y_0 = t$, $y_1 = (x_1v_1 - x_2v_2)(v_1 - v_2)^{-1}$, $y_2 = x_{12}$, $y_3 = v_1$, and $y_4 = v_2$. The writing out of Eqs. (CF-4) and (CF-20) then yields

$$\begin{aligned} \Gamma_{0i} &= -\Gamma_{i0} = -\frac{\partial H}{\partial y_i}, \\ \Gamma_{1i} &= -\Gamma_{i1} = \frac{\partial P}{\partial y_i}, \\ \Gamma_{23} &= -\Gamma_{32} = -(y_2y_3)^{-1}(1 - y_4^2)\Gamma_{34}, \\ \Gamma_{24} &= -\Gamma_{42} = (y_2y_4)^{-1}(1 - y_3^2)\Gamma_{34}. \end{aligned} \tag{A8}$$

By writing out the integrability condition (CF-21) for $(i, j, k) = (2, 3, 4)$ and using (A8), it can be shown that Γ_{34} has the form

$$\Gamma_{34} = 2y_3^2y_4^2(y_3^2 - y_4^2)^{-2}z_1\frac{\partial G(z_1, z_2)}{\partial z_1}, \tag{A9}$$

where

$$\begin{aligned} z_1 &\equiv y_2^2(y_3 + y_4)(y_3 - y_4)^{-1}, \\ z_2 &\equiv (y_3^2 + y_4^2 - 2y_3^2y_4^2)(y_3^2 - y_4^2)^{-1}, \end{aligned} \tag{A10}$$

and G is an arbitrary function of the two indicated variables. Different choices of μ and G yield canonically inequivalent Hamiltonizations. With the Γ_{ij} given by (A8) and (A9), a set of U_i can be found and Pfaff's problem solved. A particular solution yields for coordinates and momenta

$$\begin{aligned} q_1 &= (x_1v_1 - x_2v_2)(v_1 - v_2)^{-1}, \\ p_1 &= \mu x_{12}v_1v_2(v_1 - v_2)^{-1}, \\ q_2 &= z_2, \\ p_2 &= G(z_1, z_2), \end{aligned}$$

with generators $H = \mu q_1$, $P = \mu t + p_1$, and $K = \frac{1}{2}\mu^{-1}(H^2 - P^2)$. The general solution (for given μ and G) is obtained by making an arbitrary canonical transformation.

APPENDIX B: THE CHOICES OF f AND g FOR WHICH $J \equiv \frac{\partial(x_{12}, v_1, v_2)}{\partial(\xi, \eta, \zeta)}$ IS IDENTICALLY ZERO OR INFINITY

We investigate first the case in which J is zero as a consequence of J_1 vanishing identically. If $J_1 \equiv 0$, then also $\partial^2 J_1/\partial\xi\partial\eta \equiv 0$. Using (41), we find

$$\frac{\partial^2 J_1}{\partial\xi\partial\eta} = (\xi - \eta)\left[\left(\xi\frac{\partial^3 f}{\partial\xi^3} + \frac{3}{2}\frac{\partial^2 f}{\partial\xi^2}\right)\frac{\partial^3 g}{\partial\eta^2\partial\zeta} - \left(\eta\frac{\partial^3 g}{\partial\eta^3} + \frac{3}{2}\frac{\partial^2 g}{\partial\eta^2}\right)\frac{\partial^3 f}{\partial\xi^2\partial\zeta}\right]. \quad \text{(B1)}$$

It now follows from (B1) by use of the standard argument for separating variables that $\partial^2 J_1/\partial\xi\partial\eta = 0$ if and only if

$$\xi\frac{\partial^3 f}{\partial\xi^3} + \frac{3}{2}\frac{\partial^2 f}{\partial\xi^2} = \theta(\zeta)\frac{\partial^3 f}{\partial\xi^2\partial\zeta} \quad \text{(B2)}$$

and

$$\eta\frac{\partial^3 g}{\partial\eta^3} + \frac{3}{2}\frac{\partial^2 g}{\partial\eta^2} = \theta(\zeta)\frac{\partial^3 g}{\partial\eta^2\partial\zeta}, \quad \text{(B3)}$$

where the "separation constant" θ depends only on ζ. The general solution to Eq. (B2) is found by integrating twice with respect to ξ and then applying standard methods for first-order equations; the result is

$$f = \xi^{\frac{1}{2}}h_1[\xi h_2(\zeta)] + \xi h_3(\zeta) + h_4(\zeta). \quad \text{(B4)}$$

Here h_1, h_3, and h_4 are arbitrary functions; h_2 is related to $\theta(\zeta)$ by

$$h_2(\zeta) - \theta(\zeta)h_2'(\zeta) = 0. \quad \text{(B5)}$$

Similarly, the general solution of Eq. (B3) is

$$g = \eta^{\frac{1}{2}}h_5[\eta h_2(\zeta)] + \eta h_6(\zeta) + h_7(\zeta), \quad \text{(B6)}$$

where h_5, h_6, and h_7 are arbitrary. If (B4) and (B6) are now inserted in the definition (41) of J_1, we obtain

$$\begin{aligned} J_1 = {} & [\tfrac{1}{2}(h_4 + h_7)h_2' + (h_4' + h_7')h_2] \\ & \times [\tfrac{3}{2}\xi^{\frac{1}{2}}h_1' + \xi^{\frac{3}{2}}h_1''h_2 + \tfrac{3}{2}\eta^{\frac{1}{2}}h_5' + \eta^{\frac{3}{2}}h_5''h_2] \\ & + [-\tfrac{1}{2}(h_3 + h_6)h_2' + (h_3' + h_6')h_2] \\ & \times [\tfrac{1}{2}\xi^{\frac{3}{2}}h_1' + \xi^{\frac{5}{2}}h_1''h_2 + \tfrac{1}{2}\eta^{\frac{3}{2}}h_5' + \eta^{\frac{5}{2}}h_5''h_2] \\ & + \tfrac{1}{2}[(h_3 + h_6)(h_4' + h_7') + (h_4 + h_7)(h_3' + h_6')]. \end{aligned} \quad \text{(B7)}$$

From (B7),

$$\begin{aligned} \frac{\partial J_1}{\partial\xi} = {} & [\tfrac{1}{2}(h_4 + h_7)h_2' + (h_4' + h_7')h_2] \\ & \times (\tfrac{3}{4}\xi^{-\frac{1}{2}}h_1' + 3\xi^{\frac{1}{2}}h_1''h_2 + \xi^{\frac{3}{2}}h_1'''h_2^2) \\ & + [-\tfrac{1}{2}(h_3 + h_6)h_2' + (h_3' + h_6')h_2] \\ & \times (\tfrac{3}{4}\xi^{\frac{1}{2}}h_1' + 3\xi^{\frac{3}{2}}h_1'h_2 + \xi^{\frac{5}{2}}h_1'''h_2^2), \end{aligned} \quad \text{(B8)}$$

$$\begin{aligned} \frac{\partial J_1}{\partial\eta} = {} & [\tfrac{1}{2}(h_4 + h_7)h_2' + (h_4' + h_7')h_2] \\ & \times (\tfrac{3}{4}\eta^{-\frac{1}{2}}h_5' + 3\eta^{\frac{1}{2}}h_5''h_2 + \eta^{\frac{3}{2}}h_5'''h_2^2) \\ & + [-\tfrac{1}{2}(h_3 + h_6)h_2' + (h_3' + h_6')h_2] \\ & \times (\tfrac{3}{4}\eta^{\frac{1}{2}}h_5' + 3\eta^{\frac{3}{2}}h_5''h_2 + \eta^{\frac{5}{2}}h_5'''h_2^2). \end{aligned} \quad \text{(B9)}$$

The investigation of $J_1 \equiv 0$ now breaks up into two cases:

$$\text{Case I} \quad \begin{cases} \tfrac{1}{2}(h_4 + h_7)h_2' + (h_4' + h_7')h_2 = 0, \\ -\tfrac{1}{2}(h_3 + h_6)h_2' + (h_3' + h_6')h_2 = 0, \\ (h_3 + h_6)(h_4' + h_7') + (h_4 + h_7)(h_3' + h_6') = 0 \end{cases} \quad \text{(B10)}$$

or

$$\text{Case II} \quad \begin{cases} \tfrac{3}{4}h_1' + 3\xi h_2 h_1'' + (\xi h_2)^2 h_1''' = 0, \\ \tfrac{3}{4}h_5' + 3\eta h_2 h_5'' + (\eta h_2)^2 h_5''' = 0. \end{cases} \quad \text{(B11)}$$

Equations (B10) are easily integrated to obtain, for Case I,

$$\begin{aligned} & h_2(h_4 + h_7)^2 = \text{const}, \\ & h_2^{-1}(h_3 + h_6)^2 = \text{const} \quad \text{for} \quad h_2 \neq 0, \\ & (h_3 + h_6)(h_4 + h_7) = \text{const}. \end{aligned} \quad \text{(B12)}$$

The relations (B12) are clearly sufficient to guarantee the vanishing of J_1 as given by (B7). Equations (B11) can also be easily integrated to obtain

$$\begin{aligned} h_1[\xi h_2(\zeta)] &= C_1[\xi h_2(\zeta)]^{\frac{1}{2}} + C_2[\xi h_2(\zeta)]^{-\frac{1}{2}} + C_3, \\ h_5[\eta h_2(\zeta)] &= C_4[\eta h_2(\zeta)]^{\frac{1}{2}} + C_5[\xi h_2(\zeta)]^{-\frac{1}{2}} + C_6. \end{aligned} \quad \text{(B13)}$$

The use of (B13) in (B7) yields

$$\begin{aligned} J_1 = {} & [\tfrac{1}{2}(h_4 + h_7)h_2' + (h_4' + h_7')h_2][\tfrac{1}{2}(C_1 + C_4)h_2^{-\frac{1}{2}}] \\ & + [-\tfrac{1}{2}(h_3 + h_6)h_2' + (h_3' + h_6')h_2] \\ & \times [\tfrac{1}{2}(C_2 + C_5)h_2^{-\frac{3}{2}}] \\ & + \tfrac{1}{2}[(h_3 + h_6)(h_4' + h_7') + (h_4 + h_7)(h_3' + h_6')]. \end{aligned}$$

Integrating, we find that $J_1 = 0$ if

$$\begin{aligned} & (C_1 + C_4)(h_4 + h_7)h_2^{\frac{1}{2}} + (C_2 + C_5)(h_3 + h_6)h_2^{-\frac{1}{2}} \\ & \qquad + (h_3 + h_6)(h_4 + h_7) = \text{const}. \end{aligned} \quad \text{(B14)}$$

The cases where $J \equiv 0$ because either $\alpha \equiv 0$ or $\beta \equiv 0$ have already been included in (B4) and (B6) as special cases: $\alpha \equiv 0$ if $h_1 = h_5 = 0$ and $h_4 = -h_7$; $\beta \equiv 0$ if $h_1 = h_5 = 0$ and $h_3 = -h_6$. The case where

J is infinite because $\alpha + \beta\xi \equiv 0$ or $\alpha + \beta\eta \equiv 0$ has also been included, since either of these factors can vanish identically only if $\alpha \equiv 0$ and $\beta \equiv 0$.

APPENDIX C: POISSON BRACKETS AMONG PHYSICAL VARIABLES

The computation of Poisson brackets involving physical coordinates can be simplified by using Eqs. (21), (73a), (75), and (78) to write

$$x_i = H^{-1}(K + Pt + k_i), \tag{C1}$$

where k_1, k_2 are defined by (113). It now follows from (C1) (and the fact that H, P, and K generate respectively the infinitesimal space, time, and Lorentz transformations) that, for any function w,

$$[x_i, w] = H^{-1}\{x_i L_{\mathrm{CTT}} w - tL_{\mathrm{ST}} w - L_{\mathrm{LT}} w + [k_i, w]\}. \tag{C2}$$

The use of (C2), (28a), (32), (34), (35), (37), (64), (67), (68), (73a), and (115) now yields

$$[x_1, x_2] = H^{-1}x_{12}(v_1 + v_2) + H^{-2}(A\beta - B\alpha + [k_1, k_2]), \tag{C3}$$

$$[x_1, v_1] = 2H^{-1}(\Phi + \xi)^{-2}(2\Phi\xi - \Phi[k_1, \xi] + \xi[k_1, \Phi]), \tag{C4}$$

$$[x_1, v_2] = H^{-1}\{x_{12}a_2 + 2(\Phi + \eta)^{-2}(2\Phi\eta - \Phi[k_1, \eta] + \eta[k_1, \Phi])\}, \tag{C5}$$

$$[x_2, v_1] = H^{-1}\{-x_{12}a_1 + 2(\Phi + \xi)^{-2}(2\Phi\xi - \Phi[k_2, \xi] + \xi[k_2, \Phi])\}, \tag{C6}$$

$$[x_2, v_2] = 2H^{-1}(\Phi + \eta)^{-2}(2\Phi\eta - \Phi[k_2, \eta] + \eta[k_2, \Phi]), \tag{C7}$$

$$[v_1, v_2] = 4(\Phi + \xi)^{-2}(\Phi + \eta)^{-2}\Phi(-\xi[\Phi, \eta] + \eta[\Phi, \xi] + \Phi[\xi, \eta]). \tag{C8}$$

The Poisson brackets which appear on the right-hand sides of (C3)–(C8) require for their computation a knowledge of the brackets $[\xi, \eta] = [y_2, y_3]$, $[\xi, \zeta] = [y_2, y_4]$, and $[\eta, \zeta] = [y_3, y_4]$; by using the relation (75) and the generators, we have avoided the need to compute $[y_i, y_j]$ explicitly. The needed brackets can be computed by inverting the matrix of the Γ_{ij} [see Sec. IA and Eq. (78) of CF]; the result is

$$\begin{aligned}[\xi, \eta] &= -\Gamma_{14}/\Gamma,\\ [\xi, \zeta] &= \Gamma_{13}/\Gamma,\\ [\eta, \zeta] &= -\Gamma_{12}/\Gamma,\end{aligned} \tag{C9}$$

where $\Gamma \equiv -\Gamma_{12}\Gamma_{34} + \Gamma_{13}\Gamma_{24} - \Gamma_{14}\Gamma_{23}$. Explicit computation, using (28a), (32), (34), (73), (96), (101b), (102), and (107) yields

$$\Gamma = -\tfrac{1}{2}\beta^{-1}\Phi^{-\frac{3}{2}}(\Phi + \xi)(\Phi + \eta)\left(\frac{\partial^2 f}{\partial \xi^2}\right) \times \left(\frac{\partial^2 g}{\partial \eta^2}\right)\left(\frac{d(AB)}{d\zeta}\right), \tag{C10}$$

$$[\xi, \eta] = (\Phi + \xi)^{-1}(\Phi + \eta)^{-1}\left(\frac{\partial^2 f}{\partial \xi^2}\right)^{-1} \times \left(\frac{\partial^2 g}{\partial \eta^2}\right)^{-1}\left(\frac{\partial(AB)}{\partial \zeta}\right)^{-1}\left\{2\Phi\left[-\beta\left(\frac{dA}{d\zeta}\right) + \alpha\left(\frac{dB}{d\zeta}\right)\right] + H\Phi^{\frac{1}{2}}\left[\left(\frac{\partial \alpha}{\partial \zeta}\right) - \Phi\left(\frac{\partial \beta}{\partial \zeta}\right)\right]\right\}, \tag{C11}$$

$$[\xi, \zeta] = H\Phi^{\frac{1}{2}}(\Phi + \xi)^{-1}\left(\frac{\partial^2 f}{\partial \xi^2}\right)^{-1}\left(\frac{\partial(AB)}{\partial \zeta}\right)^{-1}, \tag{C12}$$

$$[\eta, \zeta] = -H\Phi^{\frac{1}{2}}(\Phi + \eta)^{-1}\left(\frac{\partial^2 g}{\partial \eta^2}\right)^{-1}\left(\frac{\partial(AB)}{\partial \zeta}\right)^{-1}. \tag{C13}$$

The Poisson brackets on the right-hand side of Eqs. (C3)–(C8) can now be computed via the prescription

$$[u, v] = \sum_{i,j}\left(\frac{\partial u}{\partial y_i}\right)\left(\frac{\partial v}{\partial y_j}\right)[y_i, y_j].$$

The results, when inserted in (C3)–(C8), yield (114).

APPENDIX D: THE SOLUTION OF EQUATION (139)

We begin by finding an intermediate integral of the system (139). To do this, we look for a constant of the motion w which will satisfy

$$L_{\mathrm{TT}} w = L_{\mathrm{ST}} w = L_{\mathrm{LT}} w = 0. \tag{D1}$$

It is obvious from Eq. (138) that $v_1 + v_2$ is conserved. From Eqs. (67) and (69) of CF,

$$L_{\mathrm{LT}}[\tfrac{1}{2}(v_1 + v_2)] = -1 + [\tfrac{1}{2}(v_1 + v_2)]^2. \tag{D2}$$

Quite generally, $L_{\mathrm{LT}}\Phi = -2\Phi$. Hence, we can try

$$w = \Phi[1 - \tfrac{1}{2}(v_1 + v_2)]/[1 + \tfrac{1}{2}(v_1 + v_2)]. \tag{D3}$$

If we use (28a) and (35) in (D3), we find

$$w = \frac{(\eta + \xi)\alpha + 2\eta\xi\beta}{(\eta + \xi)\beta + 2\alpha}. \tag{D4}$$

By the use of (139), it follows that $\partial w/\partial \xi = \partial w/\partial \eta = 0$. Hence, w is an intermediate integral of the system (139), depending only on ζ. The use of (32) and (34) in (D4) yields

$$(2w - \eta - \xi)(f + g) + (\eta - \xi)\left[(w - \xi)\left(\frac{\partial f}{\partial \xi}\right) - (w - \eta)\left(\frac{\partial g}{\partial \eta}\right)\right] = 0. \tag{D5}$$

It follows from operating on (D5) with $\partial^2/\partial\xi\partial\eta$ that

$$(w-\xi)\left(\frac{\partial^2 f}{\partial\xi^2}\right)-2\left(\frac{\partial f}{\partial\xi}\right)=-(w-\eta)\left(\frac{\partial^2 g}{\partial\eta^2}\right)+2\left(\frac{\partial g}{\partial\eta}\right). \quad \text{(D6)}$$

The variables ξ and η are now separated in (D6). The usual separation of variables argument now leads to

$$f(\xi)=\xi f_1(\zeta)+f_2(\zeta)+f_3(\zeta)[\xi-w(\zeta)]^{-1},$$
$$g(\eta)=-\eta f_1(\zeta)+g_2(\zeta)+g_3(\zeta)[\eta-w(\zeta)]^{-1}. \quad \text{(D7)}$$

Here $f_1(\zeta)$ is the separation constant. If (C7) is reintroduced into (C5), we find that $g_2=-f_2$ and $g_3=-f_3$. The result (140) follows.

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[12] See Ref. 3, Secs. II and IV. Equation (149) of the present paper follows from Eq. (21) of Ref. 3.
[13] With the choice $C_0(\zeta)=0$, the result (157) should agree with Eq. (26) of Ref. 10. The two results agree only to lowest order in the velocities for small velocities; the discrepancy is evidently a consequence of the authors' of Ref. 10 having used $a_1=-a_2=e^2x_{12}^{-2}$ for the asymptotic equations of motion of electrodynamics in the center of momentum frame. A factor of $(1-v^2)^{\frac{3}{2}}$ from the relativistic variation of mass with velocity and a factor of $(1-v^2)$ from the asymptotic field [see Eq. (149)] should have been included; the correct asymptotic equations of motion of electrodynamics in the center-of-momentum frame are $a_1=-a_2=e^2(1-v^2)^{\frac{5}{2}}x_{12}^{-2}$. Use of these leads to the replacement of Eq. (24) of Ref. 10 by

$$x_1=-x_2=a+vt-\tfrac{1}{2}e^2v^{-2}(1-v^2)^{\frac{3}{2}}\ln(t/t_0);$$

Eq. (26) is then replaced by

$$M'=\tfrac{1}{2}e^2v^{-2}(1-v^2)^2\ln[(C+Sv)/(C-Sv)]$$

which agrees with (157) when $e_1=e_2=e$, $m_1=m_2=1$, and $C_0=0$.

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Green's Function for the Nonlocal Wave Equation

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The Green's function for the nonlocal wave equation in a semi-infinite medium is calculated using the Wiener–Hopf technique and shown to be given by an integral whose integrand contains only the source-free solution of that same equation.

1. INTRODUCTION AND SUMMARY

The equation

$$\frac{d^2e(x)}{dx^2} + \alpha^2 e(x) + \int_0^\infty K(|x - x'|)e(x')\,dx' = 0, \quad x > 0, \tag{1.1a}$$

with

$$e(x = 0) = 1, \tag{1.1b}$$

$$e(x \to \infty) = 0, \tag{1.1c}$$

appears in several branches of mathematical physics, among them:

(a) electromagnetic wave propagation through a bounded medium wherein the relation between the electric current and the field driving it is nonlocal,[1] and

(b) electromagnetic or acoustic wave propagation through a bounded, homogeneous, random medium.[2,3]

The equation can be solved in principle by a variety of means, among them, the Wiener–Hopf technique,[4] the method of singular eigenfunctions,[5] and perhaps by some of the other techniques which have been especially developed for handling related problems which arise in neutron transport theory.[6] In what follows, we assume that the solution to (1.1) is available, either in numerical or analytic form, as a result of carrying through the details of one or another of the possible methods of solution.

Our concern here is with the Green's function of Eq. (1.1), a quantity which arises naturally in the study of perturbations of that equation. More precisely, the Green's function for Eq. (1.1) is the solution of

$$\frac{d^2G(x, x_0)}{dx^2} + \alpha^2 G(x, x_0) + \int_0^\infty K(|x - x'|)G(x', x_0)\,dx' = \delta(x - x_0), \quad x > 0, \tag{1.2a}$$

with

$$G(x = 0, x_0) = 0, \tag{1.2b}$$

$$G(x = \infty, x_0) = 0. \tag{1.2c}$$

In this paper, we solve (1.2) using the Wiener–Hopf method and show that the Green's function G is given by either of the two equivalent forms

$$G(x, x_0) = -\int_0^{x_0} e(s)e(s + x - x_0)\,ds \tag{1.3a}$$

$$= \int_0^\infty e(s + x)e(s + x_0)\,ds + G_0(x - x_0), \tag{1.3b}$$

where $G_0(x - x_0)$ is the Green's function for the *infinite* medium, i.e., where

$$\frac{d^2G_0(x - x_0)}{dx^2} + \alpha^2 G_0(x - x_0) + \int_{-\infty}^\infty K(|x - x'|)G_0(x' - x_0)\,dx' = \delta(x - x_0), \tag{1.4a}$$

$$G_0(x, x_0) = 0 \quad \text{as} \quad x \to \pm\infty, \tag{1.4b}$$

and where $e(x)$ is taken as identically zero for negative values of the argument. The result is a general one; the only restriction is that the kernel K decay exponentially at large distances, so that the Wiener–Hopf method can be used.

2. FOURIER TRANSFORM OF THE GREEN'S FUNCTION

Equation (1.3) defines the Green's function only for x and x_0 greater than, or equal to, zero. We consider x_0 to be positive, and we define

$$G(x < 0, x_0) \equiv 0. \tag{2.1}$$

Because of (2.1), Eq. (1.3) is not satisfied for $x < 0$ but, according to the standard Wiener–Hopf procedure, the following equation is true for all x:

$$\frac{d^2G(x, x_0)}{dx^2} + \alpha^2 G(x, x_0) + \int_{-\infty}^{+\infty} K(x - x')G(x', x_0)\,dx' = \delta(x - x_0) + g(x, x_0), \tag{2.2}$$

where

$$g(x, x_0) \equiv 0, \quad x \geq 0, \tag{2.3a}$$

$$\equiv \int_{-\infty}^\infty K(x - x')G(x', x_0)\,dx', \quad x < 0. \tag{2.3b}$$

The Fourier transform of Eq. (2.2) is to be taken. We define

$$G(k, x_0) \equiv \int_{-\infty}^{\infty} G(x, x_0)e^{-ikx}\,dx, \tag{2.4a}$$

$$g(k, x_0) \equiv \int_{-\infty}^{\infty} g(x, x_0)e^{-ikx}\,dx, \tag{2.4b}$$

$$V(k) \equiv \int_{-\infty}^{\infty} K(|x|)e^{-ikx}\,dx. \tag{2.4c}$$

We assumed that the kernel $K(|x|)$ has a spatial range of L, i.e., that at large distances $K \sim e^{-|x|/L}$. It is convenient to take L as the unit of length. Having done so, the function $V(k)$ is analytic in the strip $-1 < \operatorname{Im} k < +1$. The definitions (2.1) and (2.3) guarantee that $G(k, x_0)$ is analytic for $\operatorname{Im} k < 0$ and that $g(k, x_0)$ is analytic for $-1 < \operatorname{Im} k$. Hence, for $-1 < \operatorname{Im} k < 0$, the Fourier transform of each term in (2.2) is analytic and the transform of the equation may be taken, yielding

$$-[k^2 - \alpha^2 - V(k)]G(k, x_0) = g(k, x_0) + ikG(0, x_0) + G'(0, x_0) + e^{-ikx_0}, \tag{2.5}$$

where

$$G'(0, x_0) \equiv \left[\frac{dG(x, x_0)}{dx}\right]_{x=0}.$$

At this stage, we perform a Wiener–Hopf factorization; that is, we assert that we have a pair of functions $f^+(k)$ and $f^-(k)$ with the following five properties:

$$f^-(k)/f^+(k) = k^2 - \alpha^2 - V(k), \quad -1 \leq -\eta < \operatorname{Im} k < \eta \leq 1, \tag{2.6a}$$

$f^-(k)$ is analytic for $\operatorname{Im} k < \eta$, (2.6b)

$f^+(k)$ is analytic for $-\eta < \operatorname{Im} k$, (2.6c)

$f^+(k)$ has no zeros for $-\eta < \operatorname{Im} k$, (2.6d)

the growth of $f^+(k)$ and $f^-(k)$, as $k \to \infty$, in the strip $-\eta < \operatorname{Im} k < \eta$ is algebraic, not exponential. (2.6e)

The quantity η appearing in (2.6a) is chosen small enough so that the equation $k^2 - \alpha^2 - V(k) = 0$ has no roots in the strip $-\eta < \operatorname{Im} k < \eta$. It can be arbitrarily small, if necessary; its use is a convenience, not a necessity, in formulating the factorization. We exhibit $f^+(k)$ and $f^-(k)$ later. For now, we use (2.6a) to rewrite (2.5) as

$$f^-(k)G(k, x_0) = -f^+(k)[g(k, x_0) + ikG(0, x_0) + G'(0, x_0)] - f^+(k)e^{-ikx_0}. \tag{2.7}$$

Consider the last term in (2.7): Since it is analytic in the strip $-\eta < \operatorname{Im} k < 0$, we can use Cauchy's theorem to write

$$f^+(k)e^{-ikx_0} = \frac{1}{2\pi i}\int_{-\infty-i\eta}^{+\infty-i\eta} \frac{f^+(z)e^{-izx_0}}{z-k}\,dz - \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{f^+(z)e^{-izx_0}}{z-k}\,dz, \quad \eta < \operatorname{Im} k < 0, \tag{2.8}$$

$$\equiv h^+(k, x_0) - h^-(k, x_0). \tag{2.9}$$

An argument for neglecting the contribution from the ends of the strip is given in Ref. 7 (p. 988).

The two functions h^+ and h^- defined in this way have the following properties: h^+ is analytic for $\operatorname{Im} k > -\eta$ and has $1/k$ behavior at infinity, and h^- is analytic for $\operatorname{Im} k < 0$. Hence, if we rewrite (2.7) as

$$f^-(k)G(k, x_0) - h^-(k, x_0) = -f^+(k)[g(k, x_0) + ikG(0, x_0) + G'(0, x_0)] - h^+(k, x_0), \tag{2.10}$$

then the standard Wiener–Hopf analyticity arguments apply and we conclude that each side of (2.10) must be equal to some polynomial in k. We write this as

$$P(k, x_0) \equiv \sum_{N=0}^{M} A_n(x_0)k^n \tag{2.11}$$

and, solving for G, we have

$$G(k, x_0) = [P(k, x_0) + h^-(k, x_0)]/f^-(k). \tag{2.12}$$

We turn now to the actual Wiener–Hopf factorization: Since $K(|x|)$ is an even function of x, the transform $V(k)$ is an even function of k and all singularities occur in pairs, at $\pm k$. Assume that there is at least one pair of branch points at $k = \pm\beta$. (If there are no branch points, the problem is trivial and can be done almost by inspection.) The function

$$Q(k) \equiv [k^2 - \alpha^2 - V(k)]/(k^2 - \beta^2) \tag{2.13}$$

is an even function of k which goes to unity as $k \to \pm\infty$, and is analytic and free from zeros in the strip $-\eta < \operatorname{Im} k < \eta$. Hence, again using Cauchy's theorem for k within the strip,

$$\ln Q(k) = \frac{1}{2\pi i}\int_{-\infty-i\eta}^{\infty-i\eta} \frac{\ln Q(z)\,dz}{z-k} - \frac{1}{2\pi i}\int_{-\infty+i\eta}^{\infty+i\eta} \frac{\ln Q(z)\,dz}{z-k} \tag{2.14a}$$

$$= S^+(k) - S^-(k). \tag{2.14b}$$

The analytic properties here are that S^+ is analytic for $-\eta < \operatorname{Im} k$ and has $1/k$ behavior at infinity. S^- is analytic for $\operatorname{Im} k < \eta$ and it, too, has analytic behavior at infinity.

Recombining (2.13) and (2.15), we have

$$k^2 - \alpha^2 - V(k) = (k^2 - \beta^2)e^{S^+(k)-S^-(k)}. \quad (2.15)$$

The analytic properties demanded by (2.6) are satisfied by

$$f^-(k) = (k^2 - \beta^2)e^{-S^-(k)}, \quad (2.16a)$$

$$f^+(k) = e^{-S^+(k)}. \quad (2.16b)$$

The procedure we have used to arrive at (2.16) and at (2.12) is virtually identical with that described in the text by Morse and Feshbach,[7] to which the reader is referred for greater detail on the arguments we have sketched above.

To proceed further than this, we combine (2.16) and (2.12), obtaining

$$G(k, x_0) = [P(k, x_0) + h^-(k, x_0)]e^{S^-(k)}/(k^2 - \beta^2). \quad (2.17)$$

Note that the initial condition (1.2b) demands that $G(k, x_0)$ behave like $1/k^2$ as $k \to \infty$ rather than the usual $1/k$ behavior which Fourier transforms usually exhibit. This requirement, in connection with (2.17), limits P to be a polynomial of zero order, i.e.,

$$P(k, x_0) = A_0(x_0).$$

The single constant A_0 may be fixed by noting that G, as given by (2.17), seems to be singular at $k = -\beta$ in the lower half-plane, contrary to what we know its analytic properties to be. By taking

$$A_0(x_0) = -h^-(-\beta, x_0),$$

we remove the singularity which would otherwise appear. Hence, the Fourier transform of the Green's function is given by

$$G(k, x_0) = [h^-(k, x_0) - h^-(-\beta, x_0)]e^{S^-(k)}/(k^2 - \beta^2), \quad \text{Im } \beta > 0. \quad (2.18)$$

Consider h^-: From (2.8), (2.9), and (2.16b), we have

$$h^-(k, x_0) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{\exp[-S^+(z) - izx_0]}{z - k}\, dz. \quad (2.19)$$

Hence,

$$\frac{h^-(k, x_0) - h(-\beta, x_0)}{k^2 - \beta^2} = \frac{1}{k - \beta}\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{dz \exp[S^+(z) - izx_0]}{(z - k)(z + \beta)},$$

or, on replacing z by $-z$ in the integral,

$$= \frac{1}{k - \beta}\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{dz \exp[-S^+(-z) + izx_0]}{(z + k)(z - \beta)}. \quad (2.20)$$

However, it is evident, from Eqs. (2.14) and the fact that $Q(z)$ is an even function of z, that

$$S^+(-z) = -S^-(z). \quad (2.21)$$

Hence, (2.18) takes the form

$$G(k, x_0) = \left(\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{dz \exp[S^-(z) + izx_0]}{(z + k)(z - \beta)}\right)\left(\frac{\exp[S^-(k)]}{k - \beta}\right), \quad -\eta < \text{Im } k < 0. \quad (2.22)$$

We shall need to evaluate (2.22) with k in the upper half-plane. Letting k go through the contour of the z integration gives us an extra contribution from the z integral, namely, $-\exp[S^-(-k) - ikx_0]/(k + \beta)$ or, using (2.21), $-\exp[-S^+(k) - ikx_0]/(k + \beta)$. This extra piece, inserted in (2.22), adds the following term to $G(k, x_0)$:

$$-\exp[-S^+(k) - ikx_0 + S^-(k)]/(k^2 - \beta^2) = -e^{-ikx_0}/[k^2 - \alpha^2 - V(k)]. \quad (2.23)$$

The equality here follows by use of (2.15). This gives us the continuation of (2.22) to the upper half k plane, namely,

$$G(k, x_0) = \left(\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{dz \exp[S^-(z) + izx_0]}{(z + k)(z - \beta)}\right)\left(\frac{\exp[S^-(k)]}{k - \beta}\right) - \frac{e^{-ikx_0}}{k^2 - \alpha^2 - V(k)}, \quad \text{Im } k > 0. \quad (2.24)$$

3. FOURIER TRANSFORM OF THE SOURCE-FREE SOLUTION

Equation (1.1) may also be solved by the Wiener–Hopf method. As before, the solution is defined for negative argument by choosing

$$e(x) \equiv 0, \quad x < 0. \quad (3.1)$$

Fourier transforms are introduced,

$$e(k) \equiv \int_{-\infty}^{\infty} e(x)e^{-ikx}\, dx, \quad (3.2)$$

and the entire procedure goes through as before. This time, however, there is no inhomogeneous term in the integral equation, no e^{-ikx_0} in the transformed equation, and no $h^{\pm}(k)$ appears. Instead of (2.17), one obtains

$$e(k) = P(k) \exp[S^-(k)]/(k^2 - \beta^2). \quad (3.3)$$

Since $e(k)$ is the Fourier transform of a quantity with a finite value at $x = 0$, its behavior is like $1/k$ at infinity, and the polynomial $P(k)$ appearing in (3.3) must be of first order

$$P(k) = A_0 + A_1 k = A_1(k + A_0/A_1).$$

As before, $E(k)$ has a singularity in the lower half-plane at $k = -\beta$, in contradiction to the known analytic behavior following from (3.1) and (3.2). We remove this singularity by taking $A_0/A_1 = \beta$. Finally, the value of A_1 is fixed by the condition (1.1b), which results in

$$\lim_{k\to\infty} E(k) = \frac{1}{ik}.$$

Thus,

$$E(k) = -i \exp[S^-(k)]/(k - \beta). \tag{3.4}$$

4. RELATION BETWEEN THE GREEN'S FUNCTION AND THE SOURCE-FREE SOLUTION

We insert (3.4) into (2.24) and take the Fourier inverse of (2.4a):

$$G(x, x_0) = \frac{i}{2\pi}\int dk e^{ikx}E(k)\cdot\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dzE(z)e^{izx_0}}{z+k} - \frac{1}{2\pi}\int\frac{dke^{ik(x-x_0)}}{k^2\cdot\alpha^2 + V(k)}. \tag{4.1}$$

Note that, for Im $(z + k) > 0$,

$$\frac{i}{z+k} = \int_0^\infty ds e^{is(k+z)}.$$

Hence, the first term in (4.1) is

$$\int_0^\infty ds\left(\frac{1}{2\pi}\int dkE(k)e^{ik(x+s)}\right)\left(\frac{1}{2\pi}\int dzE(z)e^{iz(x_0+s)}\right) = \int_0^\infty ds e(x+s)e(x_0+s). \tag{4.2}$$

The second term in (4.1) is obviously the infinite-medium Green's function, i.e., the solution to (1.4). We have, therefore,

$$G(x, x_0) = \int_0^\infty ds e(s+x)e(s+x_0) + G_0(|x - x_0|) \tag{4.3}$$

which is the proof of (1.3b). Setting $x = 0$ above, using the boundary condition (1.2a), and replacing x_0 by $x - x_0$ in (4.3) gives

$$0 = \int_0^\infty ds e(s)e(s + x - x_0) + G_0(|x - x_0|). \tag{4.4}$$

Changing the variable of integration from s to $s + x_0$ in (4.3) and subtracting (4.4) from that gives

$$G(x, x_0) = -\int_0^{x_0} ds e(s)e(s + x - x_0), \tag{4.5}$$

which is the proof of (1.3a).

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Scattering in General Higher Sectors of the Lee Model*

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(Received 1 August 1969)

The technique of an iterative expansion in terms of the 2-body solution used in V–2θ sector of the Lee model has been extended to the general higher sector, i.e., V–$n\theta$ sector with $n > 2$ so that S matrices for the general cases of scattering $(n-1)\theta$ particles off the $(V\theta)$ bound state can be calculated. Again, as in V–2θ sector, each term of the expansion preserves the properties of the $(V\theta)$ bound state, the analytic structure, and symmetries of the τ functions.

I. INTRODUCTION

In the previous paper,[1] we solved the τ functions in the V–2θ sector of the Lee model by an iterative expansion in terms of the known V–θ interaction, in other words, the known 2-body solution. The results of the τ functions led to the S matrices for the processes of scattering a θ particle off the $(V\theta)$ bound state, also for the processes involving 3-body problems.

The purpose of this paper is to illustrate that we can extend this iterative expansion technique to the general higher sector, i.e., V–$n\theta$ sector, with $n > 2$ of the Lee model. The reason that this can be done is essentially due to the assumption that there is no interaction among the θ particles in the Lee model. With the solutions of the τ functions, we can calculate the amplitudes of scattering $(n-1)\theta$ particles off the $(V\theta)$

As before, $E(k)$ has a singularity in the lower half-plane at $k = -\beta$, in contradiction to the known analytic behavior following from (3.1) and (3.2). We remove this singularity by taking $A_0/A_1 = \beta$. Finally, the value of A_1 is fixed by the condition (1.1b), which results in

$$\lim_{k\to\infty} E(k) = \frac{1}{ik}.$$

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Note that, for Im $(z + k) > 0$,

$$\frac{i}{z+k} = \int_0^\infty ds e^{is(k+z)}.$$

Hence, the first term in (4.1) is

$$\int_0^\infty ds\left(\frac{1}{2\pi}\int dkE(k)e^{ik(x+s)}\right)\left(\frac{1}{2\pi}\int dzE(z)e^{iz(x_0+s)}\right) = \int_0^\infty ds e(x+s)e(x_0+s). \tag{4.2}$$

The second term in (4.1) is obviously the infinite-medium Green's function, i.e., the solution to (1.4). We have, therefore,

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I. INTRODUCTION

In the previous paper,[1] we solved the τ functions in the V–2θ sector of the Lee model by an iterative expansion in terms of the known V–θ interaction, in other words, the known 2-body solution. The results of the τ functions led to the S matrices for the processes of scattering a θ particle off the $(V\theta)$ bound state, also for the processes involving 3-body problems.

The purpose of this paper is to illustrate that we can extend this iterative expansion technique to the general higher sector, i.e., V–$n\theta$ sector, with $n > 2$ of the Lee model. The reason that this can be done is essentially due to the assumption that there is no interaction among the θ particles in the Lee model. With the solutions of the τ functions, we can calculate the amplitudes of scattering $(n-1)\theta$ particles off the $(V\theta)$

bound state in both elastic and inelastic cases and the amplitudes for the many-body processes, namely, V–$n\theta$, $N-(n+1)\theta$ elastic scatterings, and V–$n\theta \to N-(n+1)\theta$ production in the general V–$n\theta$ sector.

Just as in Ref. 1, the iterative expansion which we shall construct in the following sections is such that each term in the series preserves the properties of the $(V\theta)$ bound state and the analytic structures and symmetries of the τ function.

The outline of this paper is as follows: In Sec. II we derive the equations for the τ functions in the V–$n\theta$ sector. The solution of the τ function is given in Sec. III. We solve the τ functions by expanding the integral equations into a series. We then obtain soluble integral equations for each term of the series. This completely determines all the processes in the V–$n\theta$ sector. In Sec. IV we calculate to the first few terms for the S matrices

$$V+n\theta \to V+n\theta,$$
$$V+n\theta \to N+(n+1)\theta,$$
$$N+(n+1)\theta \to N+(n+1)\theta.$$

The bound-state scattering processes

$$(V\theta)+(n-1)\theta \to (V\theta)+(n-1)\theta,$$
$$(V\theta)+(n-1)\theta \to V+n\theta,$$
$$(V\theta)+(n-1)\theta \to N+(n+1)\theta$$

are calculated in Sec. V. The conclusion follows in Sec. VI.

II. V–$n\theta$ SECTOR OF LEE MODEL

The total renormalized Hamiltonian of Lee model was given in Ref. 1. The states in the V–$n\theta$ sector are eigenstates of the operators Q_1 and Q_2 and are characterized by the eigenvalues $q_1=1$ and $q_2=n+1$. Consequently, this sector is completely determined by the following four τ functions

$$\tau^{4n+1}(t; w_1, w_2, \cdots, w_{2n}) = \prod_{i=1}^{2n} \frac{(2w_i)^{\frac{1}{2}}}{u(w_i)} \langle 0| T\left(\psi_V(t) \prod_{\alpha=1}^{n} a_{k_\alpha}(t) \psi_V^+(0) \prod_{\beta=n+1}^{2n} a_{k_\beta}^+(0)\right)|0\rangle, \tag{1a}$$

$$\tau^{4n+2}(t; w_1, w_2, \cdots, w_{2n+1}) = \prod_{i=1}^{2n+1} \frac{(2w_i)^{\frac{1}{2}}}{u(w_i)} \langle 0| T\left(\psi_N(t) \prod_{\alpha=1}^{n+1} a_{k_\alpha}(t) \psi_V^+(0) \prod_{\beta=n+2}^{2n+1} a_{k_\beta}^+(0)\right)|0\rangle, \tag{1b}$$

$$\tau^{4n+3}(t; w_1, w_2, \cdots, w_{2n+1}) = \prod_{i=1}^{2n+1} \frac{(2w_i)^{\frac{1}{2}}}{u(w_i)} \langle 0| T\left(\psi_V(t) \prod_{\alpha=1}^{n} a_{k_\alpha}(t) \psi_N^+(0) \prod_{\beta=n+1}^{2n+1} a_{k_\beta}^+(0)\right)|0\rangle, \tag{1c}$$

$$\tau^{4n+4}(t; w_1, w_2, \cdots, w_{2n+2}) = \prod_{i=1}^{2n+2} \frac{(2w_i)^{\frac{1}{2}}}{u(w_i)} \langle 0| T\left(\psi_N(t) \prod_{\alpha=1}^{n+1} a_{k_\alpha}(t) \psi_N^+(0) \prod_{\beta=n+2}^{2n+2} a_{k_\beta}^+(0)\right)|0\rangle. \tag{1d}$$

By using field equations and commutation rules listed in Eqs. (5) and (4) of Ref. 1, we get the Matthews–Salam equations

$$\left(i\frac{d}{dt} - m_0 - \sum_{i=1}^{n} w_i\right)\tau^{4n+1}(t; w_1, w_2, \cdots, w_{2n}) = \frac{i\delta(t)}{Z} \prod_{i=1}^{n} \frac{2w_i}{u^2(w_i)} \sum_{P_{fi}} \delta_{fi}^n + \frac{g}{Z} \sum_k \frac{u^2(w)}{2w} \tau^{4n+2}(t; w, w_1, w_2, \cdots, w_{2n}), \tag{2a}$$

$$\left(i\frac{d}{dt} - m - \sum_{i=1}^{n+1} w_i\right)\tau^{4n+2}(t; w_1, \cdots, w_{2n+1}) = g[\tau^{4n+1}(t; w_2, w_3, \cdots, w_{2n+1}) + \tau^{4n+1}(t; w_1, w_3, \cdots, w_{2n+1}) + \cdots + \tau^{4n+1}(t; w_1, w_2, \cdots, w_n, w_{n+2}, \cdots, w_{2n+1})], \tag{2b}$$

$$\left(i\frac{d}{dt} - m - \sum_{i=n+1}^{2n+1} w_i\right)\tau^{4n+3}(t; w_1, \cdots, w_{2n+1}) = g[\tau^{4n+1}(t; w_1, \cdots, w_n, w_{n+2}, \cdots, w_{2n+1}) + \tau^{4n+1}(t; w_1, \cdots, w_n, w_{n+1}, w_{n+3}, \cdots, w_{2n+1}) + \cdots + \tau^{4n+1}(t; w_1, \cdots, w_n, w_{n+1}, \cdots, w_{2n})], \tag{2c}$$

and

$$\left(i\frac{d}{dt} - m - \sum_{i=1}^{n+1} w_i\right)\tau^{4n+4}(t; w_1, \cdots, w_{2n+2}) = i \prod_{i=1}^{n+1} \frac{2w_i}{u^2(w_i)} \sum_{P_{fi}} \delta_{fi}^{n+1} + g[\tau^{4n+3}(t; w_2, w_3, \cdots, w_{2n+2}) + \tau^{4n+3}(t; w_1, w_3, \cdots, w_{2n+2}) + \cdots + \tau^{4n+3}(t; w_1, w_2, \cdots, w_n, w_{n+2}, \cdots, w_{2n+2})], \tag{2d}$$

where

$$m_0 = m + \delta m, \quad \delta m = \frac{g^2}{Z} \sum_k \frac{u^2(w)}{2w^2},$$

and $\sum_{P_{fi}} \delta_{fi}^n$, introduced in Ref. 1, is the summation of the δ functions where P_{fi} means the permutations between final and initial states and the superscript n represents the number of incoming (outgoing) θ particles.

Just as for the V–2θ sector, the τ functions are symmetric under the interchange of θ particles in initial or final state;

$$\tau^{4n+1}(t; w_1, \cdots, w_{2n}) = \tau^{4n+1}(t; w_2, w_1, w_3, \cdots, w_{2n}) = \cdots = \tau^{4n+1}(t; w_1, \cdots, w_n, w_{n+2}, w_{n+1}, w_{n+3}, \cdots, w_{2n}) = \cdots \tag{3a}$$

and

$$\tau^{4n+2}(t; w_1, \cdots, w_{2n+1}) = \tau^{4n+2}(t; w_2, w_1, w_3, \cdots, w_{2n+1}) = \cdots = \tau^{4n+2}(t; w_1, \cdots, w_n, w_{n+2}, w_{n+1}, w_{n+3}, \cdots, w_{2n+1}) = \cdots. \quad (3b)$$

Similar symmetric relations exist for τ^{4n+3} and τ^{4n+4}.

Furthermore, we will see again in the next section that τ^{4n+1} is also symmetric under the interchange of initial and final states, i.e.,

$$\tau^{4n+1}(t; w_1, \cdots, w_n, w_{n+1}, \cdots, w_{2n}) = \tau^{4n+1}(t; w_{n+1}, \cdots, w_{2n}, w_1, \cdots, w_n). \quad (4)$$

From Eqs. (2b) and (2c) together, by using relation (4), we get

$$\tau^{4n+2}(t; w_1, \cdots, w_{2n+1}) = \tau^{4n+3}(t; w_1, \cdots, w_{2n+1}). \quad (5)$$

The Fourier transform of these τ functions satisfy the following equations:

$$\left(W - m_0 - \sum_{i=1}^{n} w_i\right)\hat{\tau}^{4n+1}(W; w_1, \cdots, w_{2n}) = \frac{1}{Z}\prod_{i=1}^{n}\frac{2w_i}{u^2(w_i)}\sum_{P_{fi}}\delta_{fi}^n + \frac{g}{Z}\sum_k \frac{u^2(w)}{2w}\hat{\tau}^{4n+2}(W; w, w_1, \cdots, w_{2n}), \quad (6a)$$

$$\left(W - m - \sum_{i=1}^{n+1} w_i\right)\hat{\tau}^{4n+2}(W; w_1, \cdots, w_{2n+1}) = g[\hat{\tau}^{4n+1}(W; w_2, w_3, \cdots, w_{n+1}, w_{n+2}, \cdots, w_{2n+1}) + \hat{\tau}^{4n+1}(W; w_1, w_3, \cdots, w_{n+1}, w_{n+2}, \cdots, w_{2n+1}) + \cdots + \hat{\tau}^{4n+1}(W; w_1, w_2, \cdots, w_n; w_{n+2}, \cdots, w_{2n+1})], \quad (6b)$$

$$\left(W - m - \sum_{i=n+1}^{2n+1} w_i\right)\hat{\tau}^{4n+3}(W; w_1, \cdots, w_{2n+1}) = g[\hat{\tau}^{4n+1}(W; w_1, \cdots, w_n, w_{n+2}, w_{n+3}, \cdots, w_{2n+1}) + \hat{\tau}^{4n+1}(W; w_1, \cdots, w_n, w_{n+1}, w_{n+3}, \cdots, w_{2n+1}) + \cdots + \hat{\tau}^{4n+1}(W; w_1, \cdots, w_n, w_{n+1}, w_{n+2}, \cdots, w_{2n})], \quad (6c)$$

$$\left(W - m - \sum_{i=1}^{n+1} w_i\right)\hat{\tau}^{4n+4}(W; w_1, \cdots, w_{2n+2}) = \prod_{i=1}^{n+1}\frac{2w_i}{u^2(w_i)}\sum_{P_{fi}}\delta_{fi}^{n+1} + g[\hat{\tau}^{4n+3}(W; w_2, w_3, \cdots, w_{n+1}, w_{n+2}, \cdots, w_{2n+2}) + \hat{\tau}^{4n+3}(W; w_1, w_3, \cdots, w_{n+1}, w_{n+2}, \cdots, w_{2n+2}) + \cdots + \hat{\tau}^{4n+3}(W; w_1, w_2, \cdots, w_n, w_{n+2}, \cdots, w_{2n+2})], \quad (6d)$$

where

$$\hat{\tau}^{\alpha}(W; w_1, w_2, \cdots) = -i\int_{-\infty}^{\infty} dt e^{iWt}\tau^{\alpha}(t; w_1, w_2, \cdots). \quad (7)$$

Substituting Eq. (6b) into Eq. (6a), we get

$$h\left(W - \sum_{i=1}^{n} w_i\right)\hat{\tau}^{4n+1}(W + m; w_1, \cdots, w_{2n}) = \prod_{i=1}^{n}\frac{2w_i}{u^2(w_i)}\sum_{P_{fi}}\delta_{fi}^n + \frac{1}{\pi}\int_{\mu}^{\infty}\frac{dw\ \mathrm{Im}\ h(w)}{\left(W - w - \sum_{i=1}^{n} w_i\right)} \times [\hat{\tau}^{4n+1}(W + m; w, w_2, \cdots, w_{2n}) + \hat{\tau}^{4n+1}(W + m; w, w_1, w_3, \cdots, w_{2n}) + \cdots + \hat{\tau}^{4n+1}(W + m; w, w_1, w_2, \cdots, w_{n-1}, w_{n+1}, \cdots, w_{2n})], \quad (8)$$

where

$$h(w + i\epsilon) \equiv h(w) \equiv w[1 - \beta(w)] \equiv w\left(1 + \frac{g^2 w}{4\pi^2}\int_{\mu}^{\infty}\frac{dw'(w'^2 - \mu^2)^{\frac{1}{2}}u^2(w')}{w' - w - i\epsilon}\right). \quad (9)$$

Let us define

$$N^{-}(W; w_1, \cdots, w_{2n}) \equiv N(W; w_1 - i\epsilon, w_2, \cdots, w_{2n}) = -\frac{1}{g^2}\prod_{i=1}^{n}\frac{2w_i}{u^2(w_i)}h\left(W - \sum_{i=n+1}^{2n} w_i\right)\sum_{P_{fi}}\delta_{fi}^n + \frac{1}{g^2}h\left(W - \sum_{i=1}^{n} w_i\right)h\left(W - \sum_{i=n+1}^{2n} w_i\right) \times \hat{\tau}^{4n+1}(W + m; w_1, \cdots, w_{2n}). \quad (10)$$

After substituting Eq. (10) into Eq. (8) and continuing w_1 into the complex z_1 plane, we get

$$\begin{aligned} N(W; z_1, w_2, \cdots, w_{2n}) = {} & \left(\prod_{i=2}^{n}\frac{2w_i}{u^2(w_i)}\right)\frac{\sum_{P_{fi}: w_f \neq w_1}\delta_{fi}^n}{\left(W - z_1 - \sum_{i=n+1}^{2n} w_i\right)} \\ & + \left(\prod_{i=1; i\neq 2}^{n}\frac{2w_i}{u^2(w_i)}\right)\frac{\sum_{P_{fi}: w_f \neq w_2}\delta_{fi}^n}{\left(W - w_2 - \sum_{i=n+1}^{2n} w_i\right)} + \cdots \\ & + \left(\prod_{i=1}^{n-1}\frac{2w_i}{u^2(w_i)}\right)\frac{\sum_{P_{fi}: w_f \neq w_n}\delta_{fi}^n}{\left(W - w_n - \sum_{i=n+1}^{2n} w_i\right)} \\ & + \frac{1}{\pi}\int_{\mu}^{\infty}\frac{dw\ \mathrm{Im}\ h(w)}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right)} \\ & \times \left(\frac{N^{-}(W; w, w_2, \cdots, w_{2n})}{h\left(W - w - \sum_{i=2}^{n} w_i\right)}\right. \\ & + \frac{N^{-}(W; w, z_1, w_3, \cdots, w_{2n})}{h\left(W - w - z_1 - \sum_{i=3}^{n} w_i\right)} + \cdots \\ & \left. + \frac{N^{-}(W; w, z_1, w_2, \cdots, w_{n-1}, w_{n+1}, \cdots, w_{2n})}{h\left(W - w - z_1 - \sum_{i=2}^{n-2} w_i\right)}\right). \end{aligned} \quad (11)$$

We can simplify Eq. (11) by noticing that

$$\hat{\tau}^{4n+1}(W+m;\, w_1, \cdots, w_{2n})$$

is symmetric under the interchange of the pairs w_1 with w_i where $i = 2, 3, \cdots, n$. By Eq. (10), we see that the function $N^-(W; w_1, \cdots, w_{2n})$ has the same symmetry properties, so that we can write Eq. (11) as

$$\begin{aligned} &N^-(W; w_1, \cdots, w_{2n}) \\ &\quad = F^-(W; w_1, w_2, \cdots, w_{2n}) \\ &\qquad + F^-(W; w_2, w_1, w_3, \cdots, w_{2n}) + \cdots \\ &\qquad + F^-(W; w_n, w_2, w_3, \cdots, w_{n-1}, w_1, w_{n+1}, \cdots, w_{2n}), \end{aligned} \tag{12}$$

where

$$\begin{aligned} &F(W; z_1, w_2, \cdots, w_{2n}) \\ &= \left(\prod_{i=2}^{n-1} \frac{2w_i}{u^2(w_i)}\right) \frac{\sum_{P_{fi}: w_f \neq w_1} \delta_{fi}^n}{\left(W - z_1 - \sum_{i=n+1}^{2n} w_i\right)} \\ &\quad + \frac{1}{\pi} \int_\mu^\infty \frac{dw\, \mathrm{Im}\, h(w) N^-(W; w, w_2, \cdots, w_{2n})}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \end{aligned} \tag{13}$$

and

$$\begin{aligned} F^-(W; w_1, \cdots, w_{2n}) &\equiv F(W; w_1 - i\epsilon, w_2, \cdots, w_{2n}) \\ &= \lim_{z_1 \to w_1 - i\epsilon} F(W; z_1, w_2, \cdots, w_{2n}). \end{aligned}$$

Substituting Eq. (12) into Eq. (13), we get the singular integral equation for $F(W; z_1, w_2, \cdots, w_{2n})$ as

$$\begin{aligned} &F(W; z_1, w_2, \cdots, w_{2n}) \\ &= \left(\prod_{i=2}^{n} \frac{2w_i}{u^2(w_i)}\right) \frac{\sum_{P_{fi}: w_f \neq w_1} \delta_{fi}^n}{\left(W - z_1 - \sum_{i=n+1}^{2n} w_i\right)} \\ &\quad + \frac{1}{\pi} \int_\mu^\infty \frac{dw\, \mathrm{Im}\, h(w) F^-(W; w, w_2, \cdots, w_{2n})}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \\ &\quad + \frac{1}{\pi} \int_\mu^\infty \frac{dw\, \mathrm{Im}\, h(w)}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \\ &\quad \times [F^-(W; w_2, w, w_3, \cdots, w_{2n}) \\ &\quad + F^-(W; w_3, w_2, w, w_4, \cdots, w_{2n}) + \cdots \\ &\quad + F^-(W; w_n, w_2, \cdots, w_{n-1}, w, w_{n+1}, \cdots, w_{2n})]. \end{aligned} \tag{14}$$

We can consider $F(W; z_1, w_2, \cdots, w_{2n})$ as a function of variable z_1 for fixed $W, w_2, \cdots, w_{2n}$. It has $n!$ poles at

$$z_1 = \left(W - \sum_{i=n+1}^{2n} w_i + i\epsilon\right) \sum_{P_{fi}: w_f \neq w_1} \delta_{fi}^n$$

and a branch cut along the real axis from $-\infty$ to $(W - \mu - \sum_{i=2}^{n} w_i)$ (cf. Fig. 1).

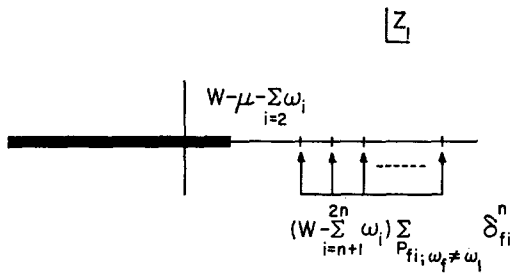


FIG. 1. Analytic structure of the function $F(W; z_1, w_2, \cdots, w_{2n})$ in the complex Z_1 plane with the assumption that $w_i < \mu$.

We are going to solve $F(W; z_1, w_2, \cdots, w_{2n})$ in the next section by constructing an iterative solution. After we get $F^-(W; w_1, w_2, \cdots, w_{2n})$ then by interchanging the pairs w_1 with w_i where $i = 2, 3, \cdots, n$, we get $F^-(W; w_2, w_1, \cdots, w_{2n})$, etc. Sum all these F's up and we have the whole solution for $N^-(W; w_1, \cdots, w_{2n})$, i.e., $\hat{\tau}^{4n+1}(W+m; w_1, \cdots, w_{2n})$. Since from Eq. (6) we know all the $\hat{\tau}^{4n+2}$(—), $\hat{\tau}^{4n+3}$(—), and $\hat{\tau}^{4n+4}$(—) can be written in terms of $\hat{\tau}^{4n+1}$(—), the solution of $F^-(W; w_1, w_2, \cdots, w_{2n})$ solves the entire V–$n\theta$ sector.

III. SOLUTION OF THE INTEGRAL EQUATION

In the last section, we derived an integral equation for the function $F(W; z_1, w_2, \cdots, w_{2n})$. It is too complicated for an exact solution, so we are going to construct an iterative method in a completely analogous way as we did in the V–2θ sector.[1] Again, it is required that each term of this expansion must preserve: (a) the properties of the bound state, (b) the analytic structure of $F(W; z_1, w_2, \cdots, w_{2n})$, and (c) the symmetry properties.

Let us now start from introducing a λ in front of the last term of Eq. (14) so that we get

$$\begin{aligned} &F(W; z_1, w_2, \cdots, w_{2n}) \\ &= \left(\prod_{i=2}^{n} \frac{2w_i}{u^2(w_i)}\right) \frac{\sum_{P_{fi}: w_f \neq w_1} \delta_{fi}^n}{\left(W - z_1 - \sum_{i=2}^{n} w_i\right)} \\ &\quad + \frac{1}{\pi} \int_\mu^\infty \frac{dw\, \mathrm{Im}\, h(w) F^-(W; w, w_2, \cdots, w_{2n})}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \\ &\quad + \frac{\lambda}{\pi} \int_\mu^\infty \frac{dw\, \mathrm{Im}\, h(w)}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \\ &\quad \times [F^-(W; w_2, w, w_3, \cdots, w_{2n}) \\ &\quad + F^-(W; w_3, w_2, w, w_4, \cdots, w_{2n}) + \cdots \\ &\quad + F^-(W; w_n, w_2, \cdots, w_{2n})] \end{aligned} \tag{15}$$

and, expressing F as a power series in λ, i.e.,

$$F(W; z_1, w_2, \cdots, w_{2n}) = \sum_{l=0}^{\infty} \lambda^l F_l(W; z_1, \cdots, w_{2n}). \tag{16}$$

Substituting Eq. (16) into Eq. (15) and equating terms of the same order in λ, we get

$$F_0(W; z_1, w_2, \cdots, w_{2n}) = \left(\prod_{i=2}^{n} \frac{2w_i}{u^2(w_i)}\right) \frac{\sum_{P_{fi}; w_f \neq w_1} \delta_{fi}^n}{\left(W - z_1 - \sum_{i=n+1}^{2n} w_i\right)} + \frac{1}{\pi} \int_{\mu}^{\infty} \frac{dw \operatorname{Im} h(w) F_0^-(W; w, w_2, \cdots, w_{2n})}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)}, \quad (17)$$

$$F_1(W; z_1, w_2, \cdots, w_{2n}) = \frac{1}{\pi} \int_{\mu}^{\infty} \frac{dw \operatorname{Im} h(w)}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \times [F_1^-(W; w, w_2, \cdots, w_{2n}) + F_0^-(W; w_2, w, w_3, \cdots, w_{2n}) + F_0^-(W; w_3, w_2, w, w_4, \cdots, w_{2n}) + \cdots + F_0^-(W; w_n, w, w_3, \cdots, w_{n-1}, w, w_{n+1}, \cdots, w_{2n})], \quad (18)$$

$$F_l(W; z_1, \cdots, w_{2n}) = \frac{1}{\pi} \int_{\mu}^{\infty} \frac{dw \operatorname{Im} h(w)}{\left(W - w - z_1 - \sum_{i=2}^{n} w_i\right) h\left(W - w - \sum_{i=2}^{n} w_i\right)} \times [F_l^-(W; w, w_2, \cdots, w_{2n}) + F_{l-1}^-(W; w_2, w, \cdots, w_{2n}) + \cdots + F_{l-1}^-(W; w_n, w_2, \cdots, w_{n-1}, w, w_{n+1}, \cdots, w_{2n})]. \quad (19)$$

At the end of the calculation, we set $\lambda = 1$ and then Eq. (15) goes back to the original equation (14).

From Eqs. (17)–(19), let us check the following properties:

(a) *The properties of the bound state:* In the following calculation, we will see that, as for the V–2θ sector, each term of the series can be written in terms of the function $U^-(W; w, w')$ which has a pole at the mass of the $(V\theta)$ bound state.[2] Thus, the properties of the $(V\theta)$ bound state are preserved by each term of the series.

(b) *Analytic structure:* In the complex z_1 plane, $F_0(W; z_1, w_2, \cdots, w_{2n})$ has $n!$ poles at

$$z_1 = \left(W - \sum_{i=n+1}^{2n} w_i + i\epsilon\right) \sum_{P_{fi}; w_f = w_1} \delta_{fi}^n.$$

Owing to the δ functions in F_0, $F_1(W; z_1, \cdots, w_{2n})$ has $n!$ poles at the same positions. Besides, all F_l's have branch cut along the real axis from $-\infty$ to $(W - \mu - \sum_{i=2}^{n} w_i)$. We compare these informations with the analytic structure of $F(W; z_1, w_2, \cdots, w_{2n})$ discussed earlier and see that each term of the series preserves the analytic structure.

(c) *Symmetry properties:* All $F_l(W; w_1, \cdots, w_{2n})$'s are symmetric under the interchange of θ particles in the initial state (i.e., w_i,where $i = n+1, n+2, \cdots, 2n$). The sums of all

$$[F_l^-(W; w_1, w_2, \cdots, w_{2n}) + F_l^-(W; w_2, w_1, \cdots, w_{2n}) + \cdots + F_l^-(W; w_n, w_2, \cdots, w_{n-1}, w_1, w_{n+1}, \cdots, w_{2n})]$$

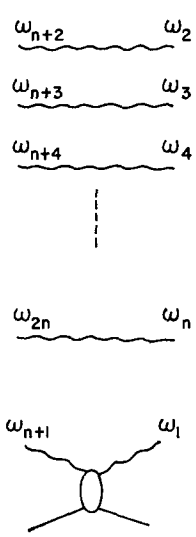
are symmetric under the interchange of the pairs w_1 with w_i, where $i = 2, 3, 4, \cdots, n$. Thus, we see each term of this series preserves the symmetry properties of the original τ function $\tau^{4n+1}(-)$.

By analogy with the solutions to Eq. (26)–(28) of Ref. 1, we can write down the solutions to Eq. (17)–(19) here as

$$F_0^-(W; w_1, w_2, \cdots, w_{2n}) = \prod_{i=2}^{n} \frac{2w_i}{u^2(w_i)} \left(\sum_{P_{fi}; w_f \neq w_1} \delta_{fi}^n\right) \times U^-\left(W - \sum_{i=2}^{n} w_i; w_1, \sum_{i=n+1}^{2n} w_i - \sum_{i=2}^{n} w_i\right) \quad (20)$$

(cf. Fig. 2),

$$F_1(W; z_1, w_2, \cdots, w_{2n}) = \frac{1}{\pi} \int_{\mu}^{\infty} \frac{dw \operatorname{Im} h(w)}{h\left(W - w - \sum_{i=2}^{n} w_i\right)} U\left(W - \sum_{i=2}^{n} w_i; z_1, w\right) \times [F_0^-(W; w_2, w, w_3, \cdots, w_{2n}) + F_0^-(W; w_3, w_2, w, w_4, \cdots, w_{2n}) + \cdots + F_0^-(W; w_n, w_2, \cdots, w_{n-1}, w, w_{n+1}, \cdots, w_{2n})], \quad (21)$$



+ (Diagrams with permutations of θ particles in initial state)

FIG. 2. Diagrams of the first-order term $F_0(W; w_1, \cdots, w_{2n})$ in the series expansion of $F^-(W; w_1, \cdots, w_{2n})$.

and

$$F_n(W; z_1, w_2, \cdots, w_{2n}) = \frac{1}{\pi}\int_\mu^\infty \frac{dw\ \mathrm{Im}\ h(w)}{h\left(W - w - \sum_{i=2}^n w_i\right)} U\left(W - \sum_{i=2}^n w_i; z_1, w\right) \times [F_{n-1}^-(W; w_2, w, w_3, \cdots, w_{2n}) + F_{n-1}^-(W; w_3, w_2, w, w_4, \cdots, w_{2n}) + \cdots + F_{n-1}^-(W; w_n, w_2, \cdots, w_{n-1}, w, w_{n+1}, \cdots, w_{2n})]. \quad (22)$$

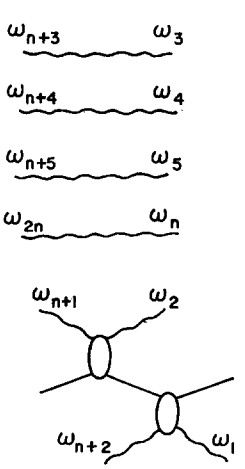
Substituting Eq. (20) into Eq. (21), we get

$$F_1^-(W; w_1, w_2, \cdots, w_{2n}) = g^2\left(\prod_{i=3}^n \frac{2w_i}{u^2(w_i)}\right)\frac{\delta_{k_2k_{n+3}}\delta_{k_4k_{n+4}}\cdots\delta_{k_nk_{2n}}}{h\left(W - w_{n+2} - \sum_{i=2}^n w_i\right)} \times U^-\left(W - \sum_{i=2}^n w_i; w_1, w_{n+2}\right) \times U^-\left(W - \sum_{i=3}^n w_i - w_{n+2}; w_2, w_{n+1}\right) + (\text{permutation of } \theta \text{ particles in the initial state}) + (\text{terms with } w_2 \text{ and } w_i \text{ interchanged where } i = 3, 4, \cdots, n) \quad (23)$$

(cf. Fig. 3).

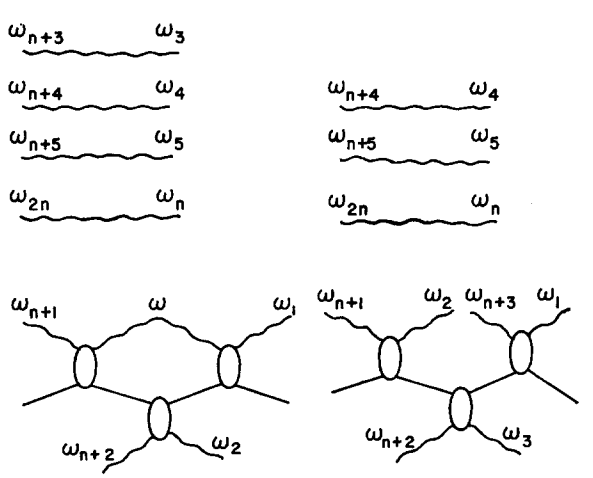
Substituting Eq. (23) into Eq. (22), we get F_2. Similarly, we can get F_3 and all the higher-order terms in the series expansion. The result of F_2 is (cf. Fig. 4)

$$\begin{aligned} F_2^-(W; w_1, \cdots, w_{2n}) = {} & g^2\left(\prod_{i=3}^n \frac{2w_i}{u^2(w_i)}\right)\delta_{k_2k_{n+3}}\delta_{k_4k_{n+4}}\cdots\delta_{k_nk_{2n}} \\ & \times \frac{1}{\pi}\int_\mu^\infty \frac{dw\ \mathrm{Im}\ h(w) U\left(W - \sum_{i=2}^n w_i; z_1, w\right) U^-\left(W - w - \sum_{i=3}^n w_i; w_2, w_{n+2}\right)}{h\left(W - w - \sum_{i=2}^n w_i\right) h\left(W - w - w_{n+2} - \sum_{i=3}^n w_i\right)} \\ & \times U^-\left(W - \sum_{i=3}^n w_i - w_{n+2}; w, w_{n+1}\right) + g^4\left(\prod_{i=4}^n \frac{2w_i}{u^2(w_i)}\right)\delta_{k_4k_{n+4}}\cdots\delta_{k_nk_{2n}} \\ & \times \frac{U^-\left(W - \sum_{i=2}^n w_i; w_1, w_{n+3}\right) U^-\left(W - \sum_{i=4}^n w_i - w_2 - w_{n+3}; w_3, w_{n+2}\right)}{h\left(W - w_{n+3} - \sum_{i=2}^n w_i\right) h\left(W - w_{n+2} - w_{n+3} - \sum_{i=4}^n w_i - w_2\right)} \\ & \times U^-\left(W - w_{n+2} - w_{n+3} - \sum_{i=4}^n w_i; w_2, w_{n+1}\right) \\ & + (\text{terms with permutations of } \theta \text{ particles in the initial state}) \\ & + (\text{terms with } w_2 \text{ and } w_i \text{ interchanged where } i = 3, 4, \cdots, n). \end{aligned} \quad (24)$$



+ (Diagrams of permutation in θ particles of initial stage)
+ (Diagrams with ω_2 and ω_i interchanged where i = 3,4,..n)

FIG. 3. Diagrams of the second-order term $F_1^-(W; w_1, \cdots, w_{2n})$.



+ (Diagrams of permutations in θ particles of initial state)
+ (Diagrams with ω_2 and ω_i interchanged where i = 3,4,..n)

FIG. 4. Diagrams of the third-order term $F_2^-(W; w_1, \cdots, w_{2n})$.

From Eqs. (20), (23), and (24) we see that each term of the series can be written in terms of the function $U^-(W; w, w')$ which can have a pole at the $(V\theta)$ bound state position,[2] so that, indeed, the properties of bound state are preserved.

Because the δ function corresponds to the θ particle without interaction and because of the above derivation, we see that for each term the number of δ functions is at least equal to $n - l$, where l is the order of the term in the expansion. So F_l for $l < n$ will not contribute to the nonforward scattering amplitude.

From Eq. (10) we have

$$\begin{aligned}
&\hat{\tau}^{4n+1}(W + m; w_1, \cdots, w_{2n}) \\
&= \left(\prod_{i=1}^{n} \frac{2w_i}{u^2(w_i)}\right) \frac{\sum_{P_{fi}} \delta_{fi}^n}{h\left(W - \sum_{i=1}^{n} w_i\right)} \\
&\quad + \frac{g^2}{h\left(W - \sum_{i=1}^{n} w_i\right) h\left(W - \sum_{i=n+1}^{2n} w_i\right)} \\
&\quad \times [F^-(W; w_1, w_2, \cdots, w_{2n}) \\
&\quad + F^-(W; w_2, w_1, \cdots, w_{2n}) + \cdots \\
&\quad + F^-(W; w_n, w_2, \cdots, w_{n-1}; w_1, w_{n+1}, \cdots, w_{2n})].
\end{aligned} \tag{25}$$

Substituting Eqs. (20), (23), and (24) into Eq. (25), we see that the first few terms of $\hat{\tau}^{4n+1}$ are (cf. Fig. 5)

$$\begin{aligned}
&\hat{\tau}^{4n+1}(W + m; w_1, \cdots, w_{2n}) \\
&= \left(\prod_{i=1}^{n} \frac{2w_i}{u^2(w_i)}\right) \frac{\sum_{P_{fi}} \delta_{fi}^n}{h\left(W - \sum_{i=1}^{n} w_i\right)} + \frac{g^2}{h\left(W - \sum_{i=1}^{n} w_i\right) h\left(W - \sum_{i=n+1}^{2n} w_i\right)} \\
&\quad \times \Bigg\{ \left(\prod_{i=2}^{n} \frac{2w_i}{u^2(w_i)}\right) \left(\sum_{P_{fi}; w_f \neq w_1} \delta_{fi}^n\right) U^-\left(W - \sum_{i=2}^{n} w_i; w_1, \sum_{i=n+1}^{2n} w_i - \sum_{i=2}^{n} w_i\right) \\
&\quad + \Bigg[\left(\prod_{i=3}^{n} \frac{2w_i}{u^2(w_i)}\right) \frac{\delta_{k_3 k_{n+3}} \delta_{k_4 k_{n+4}} \cdots \delta_{k_n k_{2n}}}{\left(hW - w_{n+2} - \sum_{i=2}^{n} w_i\right)} g^2 U^-\left(W - \sum_{i=2}^{n} w_i; w_1, w_{n+2}\right) U^-\left(W - \sum_{i=3}^{n} w_i - w_{n+2}; w_2, w_{n+1}\right) \\
&\quad + \left(\prod_{i=3}^{n} \frac{2w_i}{u^2(w_i)}\right) \delta_{k_3 k_{n+3}} \delta_{k_4 k_{n+4}} \cdots \delta_{k_n k_{2n}} \frac{g^4}{4\pi^2} \int_{\mu}^{\infty} \frac{dw (w^2 - \mu^2)^{\frac{1}{2}} u^2(w)}{h\left(W - w - \sum_{i=2}^{n} w_i\right) h\left(W - w - w_{n+2} - \sum_{i=3}^{n} w_i\right)} \\
&\quad \times U^-\left(W - \sum_{i=2}^{n} w_i; w_1, w\right) U^-\left(W - w - \sum_{i=3}^{n} w_i; w_2, w_{n+2}\right) U^-\left(W - \sum_{i=3}^{n} w_i - w_{n+2}; w, w_{n+1}\right) \\
&\quad + \left(\prod_{i=4}^{n} \frac{2w_i}{u^2(w_i)}\right) \delta_{k_4 k_{n+4}} \cdots \delta_{k_n k_{2n}} \times \frac{g^4 U^-\left(W - \sum_{i=2}^{n} w_i; w_1, w_{n+3}\right)}{h\left(W - w_{n+3} - \sum_{i=2}^{n} w_i\right)} \\
&\quad \times \frac{U^-\left(W - \sum_{i=4}^{n} w_i - w_2 - w_{n+3}; w_3, w_{n+2}\right) U^-\left(W - w_{n+2} - w_{n+3} - \sum_{i=4}^{n} w_i; w_2, w_{n+1}\right)}{h\left(W - w_{n+2} - w_{n+3} - \sum_{i=4}^{n} w_i - w_2\right)} \\
&\quad + (\text{terms with permutations of } \theta \text{ particles in the initial state}) \\
&\quad + (\text{terms with } w_2 \text{ and } w_i \text{ interchanged where } i = 3, 4, \cdots, n) \Bigg] \\
&\quad + (\text{terms with } w_1 \text{ and } w_i \text{ interchanged where } i = 2, 3, \cdots, n) \Bigg\}.
\end{aligned} \tag{26}$$

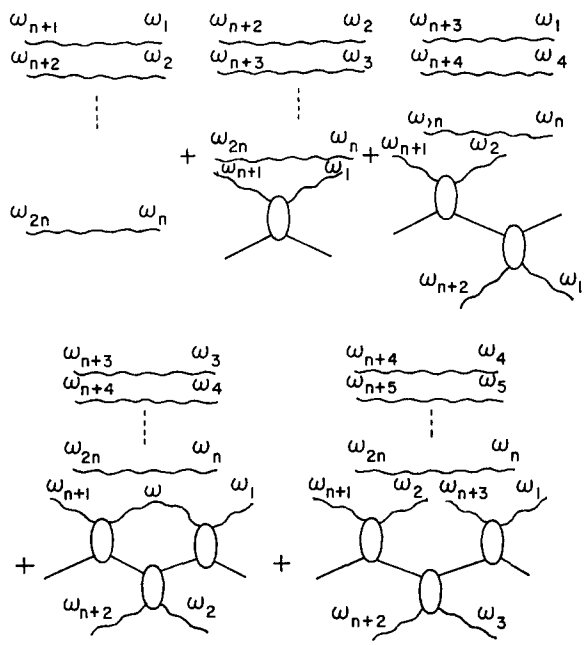


FIG. 5. Diagrams of the zeroth-, first-, second-, and third-order terms in $\hat{\tau}^{4n+1}(\hat{W}+m; w_1, \cdots, w_{2n})$.

From Eq. (26) we see that the key function $\hat{\tau}^{4n+1}$ in V–$n\theta$ sector can be written in terms of the function $U^-(W; w, w')$ which represents the fundamental V–θ interaction. By setting $n=2$, we can reduce Eq. (26) to the result for τ function in V–2θ sector[1] (i.e., $\hat{\tau}^9$).

Again, owing to the fact that $U^-(W; w, w') = U^-(W; w', w)$ we get the following symmetry property which was mentioned in Sec. II:

$$\hat{\tau}^{4n+1}(W+m; w_1, w_2, \cdots, w_n, \cdots, w_{2n}) = \hat{\tau}^{4n+1}(W+m; w_{n+1}, \cdots, w_{2n}, w_1, \cdots, w_n).$$

Just as the case in V–2θ sector, by this iterative expansion, we can approximate the function $\hat{\tau}^{4n+1}(W; w_1, \cdots, w_{2n})$ to an arbitrary order of the series in Eq. (16). Now let us write the rules for calculating to arbitrary order of $\hat{\tau}^{4n+1}(W; w_1, \cdots, w_{2n})$.

Notation

(1) A straight line ——— corresponds to a V particle.

(2) A wavy line ~~~~ corresponds to a θ particle.

(3) A bubble diagram ≈≈≈ corresponds to the function $U^-(W; w, w')$.

(4) $(w_{n+1}, w_{n+2}, \cdots, w_{2n})$ and $(w_1, w_2, \cdots, w_n)$ correspond to the energies of n incoming and outgoing θ particles, respectively.

Rules

$\hat{\tau}^{4n+1}$ is computed by drawing all generalized Feynman diagrams for a V and $n\theta$ particles coming in and going out. This indicates that both the connected and disconnected diagrams are included. The diagrams can have at most a four-point vertex because $\hat{\tau}^{4n+1}$ is in terms of $U^-(W; w, w')$. Specially we have the following:

(1) We integrate over each internal wavy line with energy w and multiply by a factor

$$\int_\mu^\infty \frac{dw u^2(w)(w^2-\mu^2)^{\frac{1}{2}}}{4\pi^2}.$$

(2) We multiply by an over-all factor

$$\left[h\left(W-\sum_{i=1}^{n} w_i\right)h\left(W-\sum_{i=n+1}^{2n} w_i\right)\right]^{-1}$$

for each individual diagram.

(3) The order of the series corresponds to the number of the bubble diagrams. We multiply by a factor g^2 for each bubble diagram.

(4) We multiply by a factor $[2w_0/u^2(w_0)]\delta_{k_0 k_i}$ for each wavy line without interaction [cf. Fig. 6(a)].

(5) We multiply by a factor

$$\left[h\left(W-w_l-\sum_{j=n+1;j\neq k}^{2n} w_j\right)\right]^{-1}$$

[cf. Fig. 6(a)] or

$$\left[h\left(W-w_k-\sum_{j=1;j\neq l}^{n} w_j\right)\right]^{-1}$$

[cf. Fig. 6(c)] for each internal straight line between two bubble diagrams.

(6) We multiply by a factor

$$U^-\left(W-\sum_{j=1;j\neq l}^{n} w_j; w_l, w_k\right)$$

for each bubble diagram with four external lines [cf. Fig. 6(d)].

(7) We multiply by a factor

$$U^-\left(W-\sum_{j=n+1;j\neq k}^{2n} w_j; w_l, w_k\right)$$

[cf. Fig. 6(e)] or

$$U^-\left(W-\sum_{j=1;j\neq l}^{n} w_j; w_l, w_k\right)$$

[cf. Fig. 6(f)] for each bubble diagram with one internal straight line or with a pair of external straight and wavy lines.

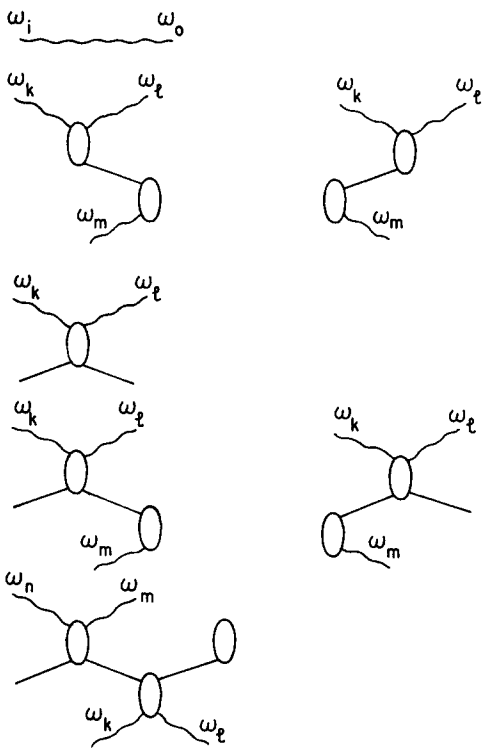


FIG. 6. Feynman rules correspond to (a) a wavy line without interaction, (b) and (c) each internal straight line between two bubbles, (d) each bubble diagram with four external lines, (e) and (f) each bubble diagram with one internal straight line or with a pair of external straight and wavy lines, (g) each bubble diagram with at least two internal straight lines.

(8) We multiply by a factor

$$U^{-}\left(W - w_m - \sum_{\substack{j=n+1 \\ j\neq n\neq k}}^{2n} w_j;\, w_l,\, w_k\right)$$

for each bubble diagram with at least two internal straight lines [cf. Fig. 6(g)].

IV. NONBOUND-STATE S-MATRIX ELEMENTS

Using the reduction formula and asymptotic conditions,[3] together with the definitions of the functions $\hat{\tau}^{4n+1}$, $\hat{\tau}^{4n+2}$, $\hat{\tau}^{4n+3}$, and $\hat{\tau}^{4n+4}$ (Eq. 1). S matrices corresponding to the processes

$$V + n\theta \to V + n\theta,$$
$$V + n\theta \to N + (n+1)\theta,$$
$$N + (n+1)\theta \to N + (n+1)\theta$$

can be written respectively as

$$S^{Vn\theta}_{k_1k_2\cdots k_n,k_{n+1}\cdots k_{2n}} = \frac{1}{n!}\sum_{P_{fi}}\delta^n_{fi} + 2\pi i\delta\left(\sum_{i=n+1}^{2n} w_i - \sum_{i=1}^{n} w_i\right) \times \frac{\left(\sum_{i=n+1}^{2n} w_i - \sum_{i=1}^{n} w_i\right)^2}{n!}\prod_{i=1}^{2n}\frac{u(w_i)}{(2w_i)^{\frac{1}{2}}} \times \hat{\tau}^{4n+1}(W+m; w_1,\cdots,w_{2n})\big|_{W=\sum_{i=1}^{n} w_i}, \quad (27)$$

$$S^{P}_{k_{n+2}k_{n+3}\cdots k_{2n+1},k_1\cdots k_{n+1}} = 2\pi i\delta\left(\sum_{i=n+2}^{2n+1} w_i - \sum_{i=1}^{n+1} w_i\right) \times \frac{\left(\sum_{i=n+2}^{2n+1} w_i - \sum_{i=1}^{n} w_i\right)^2}{[n!\,(n+1)!]^{\frac{1}{2}}} \times \prod_{i=1}^{2n+1}\frac{u(w_i)}{(2w_i)^{\frac{1}{2}}} \times \hat{\tau}^{4n+2}(W+m; w_1,\cdots,w_{2n+1})\big|_{W=\sum_{i=n+2}^{2n+1} w_i}, \quad (28)$$

$$S^{N(n+1)\theta}_{k_1k_2\cdots k_{n+1},k_{n+2}\cdots k_{2n+2}} = \frac{1}{(n+1)!}\sum_{P_{fi}}\delta^{n+1}_{fi} + 2\pi i\delta\left(\sum_{i=n+2}^{2n+2} w_i - \sum_{i=1}^{n+1} w_i\right) \times \frac{\left(\sum_{i=n+2}^{2n+2} w_i - \sum_{i=1}^{n+1} w_i\right)^2}{(n+1)!} \times \prod_{i=1}^{2n+2}\frac{u(w_i)}{(2w_i)^{\frac{1}{2}}} \times \hat{\tau}^{4n+4}(W+m; w_1,\cdots,w_{2n+2})\big|_{W=\sum_{i=1}^{n+1} w_i}. \quad (29)$$

Using the result of $\hat{\tau}^{4n+1}(-)$ in Eq. (26), the first few terms of the S-matrix element in Eq. (27) are

$$\begin{aligned} S^{Vn\theta}_{k_1k_2\cdots k_n,k_{n+1}\cdots k_{2n}} &= \frac{1}{n!}\sum_{P_{fi}}\delta^n_{fi} + 2\pi i\,\frac{\delta\left(\sum_{i=n+1}^{2n} w_i - \sum_{i=1}^{n} w_i\right)}{n!} \\ &\times \left\{\left(\prod_{i=2}^{n}\frac{2w_i}{u^2(w_i)}\right)\left(\sum_{P_{fi};w_f\neq w_1}\delta^n_{fi}\right)g^2 \right. \\ &\times U^{-}\left(w_1; w_1, \sum_{i=n+1}^{2n} w_i - \sum_{i=2}^{n} w_i\right) \\ &+ \left[\left(\prod_{i=3}^{n}\frac{2w_i}{u^2(w_i)}\right)\frac{g^4\delta_{k_3k_{n+3}}\cdots\delta_{k_nk_{2n}}}{h(w_1-w_{n+2})}\right. \\ &\times U^{-}(w_1; w_1, w_{n+2})U^{-}(w_{n+1}; w_2, w_{n+1}) \\ &+ \left(\prod_{i=3}^{n}\frac{2w_i}{u^2(w_i)}\right)\delta_{k_3k_{n+3}}\cdots\delta_{k_nk_{2n}}\frac{g^4}{4\pi^2} \\ &\times \int_{\mu}^{\infty}\frac{dwu^2(w)(w^2-u^2)}{h(w_1-w)h(w_{n+1}-w)}\,U^{-}(w_1; w_1, w) \\ &\times U^{-}(w_1+w_2-w; w_2, w_{n+2})U^{-}(w_{n+1}; w, w_{n+1}) \\ &+ g^4\left(\prod_{i=4}^{n}\frac{2w_i}{u^2(w_i)}\right) \\ &\times \frac{\delta_{k_4k_{n+4}}\cdots\delta_{k_nk_{2n}}}{h(w_1-w_{n+3})h(w_1+w_3-w_{n+2}-w_{n+3})} \\ &\times U^{-}(w_1; w_1, w_{n+3}) \\ &\times U^{-}(w_{n+1}+w_{n+2}-w_2; w_3, w_{n+2}) \\ &\times U^{-}(w_{n+1}; w_2, w_{n+1}) \\ &+ (\text{terms with permutations of } \theta \text{ particles in the initial state}) \\ &+ (\text{terms with } w_2 \text{ and } w_i \text{ interchanged where } i = 3, 4, \cdots, n)\Big] \\ &+ \left.(\text{terms with } w_1 \text{ and } w_i \text{ interchanged where } i = 2, 3, \cdots, n)\right\}. \end{aligned} \quad (30)$$

By using Eqs. (6b)–(6d), we can write the S matrices in Eq. (28) and (29) in terms of the functions $\hat{\tau}^{4n+1}(—)$

$$S^{P}_{k_{n+2}k_{n+3}\cdots k_{2n+1},k_1\cdots k_{n+1}} = 2\pi i\delta\left(\sum_{i=n+2}^{2n+1} w_i - \sum_{i=1}^{n+1} w_i\right) \frac{\left(\sum_{i=n+2}^{2n+1} w_i - \sum_{i=1}^{n} w_i\right)}{[n!\,(n+1)!]^{\frac{1}{2}}} \left(\prod_{i=1}^{2n+1} \frac{u(w_i)}{(2w_i)^{\frac{1}{2}}}\right)$$
$$\times g[\hat{\tau}^{4n+1}(W+m; w_2, w_3, \cdots, w_{2n+1}) + \hat{\tau}^{4n+1}(W+m; w_1, w_3, \cdots, w_{2n+1})$$
$$+ \cdots + \hat{\tau}^{4n+1}(W+m; w_1, w_2, \cdots, w_n, w_{n+2}, \cdots, w_{2n+1})]_W\Big|_{=\sum_{i=n+2}^{2n+1} w_i} \quad (31)$$

and

$$S^{N(n+1)\theta}_{k_1k_2\cdots k_{n+1},k_{n+2}\cdots k_{2n+2}} = \frac{1}{(n+1)!}\sum_{P_{fi}} \delta_{fi}^{n+1} + 2\pi i\delta\left(\sum_{i=n+2}^{2n+2} w_i - \sum_{i=1}^{n+1} w_i\right)$$
$$\times \frac{1}{(n+1)!}\prod_{i=1}^{2n+2} \frac{u(w_i)}{(2w_i)^{\frac{1}{2}}}\, g^2[\hat{\tau}^{4n+1}(W; w_2, \cdots, w_{n+1}, w_{n+3}, \cdots, w_{2n+2})$$
$$+ \hat{\tau}^{4n+1}(W; w_2, \cdots, w_{n+2}, w_{n+4}, \cdots, w_{2n+2})$$
$$+ \cdots + \hat{\tau}^{4n+1}(W; w_1, \cdots, w_n, w_{n+2}, \cdots, w_{2n+1})]\Big|_{W=\sum_{i=1}^{n+1} w_i}. \quad (32)$$

From Eqs. (30)–(32) we see that all the nonbound-state scattering amplitudes in V–$n\theta$ sector can be written in terms of $U^{-}(W; w, w')$, a key function in V–θ sector.

V. BOUND STATE SCATTERING IN V–$n\theta$ SECTOR

Since our iterative solutions for the τ functions in the V–$n\theta$ sector do preserve the information of the $\theta(V)$ bound state, we can start to study the following bound-state scattering processes:

(i) $(V\theta) + (n-1)\theta \to (V\theta) + (n-1)\theta$,

(ii) $(V\theta) + (n-1)\theta \to V + n\theta$,

(iii) $(V\theta) + (n-1)\theta \to N + (n+1)\theta$.

All necessary information and notations for studying bound-state scattering processes are referred to in Ref. 1.

Now let us work with case (i) by using the reduction formula[3] and the asymptotic condition.[4] The corresponding S matrix is

$$S_{k_1k_2\cdots k_{n-1},k_n\cdots k_{2n-2}} = \frac{1}{(n-1)!}\sum_{P_{fi}} \delta_{fi}^{n-1} - \frac{1}{|Z_{V\theta}|}\iint dt\,dt' \exp\left(i\sum_{i=1}^{n-1} w_i t' - i\sum_{i=n}^{2n-2} w_i t\right) \times \overrightarrow{\left(i\frac{d}{dt'} - \sum_{i=1}^{n-1} w_i - m_B\right)}$$
$$\times \langle 0|\, T(B_0^{V\theta}(t')a_{k_1}(t')a_{k_2}(t')\cdots a_{k_{n-1}}(t')\beta_0^{V\theta+}(t)a_{k_n}^{+}(t)\cdots a_{k_{2n-2}}^{+}(t))\,|0\rangle$$
$$\times \overleftarrow{\left(i\frac{d}{dt} + m_B + \sum_{i=n}^{2n-2} w_i\right)}, \quad (33)$$

where $B_0^{V\theta}(t)$, m_B, and $Z_{V\theta}$ are the general field operator, mass, and renormalization constant of the $(V\theta)$ bound state, respectively, and

$$B_0^{V\theta}(t) = A\psi_V(t)\int d^3k\, a_k(t) + C\psi_N(t)\iint d^3k\, d^3k' a_k(t)a_{k'}(t), \quad (34)$$

where A and C are arbitrary C-numbers.

From Eqs. (1), (6), and (34) we can reduce this S matrix to

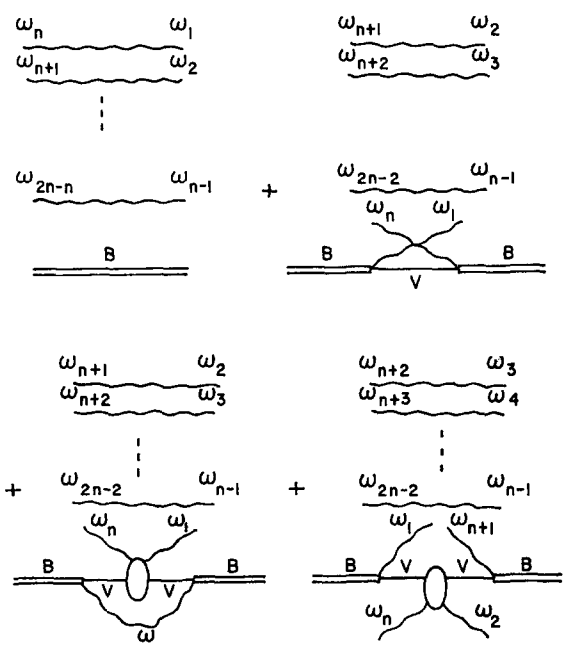
$$
\begin{aligned}
&S_{k_1 k_2 \cdots k_{n-1},\, k_n \cdots k_{2n-2}} \\
&= \frac{1}{(n-1)!}\sum_{P_{fi}} \delta_{fi}^{n-1} + \frac{2\pi i \delta\left(\sum_{i=n}^{2n-2} w_i - \sum_{i=1}^{n-1} w_i\right)}{|Z_{V\theta}|\,(n-1)!} \times \left(\sum_{i=n}^{2n-2} w_i - \sum_{i=1}^{n} w_i\right)^2 \\
&\quad \times \prod_{i=1}^{2n-2} \frac{u(w_i)}{(2w_i)^{\frac{1}{2}}} \Bigg\{ \iint d^3p_1\, d^3p_1' \, \frac{u(w_{p_1})u(w_{p_1'})}{(4w_{p_1}w_{p_1'})^{\frac{1}{2}}} \hat{\tau}^{4n+1}(W; w_{p_1}, w_1, w_2, \cdots, w_{n-1}, w_{p_1'}, w_n, \cdots, w_{2n-2}) \\
&\quad \times \left(A + 2gC \int d^3p_2 \frac{u(w_{p_2})}{(2w_{p_2})^{\frac{1}{2}}\left(W - m - w_{p_1} - w_{p_2} - \sum_{i=1}^{n-1} w_i\right)} \right) \\
&\quad \times \left(A^+ + 2gC^+ \int d^3p_2' \frac{u(w_{p_2'})}{(2w_{p_2'})^{\frac{1}{2}}\left(W - m - w_{p_1'} - w_{p_2'} - \sum_{i=n}^{2n-2} w_i\right)} \right) \\
&\quad + gC \iiint \frac{d^3p_1\, d^3p_2\, d^3p_1' u(w_{p_1})u(w_{p_2})u(w_{p_1'})}{(8w_{p_1}w_{p_2}w_{p_1'})^{\frac{1}{2}}\left(W - m - w_{p_2} - w_{p_2} - \sum_{i=1}^{n-1} w_i\right)} \\
&\quad \times \left(A^+ + 2gC^+ \int \frac{d^3g u(w_q)}{(2w_q)^{\frac{1}{2}}\left(W - m - w_q - w_{p_1'} - \sum_{i=n}^{2n-2} w_i\right)} \right) \\
&\quad \times [\hat{\tau}^{4n+1}(W; w_{p_1}, w_{p_2}, w_2, \cdots, w_{n-1}, w_{p_1'}, w_n, \cdots, w_{2n-2}) \\
&\quad + \hat{\tau}^{4n+1}(W; w_{p_1}, w_{p_2}, w_1, w_3, \cdots, w_{n-1}, w_{p_1'}, w_n, \cdots, w_{2n-2}) + \cdots \\
&\quad + \hat{\tau}^{4n+1}(W; w_{p_1}, w_{p_2}, w_1, \cdots, w_{n-2}, w_{p_1'}, w_n, \cdots, w_{2n-2})] \\
&\quad + gC^+ \iiint \frac{d^3p_1\, d^3p_1'\, d^3p_2' u(w_{p_1})u(w_{p_1'})u(w_{p_2'})}{(8w_{p_1}w_{p_1'}w_{p_2'})^{\frac{1}{2}}\left(W - m - w_{p_1'} - w_{p_2'} - \sum_{i=n}^{2n-2} w_i\right)} \\
&\quad \times \left(A + 2gC \int \frac{d^3q u(w_q)}{(2w_q)^{\frac{1}{2}}\left(W - m - w_q - w_{p_1} - \sum_{i=1}^{n-1} w_i\right)} \right) \\
&\quad \times [\hat{\tau}^{4n+1}(W; w_{p_1}, w_1, \cdots, w_{n-1}, w_{p_1'}, w_{p_2'}, w_{n+1}, \cdots, w_{2n-2}) \\
&\quad + \hat{\tau}^{4n+1}(W; w_{p_1}, w_1, \cdots, w_{n-1}, w_{p_1'}, w_{p_2'}, w_n, w_{n+2}, \cdots, w_{2n-2}) + \cdots \\
&\quad + \hat{\tau}^{4n+1}(W; w_{p_1}, w_1, \cdots, w_{n-1}, w_{p_1'}, w_{p_2'}, w_n, w_{n+1}, \cdots, w_{2n-3})] \\
&\quad + g^2 CC^+ \iiiint \frac{d^3p_1\, d^3p_2\, d^3p_1'\, d^3p_2' u(w_{p_1})u(w_{p_2})u(w_{p_1'})u(w_{p_2'})}{(16w_{p_1}w_{p_2}w_{p_1'}w_{p_2'})^{\frac{1}{2}}\left(W - m - w_{p_1} - w_{p_2} - \sum_{i=1}^{n-1} w_i\right)\left(W - m - w_{p_1'} - w_{p_2'} - \sum_{i=n}^{2n-2} w_i\right)} \\
&\quad \times [\hat{\tau}^{4n+1}(W; w_{p_1}, w_{p_2}, w_2, \cdots, w_{n-1}, w_{p_1'}, w_{p_2'}, w_{n+1}, \cdots, w_{2n-2}) \\
&\quad + \hat{\tau}^{4n+1}(W; w_{p_1}, w_{p_2}, w_1, w, \cdots, w_{n-1}, w_{p_1'}, w_{p_2'}, w_n, w_{n+2}, \cdots, w_{2n-2}) + \cdots \\
&\quad + \hat{\tau}^{4n+1}(W; w_{p_1}, w_{p_2}, w_1, w_2, \cdots, w_{n-2}, w_{p_1'}, w_{p_2'}, w_n, w_{n+1}, \cdots, w_{2n-3})] \\
&\quad + CC^+ \iiiint \frac{d^3p_1\, d^3p_2\, d^3p_1'\, d^3p_2'}{\left(W - m - w_{p_1} - w_{p_2} - \sum_{i=1}^{n-1} w_i\right)} \times \frac{4w_{p_1}w_{p_2}\prod_{i=1}^{n-1} 2w_i}{u^2(w_{p_1})u^2(w_{p_2})\prod_{i=1}^{n-1} u^2(w_i)} \times \sum_{P_{fi}} \delta_{fi}^{n+1} \Bigg\} \Bigg|_{W = m_{B^+} \sum_{i=1}^{n-1} w_i} .
\end{aligned}
\tag{35}
$$

From Eq. (26) we see that only the term with $\hat{\tau}^{4n+1}(W; w_{p_1}, w_1, \cdots, w_{n-1}, w_{p_1'}, w_n, \cdots, w_{2n-2})$ will contribute to the S matrix. All other terms in Eq. (35) will vanish as

$$\sum_{i=1}^{n-1} w_i \to \sum_{j=n}^{2n-2} w_j$$

because of the factor $(\sum_{i=1}^{n-1} w_i - \sum_{j=n}^{2n-2} w_j)^2$ multiplying them. So by using Eq. (26), the first few terms of this S matrix are (cf. Fig. 7)

$$\begin{aligned}
&S_{k_1 k_2 \cdots k_{n-1}, k_n \cdots k_{2n-2}} \\
&= \frac{1}{(n-1)!} \sum_{P_{fi}} \delta_{fi}^{n-1} + \frac{2\pi i \delta\left(\sum_{i=n}^{2n-2} w_i - \sum_{j=1}^{n-1} w_j\right)}{(n-1)!} \prod_{i=1}^{2n-2} \frac{u(w_i)}{(2w_i)^{\frac{1}{2}}} \\
&\times \Bigg[\left(\prod_{i=2}^{n-1} \frac{2w_i}{u^2(w_i)} \right) \delta_{k_2 k_{n+1}} \cdots \delta_{k_{n-1} k_{2n-2}} h(m_B - m - w_1) f^5(m_B; w_1) f^5(m_B; w_n) \\
&+ \left(\prod_{i=2}^{n-1} \frac{2w_i}{u^2(w_i)} \right) \delta_{k_2 k_{n+1}} \cdots \delta_{k_{n-1} k_{2n-2}} \times \frac{1}{4\pi^2} \int_\mu^\infty dw (w^2 - \mu^2)^{\frac{1}{2}} u^2(w) f^5(m_B; w) \\
&\times U^-(m_B - m - w_1; w_1, w_n) f^5(m_B; w) \\
&+ \left(\prod_{i=3}^{n-1} \frac{2w_i}{u^2(w_i)} \right) \delta_{k_3 k_{n+2}} \cdots \delta_{k_{n-1}} \delta_{2n-2} f^5(m_B; w_1) U^-(w_1 - w_{n+1} + m_B - m; w_2, w_n) f^5(m_B; w_{n+1}) \\
&+ (\text{terms with permutation of } \theta \text{ particles in the initial state}) \\
&+ (\text{terms with permutation of } \theta \text{ particles in the final state}) \Bigg]. \qquad (36)
\end{aligned}$$



+ (Diagrams with permutation of Θ particles in the initial state)

+ (Diagrams with permutation of Θ particles in the final state)

FIG. 7. Diagrams of S matrix for the elastic bound-state scattering process

$$(V\theta) + \theta_{k_n} + \cdots + \theta_{k_{2n-2}} \to (V\theta) + \theta_{k_1} + \cdots + \theta_{k_{n-1}}.$$

Similarly, we can calculate the inelastic cases (ii) and (iii) of the $(V\theta)$ bound-state scattering reactions. Leaving out the detailed calculations, we will now just write down the final results of S matrices to the first few terms as follows:

$$\text{(ii)}\quad (V\theta)+\theta_{k_n}+\theta_{k_{n+1}}+\cdots+\theta_{k_{2n-2}}\to V+\theta_k+\theta_{k_1}+\theta_{k_2}+\cdots+\theta_{k_{n-1}},$$

$$\begin{aligned}
S_{kk_1k_2\cdots k_{n-1},k_n\cdots k_{2n-2}} &= \frac{2\pi i}{[n!\,(n-1)!]^{\frac{1}{2}}}\times\frac{u(w)}{(2w)^{\frac{1}{2}}}\prod_{i=1}^{2n-2}\frac{u(w_i)}{(2w_i)^{\frac{1}{2}}}\,\delta\Big(m_B+\sum_{i=n}^{2n-2}w_i-m-w-\sum_{i=1}^{n-1}w_i\Big)\\
&\times\Bigg\{\Big(\prod_{i=2}^{n-1}\frac{2w_i}{u^2(w_i)}\Big)\delta_{k_2k_{n+1}}\cdots\delta_{k_{n-1}k_{2n-2}}\Big[g^2U^-(w;w,w_n)f^5(m_B;w_1)\\
&+\frac{g^2}{4\pi^2}\int_\mu^\infty dw''(w''^2-\mu^2)^{\frac{1}{2}}u^2(w'')U^-(w;w,w'')\\
&\times U^-(m_B-m+w_n-w'';w_1,w_n)\frac{f^5(m_B;w'')}{h(m_B-m+w_n-w_1-w'')}\Big]\\
&+g^2\prod_{i=3}^{n-1}\frac{2w_i}{u^2(w_i)}\,\delta_{k_3k_{n+2}}\cdots\delta_{k_{n-1}k_{2n-2}}U^-(w;w,w_{n+1})\\
&\times U^-(w+w_2-w_{n+1};w_2,w_n)\frac{f^5(m_B;w_1)}{h(w-w_{n+1})}\\
&+\text{(terms with permutation of }\theta\text{ particles in the initial state)}\\
&+\text{(terms with permutation of }\theta\text{ particles in the final state)}\Bigg\}
\end{aligned}\tag{37}$$

(cf. Fig. 8),

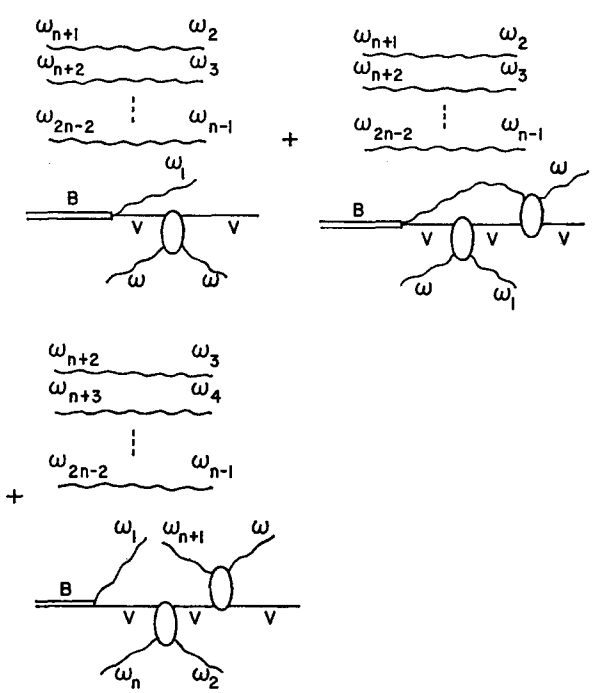


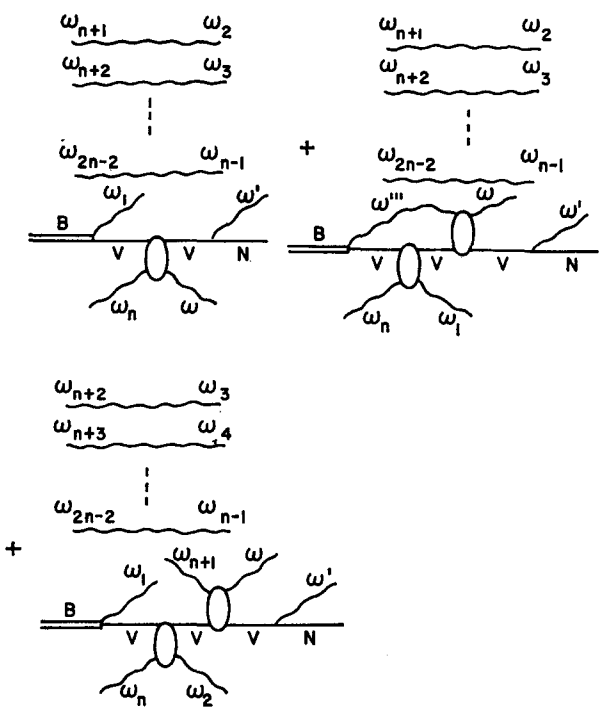
FIG. 8. Diagrams of S matrix for the inelastic bound-state scattering process

$$(V\theta)+\theta_{k_n}+\cdots+\theta_{k_{2n-2}}\to V+\theta_k+\theta_{k_1}+\cdots+\theta_{k_{n-1}}.$$

(iii) $(V\theta) + \theta_{k_n} + \cdots + \theta_{k_{2n-2}} \to N + \theta_k + \theta_{k'} + \theta_{k_1} + \cdots + \theta_{k_{n-1}}$,

$$
\begin{aligned}
&S_{kk'k_1\cdots k_{n-1},k_n\cdots k_{2n-2}} \\
&= \frac{2\pi i g^3}{[(n-1)!\,(n+1)!]^{\frac{1}{2}}}\,\delta\Big(m_B + \sum_{i=n}^{2n-2} w_i - m - w - w' - \sum_{i=1}^{n-1} w_i\Big)\frac{u(w)u(w')}{[4ww']^{\frac{1}{2}}}\prod_{i=1}^{2n-2}\frac{u(w_i)}{[2w_i]^{\frac{1}{2}}} \\
&\quad\times\Bigg[\prod_{i=2}^{n-1}\frac{2w_i}{u^2(w_i)}\,\delta_{k_2k_{n+1}}\cdots\delta_{k_{n-1}k_{2n-2}}\Bigg(\frac{U^-(w+w';w,w_n)f^5(m_B;w_1)}{h(w')} \\
&\quad+\frac{1}{4\pi^2}\int_\mu^\infty\frac{dw'''(w'''^2-\mu^2)^{\frac{1}{2}}u^2(w''')U^-(w+w';w,w''')U^-(w+w'+w_1-w''';w_1,w_n)f^5(m_B;w_1)}{h(w')h(w+w'-w''')}\Bigg) \\
&\quad+\prod_{i=3}^{n-1}\frac{2w_i}{u^2(w_i)}\,\delta_{k_3k_{n+2}}\cdots\delta_{k_{n-1}k_{2n-2}}\frac{U^-(w+w';w,w_{n+1})U^-(w+w'+w_2-w_{n+1};w_2,w_n)f^5(m_B;w_1)}{h(w')h(w+w'-w_{n+1})} \\
&\quad+(\text{terms with permutation of }\theta\text{ particles in the initial state}) \\
&\quad+(\text{terms with permutations of }\theta\text{ particles in the final state})\Bigg]
\end{aligned}
\tag{38}
$$

(cf. Fig. 9).



+ (Diagrams with permutation of θ particles in the initial state)
+ (Diagrams with permutation of θ particles in the final state)

FIG. 9. Diagrams of S matrix for the inelastic bound-state scattering process
$(V\theta) + \theta_{k_n} + \cdots + \theta_{k_{2n-2}} \to N + \theta_k + \theta_{k'} + \theta_{k_1} + \cdots + \theta_{k_{n-1}}$.

From Eqs. (36), (37), and (38) we see that once again we get the results that the S matrices of all the $(V\theta)$ bound-state scattering processes in the V–$n\theta$ sector are independent of the $(V\theta)$ bound-state field operator.

VI. CONCLUSION

In this article, we have investigated the scatterings in the general higher sector, i.e., V–$n\theta$ sector with $n > 2$ of the Lee model. The technique and procedures here are completely analogous to those in the V–2θ sector. By using an iterative expansion, we solved the τ functions $\hat{\tau}^{4n+1}(W; w_1, w_2, \cdots, w_{2n})$ in the Matthews–Salam equation of the V–$n\theta$ sector. Since all the S matrices for the bound-state and nonbound-state scattering processes can be written in terms of the function $\hat{\tau}^{4n+1}(-)$, the solution of $\hat{\tau}^{4n+1}$ solves the entire V–$n\theta$ sector.

As explained in the previous sections, each terms of the iterative expansion preserves the properties of the $(V\theta)$ bound state and the analytic structures and symmetries of the τ functions, the same as for $\hat{\tau}^9$ in V–2θ sector.[1] The result obtained for $\hat{\tau}^{4n+1}$ is again in terms of the key function $U^-(W; w, w')$ which represents the V–θ interaction. This is reasonable because there is no interaction between the θ particles in the Lee model. In other words, we essentially solved the many-body problem in terms of the 2-body solution, due to this restricted interaction assumed in the Lee model.

We have constructed the Feynman rules for calculating to an arbitrary order of the function $\hat{\tau}^{4n+1}(-)$.

Once again, in this general V–$n\theta$ sector, we obtained the interesting fact that the S matrices for the bound state scatterings are independent of the form of the $(V\theta)$ bound-state field operator. This same result was obtained elsewhere and also for the case of the $(V\theta)$ bound state in the V–2θ sector[1,4] and the V particle[5] in the Lee model.

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Multipole Moments. I. Flat Space

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There is an intimate connection between multipole moments and the conformal group. While this connection is not emphasized in the usual formulation of moments, it provides the starting point for a consideration of multipole moments in curved space. As a preliminary step in defining multipole moments in general relativity (a program which will be carried out in a subsequent paper), the moments of a solution of Laplace's equation in flat 3-space are studied from the standpoint of the conformal group. The moments emerge as certain multilinear mappings on the space of conformal Killing vectors. These mappings are re-expressed as a collection of tensor fields, which then turn out to be conformal Killing tensors (first integrals of the equation for null geodesics). The standard properties of multipole moments are seen to arise naturally from the algebraic structure of the conformal group.

INTRODUCTION

This is the first of two papers whose ultimate goal is to define the multipole moments of the gravitational field in a static asymptotically flat solution of Einstein's equations. The essential first step in this program is to reinterpret multipole moments in Euclidean 3-space in a way which emphasizes one particular aspect of flatness: the existence of conformal Killing vectors. This conformal approach to multipole moments in flat space is the subject of the present paper.

Choose an origin p for our Euclidean space. The multipole moments of a solution of $\nabla^2\psi = 0$ about this origin are, in the usual formulation, a collection of totally symmetric, trace-free tensors $Q, Q^a, Q^{ab}, \cdots$. The Q's of different ranks are completely independent. Let us now "attach" the Q's to the origin p, and permit changes in the choice of origin. Each of Q, Q^a, $Q^{ab}, \cdots$ thus becomes a tensor field. These tensor fields have the following properties: (1) a knowledge of $Q^{a_1\cdots a_s}$ as a tensor field uniquely determines all Q's of lower rank, and (2) a knowledge of $Q, Q^a, Q^{ab}, \cdots, Q^{a_1\cdots a_s}$ at a given origin uniquely determines the tensor field $Q^{a_1\cdots a_s}$. That is to say, the Q's have a very special, essentially algebraic, position dependence.

It turns out that, because of this simple position dependence, each $Q^{a_1\cdots a_s}$ is a conformal Killing tensor (a generalization of conformal Killing vectors). The fact that solutions of the conformally invariant[1] equation $\nabla^2\psi = 0$ are characterized by conformal Killing tensors suggests that it should be possible to make the transition from ψ to its multipole moments in some way which brings out the important role being played by the conformal group.

From the structure of the conformal group (in particular, from the fact that its invariant metric is nonsingular), we show that each tensor field $Q^{a_1\cdots a_s}$ may be interpreted as a multilinear mapping on the 10-dimensional vector space of conformal Killing vectors. Furthermore, these multilinear mappings can be obtained in a very simple way as 2-surface integrals of certain divergence-free vector fields constructed from ψ. We are thus able to pass from ψ to its multipole moments by the following steps: (1) introduce the collection of divergence-free vector fields, (2) integrate these fields over a 2-surface to obtain multilinear mappings on the space of conformal Killing vectors, and (3) interpret these multilinear mappings as tensor fields $Q, Q^a, Q^{ab}, \cdots$ on the original manifold.

There are three advantages to the present approach to multipole moments: (1) The multipole moments emerge directly as tensor fields on the manifold. We thus avoid both the arbitrary choice of an origin and the introduction of special coordinate systems. (2) In the usual formulation of multipole moments, it is necessary to integrate the components of tensor fields over the unit 2 sphere. While this procedure can be given a well-defined meaning in flat space, it is simpler and perhaps more within the spirit of differential geometry if all integrals involve closed forms over essentially arbitrary compact surfaces. (3) The intimate connection between multipole moments and the conformal group is almost entirely suppressed in the usual formulation. This connection is the key feature which will be needed in the subsequent paper to define the multipole moments of the gravitational field.

Some techniques and results concerning the conformal group are introduced in the appendices. Using concomitants, we develop in Appendix A an algebra of conformal Killing tensors. In Appendix B, we use conformal Killing transport to derive some of the basic properties of conformal Killing vectors and their multilinear mappings.

MULTIPOLE MOMENTS AS CONFORMAL KILLING TENSORS

Let ψ be a solution of $\nabla^2\psi = 0$ on a 3-dimensional manifold V with a flat, positive-definite metric h_{ab}. We are concerned with the definition and properties of the multipole moments of ψ. Although ψ may be considered as arising from some source distribution, we are interested only in the multipole moments themselves and not in their relation to sources. It is convenient, therefore, to have these source regions removed from V. We thus require that V be Euclidean 3-space with some region, topologically a 3-ball, removed, e.g., Euclidean space with a "hole in the middle."[2] We then demand $\nabla^2\psi = 0$ everywhere on V.

Let ξ^a be any conformal Killing vector on V, i.e., any solution of $\nabla_{(a}\xi_{b)} = \frac{1}{3}h_{ab}(\nabla_m\xi^m)$. Then the vector field $\xi^{a_1}\cdots\xi^{a_s}\nabla_m\nabla_{a_1}\cdots\nabla_{a_s}\psi$ on V is divergence free, i.e.,

$$\begin{aligned}\nabla^m(\xi^{a_1}\cdots\xi^{a_s}\nabla_m\nabla_{a_1}\cdots\nabla_{a_s}\psi)\\ = s(\nabla^m\xi^{a_1})\xi^{a_2}\cdots\xi^{a_s}\nabla_m\nabla_{a_1}\cdots\nabla_{a_s}\psi\\ + \xi^{a_1}\cdots\xi^{a_s}\nabla^m\nabla_m\nabla_{a_1}\cdots\nabla_{a_s}\psi = 0. \quad (1)\end{aligned}$$

Let K denote any closed 2-surface (topologically, a 2-sphere) surrounding the "hole" in V. (More precisely, K is to be any generator of the second homology group of V.) Then the integral

$$(4\pi)^{-1}\int_K(\xi^{a_1}\cdots\xi^{a_s}\nabla_m\nabla_{a_1}\cdots\nabla_{a_s}\psi)\,dS^m \quad (2)$$

is, by (1), independent of the choice of K. We have thus defined a multilinear mapping from the (10-dimensional) vector space $\mathcal{C}$ of conformal Killing vectors on V into the real line.

This collection ($s = 0, 1, 2, \cdots$) of multilinear mappings contains precisely the information of the multipole moments of ψ. In order to deal with such mappings, it is convenient to introduce the algebra of tensors over $\mathcal{C}$. These tensors are constructed from $\mathcal{C}$ in the standard way,[3] using tensor products and duals. They are labeled by Greek indices. Thus, for example, the conformal Killing vector ξ^a, considered as an element of $\mathcal{C}$, is written ξ^α, while V^α_β denotes a linear mapping from $\mathcal{C}$ to $\mathcal{C}$, and $W_{\alpha\beta}$ denotes a bilinear mapping from $\mathcal{C}$ to the real line. In this notation, the multilinear mapping (2) takes the form $Q_{\alpha_1\cdots\alpha_s}\xi^{\alpha_1}\cdots\xi^{\alpha_s}$, where $Q_{\alpha_1\cdots\alpha_s}$ is some totally symmetric tensor over $\mathcal{C}$. We now derive some properties of the tensors Q, Q_α, $Q_{\alpha\beta}$, $\cdots$. In particular, the Q's are shown to lead directly to the more conventional representation of multipole moments.

We first show how the Q's can be interpreted as tensor fields on our original manifold V. If ξ^a and ξ'^a are two conformal Killing vectors, then their Lie bracket $\xi''^a = \xi^m\nabla_m\xi'^a - \xi'^m\nabla_m\xi^a$ is also a conformal Killing vector. That is to say, $\mathcal{C}$ has the structure of a Lie algebra, in addition to its vector space structure. Therefore, we have a tensor $C^\mu{}_{\alpha\beta} = C^\mu{}_{[\alpha\beta]}$ (the structure constants[4]) over $\mathcal{C}$ such that the bracket operation is given by $\xi''^\mu = C^\mu{}_{\alpha\beta}\xi^\alpha\xi'^\beta$. (For example, the Jacobi identity, written in terms of $C^\mu{}_{\alpha\beta}$, takes the form $C^\mu{}_{\nu[\alpha}C^\nu{}_{\beta\gamma]} = 0$.) Now consider the symmetric tensor[4]

$$G_{\alpha\beta} = -C^\mu{}_{\nu\alpha}C^\nu{}_{\mu\beta}$$

over $\mathcal{C}$. It is shown in Appendix B that $G_{\alpha\beta}$ is nonsingular [and, in fact, that its signature is $(+, +, +, +, +, +, -, -, -, -)$]. Therefore, $G_{\alpha\beta}$ has an inverse: there is a unique symmetric tensor $G^{\alpha\beta}$ such that $G^{\alpha\mu}G_{\beta\mu} = \delta^\alpha{}_\beta$. This metric $G_{\alpha\beta}$ and its inverse can be used to raise and lower the indices of any tensor over $\mathcal{C}$.

In particular, raising the indices of the Q's, we obtain their "contravariant" versions, Q, Q^α, $Q^{\alpha\beta}$, $\cdots$. Since $Q^{\alpha_1\cdots\alpha_s}$ is a tensor over $\mathcal{C}$, it may be written (not uniquely) as a sum of the form

$$Q^{\alpha_1\cdots\alpha_s} = \xi^{\alpha_1}\cdots\xi^{\alpha_s} + \cdots + \eta^{\alpha_1}\cdots\eta^{\alpha_s}, \quad (3)$$

where each of $\xi^\alpha, \cdots, \eta^\alpha$, as an element of $\mathcal{C}$, represents a conformal Killing vector on V. The expression (3) suggests that we consider the tensor field

$$Q^{a_1\cdots a_s} = \xi^{a_1}\cdots\xi^{a_s} + \cdots + \eta^{a_1}\cdots\eta^{a_s} \quad (4)$$

on V. Clearly, this $Q^{a_1\cdots a_s}$ is independent of the particular expansion of $Q^{\alpha_1\cdots\alpha_s}$ in (3). We thus have a well-defined sequence Q, Q^a, Q^{ab}, $\cdots$ of totally symmetric tensor fields on V. Each $Q^{a_1\cdots a_s}$ is, in fact, a conformal Killing tensor. That is to say, the trace-free part of its totally symmetrized derivative vanishes. (A proof of this fact, along with a discussion of some properties of conformal Killing tensors, is given in Appendix A.) To summarize, the information of the multipole moments of ψ has now been represented as a sequence of conformal Killing tensors on V.

The tensor fields defined above have a simple interpretation. In the usual formulation of multipole moments, one first fixes an origin and then assigns to ψ a monopole, dipole, quadrupole, etc., moment with respect to that origin. These moments turn out to be precisely the values of the tensors Q, Q^a, Q^{ab}, $\cdots$ at the given origin. Since the multipole moments about an origin are trace-free, we expect the Q's to be trace-free tensor fields. Furthermore, we would expect that the change in, say, the octopole moment as we move the origin should depend only on the quadrupole, dipole, and monopole moments. Thus, it should

be possible to find an equation relating the derivative of $Q^{a_1\cdots a_s}$ to the values of the Q's of lower rank. We shall now derive these properties of the multipole moment fields.

We first consider the trace-free condition. It is shown in Appendix B that, for each integer s (≥ 2), there is a tensor $P^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s} = P^{(\alpha_1\cdots\alpha_t)}{}_{(\beta_1\cdots\beta_s)}$ over $\mathcal{C}$ which may be interpreted as the projection operator which corresponds to the operation "taking the trace-free part" of conformal Killing tensors on the manifold V. More precisely, P has the following properties:

(1) $P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s}P^{\mu_1\cdots\mu_s}{}_{\beta_1\cdots\beta_s} = P^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s}$;

(2) Let $T^{\alpha_1\cdots\alpha_s}$ be a totally symmetric tensor over $\mathcal{C}$. Then the conformal Killing tensor obtained, via (3) and (4), from $P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s}T^{\mu_1\cdots\mu_s}$ is precisely the trace-free part of the conformal Killing tensor obtained from $T^{\alpha_1\cdots\alpha_s}$.

Furthermore, this $P^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s}$ is found to satisfy the condition

$$P_{\alpha_1\cdots\alpha_s\beta_1\cdots\beta_s} = P_{\beta_1\cdots\beta_s\alpha_1\cdots\alpha_s}. \tag{5}$$

Equation (5) furnishes a simple proof that the multipole moment tensors are trace free. Since $\nabla^2\psi = 0$, it follows that the value of the integral (2) is unchanged if the conformal Killing tensor $\xi^{a_1}\cdots\xi^{a_s}$ in the integrand is replaced by its trace-free part. That is to say, we have

$$Q_{\alpha_1\cdots\alpha_s}\xi^{\alpha_1}\cdots\xi^{\alpha_s} = Q_{\mu_1\cdots\mu_s}P^{\mu_1\cdots\mu_s}{}_{\alpha_1\cdots\alpha_s}\xi^{\alpha_1}\cdots\xi^{\alpha_s}. \tag{6}$$

But (6) must hold for all ξ^α, and, therefore, holds with the ξ^α's deleted. It now follows from (5) and from the second property of P described above that $Q^{a_1\cdots a_s}$ is trace free.

The second property we expect of our multipole moment fields is that the derivative of $Q^{a_1\cdots a_s}$ be expressible in terms of the values of the Q's of lower rank. We now derive this expression. It follows from the K independence of the integral (2) that

$$\int_K \epsilon_m{}^{pq}\pounds_{\xi'}[\epsilon_{pqr}(\nabla^r\nabla_{a_1}\cdots\nabla_{a_s}\psi)\xi^{a_1}\cdots\xi^{a_s}]\,dS^m = 0, \tag{7}$$

where ξ'^a is any vector field on V. In particular, choose ξ' to be a conformal Killing vector. Defining the skew tensor F'_{ab} and the scalar φ' by $\nabla_a\xi'_b = F'_{ab} + \varphi' h_{ab}$, Eq. (7) takes the form

$$\begin{aligned}\int_K [&\xi'^b\xi^{a_2}\cdots\xi^{a_s}\nabla_m\nabla_b\nabla_{a_2}\cdots\nabla_{a_s}\psi\\ &+ (s+2)\varphi'\xi^{a_2}\cdots\xi^{a_s}\nabla_m\nabla_{a_2}\cdots\nabla_{a_s}\psi\\ &+ (s+1)\xi^{a_2}\cdots\xi^{a_s}F'_{(m}{}^x\nabla_{a_2}\cdots\nabla_{a_s)}\nabla_x\psi\\ &+ s(\pounds_{\xi'}\xi)^{a_2}\xi^{a_3}\cdots\xi^{a_s}\nabla_m\nabla_{a_2}\cdots\nabla_{a_s}\psi]\,dS^m = 0.\end{aligned} \tag{8}$$

Finally, we specialize further to the case in which F'_{ab} and φ' are both constant.[5] Each term in (8) represents a multilinear mapping on ξ^a. The first term is simply $Q_{\alpha_1\cdots\alpha_s}\xi'^{\alpha_1}\xi^{\alpha_2}\cdots\xi^{\alpha_s}$ while the subsequent terms involve only $Q_{\alpha_2\cdots\alpha_s}$. Thus, Eq. (8) represents a relation between $Q_{\alpha_1\cdots\alpha_s}$ and $Q_{\alpha_2\cdots\alpha_s}$. Re-expressing (8) in terms of the corresponding conformal Killing tensors, $Q^{a_1\cdots a_s}$ and $Q^{a_2\cdots a_s}$, we obtain the desired result

$$\begin{aligned}\nabla^m Q^{a_1\cdots a_s} = {}&\tfrac{1}{3}s(2s-1)h^{m(a_1}Q^{a_2\cdots a_s)}\\ &- \tfrac{1}{3}s(s-1)Q^{m(a_3\cdots a_s}h^{a_1a_2)}.\end{aligned} \tag{9}$$

Equation (9) (for $s = 0, 1, 2, \cdots$) is the necessary and sufficient condition that a sequence Q, Q^a, Q^{ab}, $\cdots$ of totally symmetric, trace-free tensor fields represent the multipole moments of some solution of $\nabla^2\psi = 0$. [Note that (9) automatically implies that each $Q^{a_1\cdots a_s}$ is a conformal Killing tensor.] In addition, we see from (9) that each $Q^{a_1\cdots a_s}$ uniquely determines its predecessors for, contracting (9) once, we obtain

$$\nabla_m Q^{ma_2\cdots a_s} = \tfrac{1}{3}s(2s+1)Q^{a_2\cdots a_s}.$$

On the other hand, a knowledge of all Q's of rank less than s determines $Q^{a_1\cdots a_s}$ only up to a constant tensor. That is, $Q^{a_1\cdots a_s}$ provides new information equivalent to $2s+1$ numbers, as we would expect.

In the conventional treatment of multipole moments, one often "goes to the center of mass" in order to represent the moments as tensors at a single point rather than as tensor fields. This procedure may be described in the following way. First note that, as a consequence of (9), the dipole moment Q^a is a dilation, i.e., a conformal Killing vector with vanishing curl (see Appendix B), provided the monopole moment Q does not vanish. (When $Q = 0$, Q^a is a translation.) Thus, assuming $Q \neq 0$, there is always a unique point p at which $Q^a = 0$. This point is the center of mass, and the values of the other multipole moment fields at p represent the multipole moments with respect to the center of mass.

It is convenient (particularly for applications to curved space) to reformulate this procedure in a way in which the center of mass need not be determined explicitly. This can be done very simply. Assuming $Q \neq 0$, define

$$\begin{aligned}\tilde{Q}^{a_1\cdots a_s} = {}&Q^{a_1\cdots a_s} + \mathcal{C}\sum\frac{s!}{r!}\frac{(-1)^{s-r}}{s-r}(2s-1)\\ &\times(2s-3)\cdots(2r+1)Q^{r-s}Q^{(a_1\cdots a_r}Q^{a_{r+1}}\cdots Q^{a_s)}\end{aligned}$$

for $s = 2, 3, \cdots$, where $\mathcal{C}$ denotes the operation of taking the trace-free part. Taking a derivative of $\tilde{Q}^{a_1\cdots a_s}$, using (9), we obtain zero. Clearly, the constant tensors defined by Eq. (10) represent precisely the multipole moments referred to the center of mass.

Finally, we remark that similar techniques can be used for the moments of a field of arbitrary spin in a flat space of arbitrary signature and dimension, in particular, for the linearized gravitational field in Minkowski space.

APPENDIX A: CONFORMAL KILLING TENSORS

In this appendix, we develop a formalism for dealing with conformal Killing tensors in curved space.[6]

A conformal Killing vector P^a may be defined as a vector field such that, for any null geodesic with affine[7] tangent vector l_a, $(l_a P^a)$ is constant along the geodesic. Conformal Killing vectors thus represent linear first integrals of the equations of a null geodesic. First integrals of higher order (quadratic, cubic, etc.) in l_a define conformal Killing tensors. That is, a symmetric tensor field $P^{a\cdots c}$ is a *conformal Killing tensor*[8] if, for any null geodesic[9] with affine tangent vector l_a, $(l_a \cdots l_c P^{a\cdots c})$ is constant along the geodesic. Clearly, a necessary and sufficient condition that $P^{a\cdots c}$ be a conformal Killing tensor is that, for some $T^{b\cdots c}$,

$$\nabla^{(m} P^{ab\cdots c)} = h^{(ma} T^{b\cdots c)}. \tag{A1}$$

For example, both the metric tensor h^{ab} and any symmetrized outer product of conformal Killing vectors are conformal Killing tensors.

It is convenient to view the basic algebra of conformal Killing tensors within the framework of a much more general algebra: that of all totally symmetric contravariant tensor fields on the manifold. The reason for this is that the latter can be fully developed without introducing any metric. All relevant operations on totally symmetric contravariant tensors are defined at the beginning. The metric then serves merely to pick out a certain subalgebra, consisting of the conformal Killing tensors, from this much larger algebra.

There are three basic operations on totally symmetric contravariant tensors on a manifold. The first operation is the sum, which is defined whenever the two tensors have the same rank. The second operation is the product. If $P^{a_1\cdots a_p}$ and $Q^{a_1\cdots a_q}$ are totally symmetric, we set

$$P \cap Q = P^{(a_1\cdots a_p} Q^{a_{p+1}\cdots a_{p+q})} = Q \cap P. \tag{A2}$$

[Multiplication of tensors by scalars is viewed as a special case of (A2).] The third operation is a generalization of the Lie bracket of vector fields. The bracket of $P^{a_1\cdots a_p}$ and $Q^{a_1\cdots a_q}$ is defined by

$$\begin{aligned}(P, Q) &= pP^{m(a_1\cdots a_{p-1}} D_m Q^{a_p\cdots a_{p+q-1})} \\ &\quad - qQ^{m(a_1\cdots a_{q-1}} D_m P^{a_q\cdots a_{p+q-1})} \\ &= -(Q, P),\end{aligned} \tag{A3}$$

where, in (A3), D_m is an arbitrary (torsion-free) derivative operator.[10] It is easily verified that the right-hand side of (A3) is independent of the choice of D_m, i.e., that (A3) defines a concomitant.[11] When P is a vector, (A3) reduces to the Lie derivative.

Our three operations satisfy a number of trivial relations: associativity and commutativity of the sum and product, anticommutativity of the bracket, and linearity of the product and bracket. There are, however, two further relations. The first relates the product and bracket:

$$(P, Q \cap R) = (P, Q) \cap R + (P, R) \cap Q. \tag{A4}$$

The second generalizes the Jacobi identity for vector fields to tensors of arbitrary rank:

$$(P, (Q, R)) + (Q, (R, P)) + (R, (P, Q)) = 0. \tag{A5}$$

[To prove (A5), it is only necessary to observe that it reduces to the Jacobi identity when P, Q, and R are vectors, and that if (A5) holds for P, Q, R and for P, Q, R', then, by virtue of (A4), it also holds for P, Q, $R \cap R'$.[12]]

We now return to conformal Killing tensors. Let h denote the contravariant metric h^{ab}. Then the condition (A1) that P be a conformal Killing tensor may be written in the form

$$(h, P) = h \cap T. \tag{A6}$$

The sum of two conformal Killing tensors of the same rank is, evidently, a conformal Killing tensor. Furthermore, using the definition (A6), it follows from (A4) that the product and from (A5) that the bracket of two conformal Killing tensors is a conformal Killing tensor. That is, conformal Killing tensors produce conformal Killing tensors under all three of our basic operations. The introduction of a preferred element h thus serves to define a preferred subalgebra of the algebra of all totally symmetric contravariant tensors on the manifold.[13]

APPENDIX B: THE ALGEBRA OF CONFORMAL KILLING VECTORS IN FLAT SPACE

Let V be a manifold with a flat, nonsingular metric h_{ab}. As the present discussion may be useful in various applications, we allow V to have dimension n (≥ 3) and h_{ab} to have signature with p plus's and q minus's ($p + q = n$). We next assume that (V, h_{ab}) has the property that parallel transport of any vector around any closed curve in V leaves that vector invariant. This assumption, which always holds for a simply-connected space (and which, therefore, always holds locally), is necessary to avoid certain complications of a global nature. In particular, it ensures that V will have the proper number of conformal Killing vectors.

Let $\boldsymbol{\xi}^a$ be a conformal Killing vector on V. Set

$$\begin{aligned} \mathbf{F}_{ab} &= \nabla_{[a}\boldsymbol{\xi}_{b]}, \\ \boldsymbol{\varphi} &= n\nabla_m\boldsymbol{\xi}^m, \\ \mathbf{k}_a &= \nabla_a\boldsymbol{\varphi}. \end{aligned} \tag{B1}$$

It then follows[14] from the conformal Killing equation on $\boldsymbol{\xi}^a$ that

$$\begin{aligned} &\nabla_a\boldsymbol{\xi}_b = \mathbf{F}_{ab} + \boldsymbol{\varphi}h_{ab}, \quad \nabla_a\boldsymbol{\varphi} = \mathbf{k}_a, \\ &\nabla_a\mathbf{F}_{bc} = -2h_{a[b}\mathbf{k}_{c]}, \quad \nabla_a\mathbf{k}_b = 0. \end{aligned} \tag{B2}$$

We see from (B2) that the values of the four tensors $\boldsymbol{\xi}^a$, $\mathbf{F}_{ab}$, $\boldsymbol{\varphi}$, and $\mathbf{k}_a$ at a single point p of V (called the *data* for $\boldsymbol{\xi}^a$ at p) define these tensors everywhere. Explicitly, if the data for $\boldsymbol{\xi}^a$ at p is $(\xi^a, F_{ab}, \varphi, k_a)$, then the data at p' is

$$\begin{aligned} \xi'^a &= \xi^a + F_m{}^a x^m + \varphi x^a + x^a(x^m k_m) - \tfrac{1}{2}k^a(x^m x_m), \\ F'_{ab} &= F_{ab} - 2x_{[a}k_{b]}, \\ \varphi' &= \varphi + x^m k_m, \\ k'_a &= k_a, \end{aligned} \tag{B3}$$

where x^m is the position vector[15] of p' relative to p. Thus, there is a 1-to-1 correspondence between conformal Killing vectors on V and data at a fixed point of V. By using this correspondence, we shall be able to represent certain objects in the space of conformal Killing vectors explicitly as tensors on V.

Let $\mathcal{C}$ denote the $\frac{1}{2}(n^2+3n+2)$-dimensional[16] vector space of conformal Killing vectors on V. Tensors over $\mathcal{C}$ will be labeled by Greek indices. For example, the commutator of two conformal Killing vectors, $\boldsymbol{\xi}''^a = \boldsymbol{\xi}^m\nabla_m\boldsymbol{\xi}'^a - \boldsymbol{\xi}'^m\nabla_m\boldsymbol{\xi}^a$, is again a conformal Killing vector, and so we may introduce the tensor $C^\mu{}_{\alpha\beta}$ over $\mathcal{C}$ such that $\xi''^\mu = C^\beta{}_{\alpha\beta}\xi^a\xi'^\beta$. Using (B1), we obtain an explicit expression for the action of $C^\mu{}_{\alpha\beta}$ in terms of the data for $\boldsymbol{\xi}''^a$, $\boldsymbol{\xi}^a$, and $\boldsymbol{\xi}'^a$:

$$\begin{aligned} \xi''^a &= F'_m{}^a\xi^m - F_m{}^a\xi'^m + \varphi'\xi^a - \varphi\xi'^a, \\ F''_{ab} &= 2k'_{[a}\xi_{b]} - 2k_{[a}\xi'_{b]} - 2F'_{m[a}F^m{}_{b]}, \\ \varphi'' &= \xi^m k'_m - \xi'^m k_m, \\ k''_a &= k^m F'_{ma} - k'^m F_{ma} + \varphi k'_a - \varphi' k_a. \end{aligned} \tag{B4}$$

The relation (B4) is independent of the point p at which the data are taken in the following sense: (B4) remains valid if (B3) is applied simultaneously to the data for all three conformal Killing vectors.

An important element of the algebra of conformal Killing vectors is the invariant metric,

$$G_{\alpha\beta} = -C^\mu{}_{\nu\alpha}C^\nu{}_{\mu\beta}.$$

Using (B4), we obtain an expression for $G_{\alpha\beta}$ in terms of data at an arbitrary point:

$$G_{\alpha\beta}\xi^\alpha\xi^\beta = n[F_{ab}F^{ab} - 2\varphi^2 + 4\xi^a k_a]. \tag{B5}$$

We see from (B5) that the signature of $G_{\alpha\beta}$ consists of $\frac{1}{2}(p^2+q^2+p+q)$ plus's and $(p+q+pq+1)$ minus's.[17] In particular, $G_{\alpha\beta}$ is nonsingular. On the other hand, $G_{\alpha\beta}$ *is* singular when applied only to Killing vectors (conformal Killing vectors for which $\varphi = 0$ and $k_a = 0$). It is because the conformal Killing vectors have a nonsingular metric, while the Killing vectors do not, that the algebra of the former is much simpler than that of the latter.

We may use $G_{\alpha\beta}$ and its inverse metric $G^{\alpha\beta}$ to raise and lower the indices of any tensor over $\mathcal{C}$. In particular, any tensor $T_{\alpha\cdots\beta}{}^{\mu\cdots\nu}$ over $\mathcal{C}$ can be written in its "covariant" form $T_{\alpha\cdots\beta\,\mu\cdots\nu}$. But $T_{\alpha\cdots\beta\,\mu\cdots\nu}$ represents a multilinear mapping on $\mathcal{C}$, and, therefore, a multilinear mapping at each point p on the data at p for elements of $\mathcal{C}$. Finally, multilinear mappings on data at p can be written as tensors (on V) at p. Any tensor over $\mathcal{C}$ can thus be represented explicitly as a collection of tensor fields on V. As an example, consider

$$C_{\alpha\beta\gamma} = G_{\alpha\mu}C^\mu{}_{\beta\gamma}.$$

Taking the inner product of (B4) with an arbitrary element of $\mathcal{C}$, using (B5), we find

$$\begin{aligned} &C_{\alpha\beta\gamma}\xi''^\alpha\xi'^\beta\xi^\gamma \\ &\quad = 4n(F''^{ab}k_a\xi'_b - F''^{ab}k'_a\xi_b + F^{ab}k'_a\xi''_b - F^{ab}k''_a\xi_b \\ &\qquad + F'^{ab}k''_a\xi_b - F'^{ab}k_a\xi''_b) + 2n(\varphi'\xi''^a k_a - \varphi'\xi^a k''_a \\ &\qquad + \varphi\xi'^a k''_a - \varphi\xi''^a k'_a + \varphi''\xi^a k'_a - \varphi''\xi'^a k_a) \\ &\qquad + 2nF_a{}^b F'^c_b F''^a_c. \end{aligned}$$

We conclude that $C_{\alpha\beta\gamma}$ is totally antisymmetric.

We have seen [Eqs. (3) and (4)] that a totally symmetric contravariant tensor over $\mathcal{C}$ defines a unique conformal Killing tensor on the manifold V. In fact, this construction was an essential step in expressing the multipole moments as tensor fields on the manifold. We might ask, however, whether or not this mapping sets up a correspondence between tensors over $\mathcal{C}$ and conformal Killing tensors on V. Can two distinct tensors over $\mathcal{C}$ define the same conformal Killing tensor? Are there conformal Killing tensors which do not come from any tensor over $\mathcal{C}$? Unfortunately, the answer to both questions is yes.

We consider the first question in detail only for the case of rank two. Let $T^{\alpha\beta} = T^{(\alpha\beta)}$ be a tensor over $\mathcal{C}$ which defines the zero conformal Killing tensor on V. It is easily shown that, in terms of the data for $\boldsymbol{\xi}^a$ at

p, $T_{\alpha\beta}\xi^\alpha\xi^\beta$ must be a linear combination of five expressions:

$$\begin{aligned} &n(F_{ab}F^{ab} - 2\varphi^2 + 4\xi^2 k_a) = G_{\alpha\beta}\xi^\alpha\xi^\beta, \\ &A_{ab}(\varphi F^{ab} - 2\xi^a k^b), \\ &B_{abc}F^{ab}\xi^c, \\ &C_{abc}F^{ab}k^c, \\ &D_{abcd}F^{ab}F^{cd}, \end{aligned} \tag{B6}$$

where A, B, C, and D are totally skew tensors at p. The last four of the five bilinear mappings (B6) are not individually invariant under (B3): they are taken into certain linear combinations of each other. It turns out, however, that the particular combinations which occur are such that the coefficients A, B, C, and D define a second-rank tensor over $\mathcal{C}$. We are therefore led to define the tensor $W_{\alpha\beta\gamma\delta}$ over $\mathcal{C}$ by

$$\begin{aligned} W_{\alpha\beta\gamma\delta}&\xi^\alpha\xi^\beta\xi'^\gamma\xi'^\delta \\ &= -\tfrac{4}{3}n^2(\varphi F_{ab} - 2k_{[a}\xi_{b]})(\varphi' F'^{ab} - 2k'^{[a}\xi'^{b]}) \\ &\quad + 4n^2(F_{[ab}\xi_{c]}F'^{ab}k'^c + F'_{[ab}\xi'_{c]}F^{ab}k^c) \\ &\quad + n^2 F_{[ab}F_{cd]}F'^{ab}F'^{cd} \\ &\quad + [2/(n^2 + 3n + 2)](h_{\alpha\beta}\xi^\alpha\xi^\beta)(h_{\gamma\delta}\xi'^\gamma\xi'^\delta). \end{aligned} \tag{B7}$$

The right side of (B7) *is* invariant under (B3), and hence defines a tensor over $\mathcal{C}$. It follows from (B6) that, for any $S^{\mu\nu}$, $W^{\alpha\beta}{}_{\mu\nu}S^{\mu\nu}$ is a tensor over $\mathcal{C}$ which gives the zero conformal Killing tensor and, conversely, that any such tensor over $\mathcal{C}$ can be written in the form $W^{\alpha\beta}{}_{\mu\nu}S^{\mu\nu}$. Furthermore, it follows from (B7) that $W^{\alpha\beta}{}_{\mu\nu}W^{\mu\nu}{}_{\gamma\delta} = W^{\alpha\beta}{}_{\gamma\delta}$, i.e., that W acts as a projection operator. Any symmetric second-rank tensor $T^{\alpha\beta}$ over $\mathcal{C}$ can now be decomposed uniquely into one part $W^{\alpha\beta}{}_{\mu\nu}T^{\mu\nu}$ which gives the zero conformal Killing tensor and another part $T^{\alpha\beta} - W^{\alpha\beta}{}_{\mu\nu}T^{\mu\nu}$ which similar produces the same conformal Killing tensor as $T^{\alpha\beta}$. A projection operator W and a similar decomposition is available for tensors of rank greater than two.

We can answer the second question—whether there are conformal Killing tensors which do not come from any tensor over $\mathcal{C}$—with an example. Observe that, for any scalar field f, fh^{ab} is a conformal Killing tensor. But it is impossible that every tensor of this form represent a tensor over $\mathcal{C}$, for the tensors of a given rank over $\mathcal{C}$ form a finite-dimensional vector space. One would like, therefore, to characterize in some way those conformal Killing tensors which *can* be interpreted in terms of $\mathcal{C}$. Note first of all that, if $T^{a\cdots c}$ is a conformal Killing tensor, then so is the trace-free part of T. Furthermore, if we interpret conformal Killing tensors as first integrals of null geodesics, then T and its trace-free part represent exactly the same integral. Finally, note that, for the example given above, fh^{ab} is "pure trace." These remarks suggest the following result:

Theorem: Every trace-free conformal Killing tensor can be obtained, via (3) and (4), from some tensor over $\mathcal{C}$.[18]

Outline of proof: Let $T_{a_1\cdots a_s}$ be a trace-free conformal Killing tensor. The essential step is to show that $T_{a_1\cdots a_s}$ is "algebraic" in its position dependence [more precisely, that its $(2s+1)$th derivative vanishes]. This having been done, it is a straightforward exercise, using (B3), to show that $T_{a_1\cdots a_s}$ can be written in the form of Eq. (4).

Let P be a timelike 3-dimensional space of vectors at a point p of V, and let $k^a, \cdots, l^a$ be $2s+1$ null vectors[19] which lie in P, and no two of which are parallel. Set

$$R_{a_1\cdots a_s} = k^{b_1}\cdots l^{b_{2s+1}}\nabla_{b_1}\cdots\nabla_{b_{2s+1}}T_{a_1\cdots a_s}. \tag{B8}$$

It then follows from the conformal Killing equation on $T_{a_1\cdots a_s}$ that

$$\begin{aligned} R_{a_1\cdots a_s}k^{a_1}\cdots k^{a_s} &= 0, \\ &\vdots \\ R_{a_1\cdots a_s}l^{a_1}\cdots l^{a_s} &= 0. \end{aligned} \tag{B9}$$

The $2s+1$ trace-free tensors $(k^{a_1}\cdots k^{a_s}), \cdots, (l^{a_1}\cdots l^{a_s})$ span the space of all totally symmetric, trace-free tensors of rank s in P. Since $R_{a_1\cdots a_s}$ is trace free, it now follows from (B9) that $R_{a_1\cdots a_s}$, when projected into P, gives zero. But $k^a, \cdots, l^a$ are arbitrary null vectors in P. Therefore, by (B8), the projection of $\nabla_{b_1}\cdots\nabla_{b_{2s+1}}T_{a_1\cdots a_s}$ into P gives zero. But the only tensor whose projection into an arbitrary timelike 3-space is zero is the zero tensor.

Finally, we may ask whether the operation of taking the trace-free part of a conformal Killing tensor can be extended to some operation on tensors over $\mathcal{C}$. Let $T^{\alpha_1\cdots\alpha_s}$ be a totally symmetric tensor over $\mathcal{C}$. There is associated with $T^{\alpha_1\cdots\alpha_s}$, via (3) and (4), a conformal Killing tensor $T^{a_1\cdots a_s}$ on V. This $T^{a_1\cdots a_s}$ will not, in general, be trace free. However, the trace-free part, $\tilde{T}^{a_1\cdots a_s}$, of $T^{a_1\cdots a_s}$ is also a conformal Killing tensor. It now follows from the theorem above that $\tilde{T}^{a_1\cdots a_s}$ comes from some tensor $\tilde{T}^{\alpha_1\cdots\alpha_s}$ over $\mathcal{C}$. If, in addition, we require $W^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s}\tilde{T}^{\mu_1\cdots\mu_s} = 0$, then this $\tilde{T}^{\alpha_1\cdots\alpha_s}$ is unique. Thus, for each symmetric tensor $T^{\alpha_1\cdots\alpha_s}$ over $\mathcal{C}$, we have defined a symmetric tensor $\tilde{T}^{\alpha_1\cdots\alpha_s}$. Since $\tilde{T}$ is linear in T, there is some

tensor $P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} = P^{(\alpha_1\cdots\alpha_s)}{}_{(\mu_1\cdots\mu_s)}$ over $\mathbb{C}$ such that

$$\tilde{T}^{\alpha_1\cdots\alpha_s} = P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} T^{\mu_1\cdots\mu_s}. \qquad \text{(B10)}$$

A number of properties of P follow directly from this definition. Since $\tilde{T}^{\alpha_1\cdots\alpha_s}$ necessarily comes from some conformal Killing tensor on V, we have

$$P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} = W^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s} P^{\beta_1\cdots\beta_s}{}_{\mu_1\cdots\mu_s}.$$

Furthermore, since the operation "taking the trace-free part" reduces to the identity when applied to a trace-free conformal Killing tensor on V, we have

$$P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} = P^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s} P^{\beta_1\cdots\beta_s}{}_{\mu_1\cdots\mu_s}.$$

By using the definition of P, we may write out explicitly the expression for

$$P_{\alpha_1\cdots\alpha_s\beta_1\cdots\beta_s}\xi^{\alpha_1}\cdots\xi^{\alpha_s}\xi'^{\beta_1}\cdots\xi'^{\beta_s}$$

in terms of data for ξ^a and ξ'^a at an arbitrary point. While this expression turns out to be rather complicated, it does reveal one further, and less obvious, property of P, namely, that

$$P_{\alpha_1\cdots\alpha_s\beta_1\cdots\beta_s} = P_{\beta_1\cdots\beta_s\alpha_1\cdots\alpha_s}.$$

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[1] Strictly speaking, it is $\nabla^2\psi - \frac{1}{6}R\psi = 0$ which is conformally invariant, provided ψ is assigned conformal weight $-\frac{1}{2}$. In flat space, however, this equation reduces to Laplace's equation.

[2] In particular, V will be topologically $S^2 \times R$.

[3] See, for example, T. J. Willmore, *Introduction to Differential Geometry* (Oxford U.P. London, 1959).

[4] See, for example, C. Chevalley, *Theory of Lie Groups* (Princeton U.P., Princeton, N.J., 1946).

[5] It is shown in Appendix B that the constancy of either of these tensors implies the constancy of the other.

[6] No restrictions on the dimension of the manifold or on the signature of the metric will be required in this appendix.

[7] That is, l_a is so scaled that $l^m\nabla_m l_a = 0$.

[8] Conformal Killing tensors are a generalization of Killing tensors, which represent first integrals of the equations for arbitrary geodesics. Killing tensors are discussed, for example, in L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1964), pp. 128.

[9] If the metric h_{ab} is positive definite, there are, of course, no null geodesics. In this case, (A1) is taken as the definition of a conformal Killing tensor.

[10] The difference between the actions of two derivative operators, D_m and $\tilde{D}_m$, may be expressed in terms of a tensor field $K^c{}_{ab} = K^c{}_{(ab)}$. [See S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Interscience, New York, 1963), Vol. I.] The coefficients on the right in (A3) have been so chosen that, when D_m is eliminated in favor of $\tilde{D}_m$, all K terms vanish identically.

[11] A. Nijenhuis, in *Proceedings of the International Congress of Mathematicians* (Cambridge U.P., Cambridge, England, 1960), p. 463.

[12] There is a similar algebra for totally antisymmetric contravariant tensors (Ref. 11). If P, Q, and R are skew, of ranks p, q, and r, respectively, then Eqs. (A2)–(A5) must be replaced by

$$P \cap_A Q = P^{[a_1\cdots a_p}Q^{a_{p+1}\cdots a_{p+q}]} = (-1)^{pq} Q \cap_A P,$$
$$[P, Q] = p(-1)^{p+1}Q^{m[a_1\cdots a_{p-1}}\nabla_m Q^{a_p\cdots a_{p+q-1}]} - q(-1)^{q+pq}Q^{m[a_1\cdots a_{q-1}}\nabla_m P^{a_q\cdots a_{p+q-1}]},$$
$$[P, Q \cap_A R] = [P, Q] \cap_A R + (-1)^q [P, R] \cap_A Q,$$
$$(-1)^{pr+p}[P,[Q,R]] + (-1)^{qp+q}[Q,[R,P]] + (-1)^{rq+r}[R,[P,Q]] = 0,$$

respectively.

[13] Evidently, the Killing tensors [P's which satisfy (A6) with the right side set equal to zero] form a subalgebra of the algebra of conformal Killing tensors.

[14] R. Geroch, Commun. Math. Phys. **13**, 180 (1969).

[15] The position vector of p' relative to p is defined as follows. Let γ be any curve from p to p', with parameter s and tangent vector $\eta(s)^m$, such that $\eta^m\nabla_m s = 1$. Then $x^m = \int_p^{p'} \tilde{\eta}^m(s)\, ds$, where $\tilde{\eta}^m(s)$ is the s-dependent vector at p' obtained by parallel transport of $\eta^m(s)$ along γ to p'. This x^m is certainly invariant under continuous deformations of γ: that it is totally independent of γ is a consequence of the global assumption on V mentioned earlier. Note that in certain spaces distinct points may be related by the zero position vector.

[16] This number is obtained by counting data for ξ^b: n dimensions for ξ^a, $\frac{1}{2}n(n-1)$ for F_{ab}, 1 for φ, and n for k_a.

[17] The first term in (B5) contributes $\frac{1}{2}(p^2 + q^2 - p - q)$ plus's and pq minus's, the second term, 0 plus's and 1 minus, and the third term $(p+q)$ plus's and $(p+q)$ minus's.

[18] The converse is false. The conformal Killing tensor g^{ab}, for example, is not trace free, yet it certainly comes from some tensor over $\mathbb{C}$.

[19] This proof requires a modification for the case in which the metric is positive definite: one must permit $k^a, \cdots, l^a$ to be complex.

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Partial-Tensor-Product Representations of the Canonical Commutation Relations: Classification

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Partial-tensor-product representations of the canonical commutation relations are a generalization of direct- (or tensor-) product representations as discussed by Klauder, McKenna, and Woods. A classification is given of those representations up to unitary equivalence. The equivalence or inequivalence, respectively, of two representations is expressed in terms of the corresponding reference vectors.

1. INTRODUCTION AND DEFINITIONS

The canonical commutation relations (CCR) are usually discussed in Weyl's formulation. A representation of the CCR is given by a pair of families of unitary operators $U(f)$, $V(g)$ where the f and g run over test-function spaces $\mathfrak{U}_U$ and $\mathfrak{U}_V$ which are real vector spaces such that there is a scalar product (f, g) defined between elements of $\mathfrak{U}_U$ and $\mathfrak{U}_V$. For simplicity, it is assumed that $\mathfrak{U}_U = \mathfrak{U}_V = \mathfrak{U}$. Then, it is required that

$$U(f_1)U(f_2) = U(f_1 + f_2),$$
$$V(g_1)V(g_2) = V(g_1 + g_2), \qquad (1.1)$$
$$V(g)U(f) = e^{i(f,g)}U(f)V(g), \qquad (1.2)$$

tensor $P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} = P^{(\alpha_1\cdots\alpha_s)}{}_{(\mu_1\cdots\mu_s)}$ over $\mathbb{C}$ such that

$$\tilde{T}^{\alpha_1\cdots\alpha_s} = P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} T^{\mu_1\cdots\mu_s}. \qquad \text{(B10)}$$

A number of properties of P follow directly from this definition. Since $\tilde{T}^{\alpha_1\cdots\alpha_s}$ necessarily comes from some conformal Killing tensor on V, we have

$$P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} = W^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s} P^{\beta_1\cdots\beta_s}{}_{\mu_1\cdots\mu_s}.$$

Furthermore, since the operation "taking the trace-free part" reduces to the identity when applied to a trace-free conformal Killing tensor on V, we have

$$P^{\alpha_1\cdots\alpha_s}{}_{\mu_1\cdots\mu_s} = P^{\alpha_1\cdots\alpha_s}{}_{\beta_1\cdots\beta_s} P^{\beta_1\cdots\beta_s}{}_{\mu_1\cdots\mu_s}.$$

By using the definition of P, we may write out explicitly the expression for

$$P_{\alpha_1\cdots\alpha_s\beta_1\cdots\beta_s}\xi^{\alpha_1}\cdots\xi^{\alpha_s}\xi'^{\beta_1}\cdots\xi'^{\beta_s}$$

in terms of data for ξ^a and ξ'^a at an arbitrary point. While this expression turns out to be rather complicated, it does reveal one further, and less obvious, property of P, namely, that

$$P_{\alpha_1\cdots\alpha_s\beta_1\cdots\beta_s} = P_{\beta_1\cdots\beta_s\alpha_1\cdots\alpha_s}.$$

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[1] Strictly speaking, it is $\nabla^2\psi - \frac{1}{6}R\psi = 0$ which is conformally invariant, provided ψ is assigned conformal weight $-\frac{1}{2}$. In flat space, however, this equation reduces to Laplace's equation.

[2] In particular, V will be topologically $S^2 \times R$.

[3] See, for example, T. J. Willmore, *Introduction to Differential Geometry* (Oxford U.P. London, 1959).

[4] See, for example, C. Chevalley, *Theory of Lie Groups* (Princeton U.P., Princeton, N.J., 1946).

[5] It is shown in Appendix B that the constancy of either of these tensors implies the constancy of the other.

[6] No restrictions on the dimension of the manifold or on the signature of the metric will be required in this appendix.

[7] That is, l_a is so scaled that $l^m\nabla_m l_a = 0$.

[8] Conformal Killing tensors are a generalization of Killing tensors, which represent first integrals of the equations for arbitrary geodesics. Killing tensors are discussed, for example, in L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1964), pp. 128.

[9] If the metric h_{ab} is positive definite, there are, of course, no null geodesics. In this case, (A1) is taken as the definition of a conformal Killing tensor.

[10] The difference between the actions of two derivative operators, D_m and $\tilde{D}_m$, may be expressed in terms of a tensor field $K^c{}_{ab} = K^c{}_{(ab)}$. [See S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Interscience, New York, 1963), Vol. I.] The coefficients on the right in (A3) have been so chosen that, when D_m is eliminated in favor of $\tilde{D}_m$, all K terms vanish identically.

[11] A. Nijenhuis, in *Proceedings of the International Congress of Mathematicians* (Cambridge U.P., Cambridge, England, 1960), p. 463.

[12] There is a similar algebra for totally antisymmetric contravariant tensors (Ref. 11). If P, Q, and R are skew, of ranks p, q, and r, respectively, then Eqs. (A2)–(A5) must be replaced by

$$P \cap_A Q = P^{[a_1\cdots a_p}Q^{a_{p+1}\cdots a_{p+q}]} = (-1)^{pq} Q \cap_A P,$$
$$[P, Q] = p(-1)^{p+1}Q^{m[a_1\cdots a_{p-1}}\nabla_m Q^{a_p\cdots a_{p+q-1}]} - q(-1)^{q+pq}Q^{m[a_1\cdots a_{q-1}}\nabla_m P^{a_q\cdots a_{p+q-1}]},$$
$$[P, Q \cap_A R] = [P, Q] \cap_A R + (-1)^q [P, R] \cap_A Q,$$
$$(-1)^{pr+p}[P,[Q,R]] + (-1)^{qp+q}[Q,[R,P]] + (-1)^{rq+r}[R,[P,Q]] = 0,$$

respectively.

[13] Evidently, the Killing tensors [P's which satisfy (A6) with the right side set equal to zero] form a subalgebra of the algebra of conformal Killing tensors.

[14] R. Geroch, Commun. Math. Phys. **13**, 180 (1969).

[15] The position vector of p' relative to p is defined as follows. Let γ be any curve from p to p', with parameter s and tangent vector $\eta(s)^m$, such that $\eta^m\nabla_m s = 1$. Then $x^m = \int_p^{p'} \tilde{\eta}^m(s)\, ds$, where $\tilde{\eta}^m(s)$ is the s-dependent vector at p' obtained by parallel transport of $\eta^m(s)$ along γ to p'. This x^m is certainly invariant under continuous deformations of γ: that it is totally independent of γ is a consequence of the global assumption on V mentioned earlier. Note that in certain spaces distinct points may be related by the zero position vector.

[16] This number is obtained by counting data for ξ^b: n dimensions for ξ^a, $\frac{1}{2}n(n-1)$ for F_{ab}, 1 for φ, and n for k_a.

[17] The first term in (B5) contributes $\frac{1}{2}(p^2 + q^2 - p - q)$ plus's and pq minus's, the second term, 0 plus's and 1 minus, and the third term $(p+q)$ plus's and $(p+q)$ minus's.

[18] The converse is false. The conformal Killing tensor g^{ab}, for example, is not trace free, yet it certainly comes from some tensor over $\mathbb{C}$.

[19] This proof requires a modification for the case in which the metric is positive definite: one must permit $k^a, \cdots, l^a$ to be complex.

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Partial-Tensor-Product Representations of the Canonical Commutation Relations: Classification

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Partial-tensor-product representations of the canonical commutation relations are a generalization of direct- (or tensor-) product representations as discussed by Klauder, McKenna, and Woods. A classification is given of those representations up to unitary equivalence. The equivalence or inequivalence, respectively, of two representations is expressed in terms of the corresponding reference vectors.

1. INTRODUCTION AND DEFINITIONS

The canonical commutation relations (CCR) are usually discussed in Weyl's formulation. A representation of the CCR is given by a pair of families of unitary operators $U(f)$, $V(g)$ where the f and g run over test-function spaces $\mathfrak{U}_U$ and $\mathfrak{U}_V$ which are real vector spaces such that there is a scalar product (f, g) defined between elements of $\mathfrak{U}_U$ and $\mathfrak{U}_V$. For simplicity, it is assumed that $\mathfrak{U}_U = \mathfrak{U}_V = \mathfrak{U}$. Then, it is required that

$$U(f_1)U(f_2) = U(f_1 + f_2),$$
$$V(g_1)V(g_2) = V(g_1 + g_2), \qquad (1.1)$$
$$V(g)U(f) = e^{i(f,g)}U(f)V(g), \qquad (1.2)$$

$U(\lambda f)$ and $V(\lambda g)$ are weakly continuous in the real number λ. (1.3)

As an abbreviation we put

$$U(f, g) \equiv U(f)V(g). \tag{1.4}$$

Two representations $U(f, g)$ and $\hat{U}(f, g)$, with f and $g \in \mathfrak{U}$, in Hilbert spaces H and $\hat{H}$ are said to be unitarily equivalent if there is an isometric mapping T of H onto $\hat{H}$ such that

$$\hat{U}(f, g)T = TU(f, g). \tag{1.5}$$

It is well known that, if the test-function space is finite dimensional, the CCR have only one irreducible representation up to unitary equivalence.[1] When the test-function space is infinite dimensional, it is also well known that there are uncountably many unitarily inequivalent representations.[2] A special class of such representations may be constructed by use of incomplete tensor products (ITP) of Hilbert spaces introduced by von Neumann. We give the definition and a brief outline of the basic properties of ITP.[3]

Let I be an index set and $\{H_\alpha\}$, $\alpha \in I$, a set of Hilbert spaces. A sequence of vectors $\{\varphi_\alpha : \alpha \in I, \varphi_\alpha \in H_\alpha\}$ is called a C_0-sequence if

$$\sum_{\alpha \in I} |\|\varphi_\alpha\| - 1| < \infty. \tag{1.6}$$

A scalar product between "product vectors" $\otimes\varphi_\alpha$ and $\otimes\psi_\alpha$, where $\{\varphi_\alpha\}$ and $\{\psi_\alpha\}$ are C_0-sequences, is defined by

$$\begin{aligned}\langle \otimes\varphi_\alpha, \otimes\psi_\alpha\rangle &= \prod_{\alpha \in I} \langle \varphi_\alpha, \psi_\alpha\rangle, \quad \text{if } \prod_{\alpha \in I} \langle \varphi_\alpha, \psi_\alpha\rangle \text{ converges,} \\ &= 0, \qquad \text{if } \prod_{\alpha \in I} \langle \varphi_\alpha, \psi_\alpha\rangle \text{ does not converge,}\end{aligned}$$

and is extended by linearity and continuity. The closed linear set, generated by all product vectors $\otimes\varphi_\alpha$ ($\{\varphi_\alpha\}$ a C_0-sequence), is called the complete direct or tensor product of the H_α denoted by

$$\bigotimes_{\alpha \in I} H_\alpha. \tag{1.7}$$

Two C_0-sequences $\{\varphi_\alpha\}$ and $\{\psi_\alpha\}$, or the corresponding product vectors $\otimes\varphi_\alpha$ and $\otimes\psi_\alpha$, respectively, are said to be equivalent, in symbols $\otimes\varphi_\alpha \sim \otimes\psi_\alpha$, if

$$\sum_{\alpha \in I} |\langle \varphi_\alpha, \psi_\alpha\rangle - 1| < \infty. \tag{1.8}$$

The equivalence $\sim$ for C_0-sequences decomposes the set of all C_0-sequences into mutually disjoint equivalence classes. Each equivalence class contains a (C_0-) sequence $\{\varphi_\alpha^0\}$ with $\|\varphi_\alpha^0\| = 1$ for all $\alpha \in I$.

Let $\mathfrak{C}$ be an equivalence class containing $\otimes\varphi_\alpha^0$, with $\|\varphi_\alpha^0\| = 1$ for all $\alpha \in I$. Let

$$H_{\varphi^0} \equiv \bigotimes_{\alpha \in I}^{(\otimes\varphi_\alpha^0)} H_\alpha \tag{1.9}$$

be the closed linear set determined by all $\otimes\varphi_\alpha$ where $\{\varphi_\alpha\}$ is any C_0-sequence from $\mathfrak{C} \equiv \mathfrak{C}(\otimes\varphi_\alpha^0)$. This H_{φ^0} is the incomplete direct or tensor product (ITP) of the H_α with respect to the reference vector $\varphi^0 = \otimes\varphi_\alpha^0$. By definition, equivalent reference vectors determine the same ITP. Different ITP are pairwise orthogonal, and the closed linear set determined by all ITP is $\otimes_{\alpha \in I} H_\alpha$.

Two C_0-sequences $\{\varphi_\alpha\}$ and $\{\psi_\alpha\}$, or the corresponding product vectors $\otimes\varphi_\alpha$ and $\otimes\psi_\alpha$, respectively, are called weakly equivalent, in symbols

$$\otimes\varphi_\alpha \underset{\mathfrak{W}}{\sim} \otimes\psi_\alpha,$$

if there are complex numbers

$$z_\alpha, \quad |z_\alpha| = 1, \quad \alpha \in I \quad \text{such that} \quad \otimes z_\alpha\varphi_\alpha \sim \otimes\psi_\alpha. \tag{1.10}$$

A necessary and sufficient condition for weak equivalence is

$$\sum_{\alpha \in I} |\,|\langle \varphi_\alpha, \psi_\alpha\rangle| - 1| < \infty. \tag{1.11}$$

The decomposition of the set of all C_0-sequences into mutually disjoint weak-equivalence classes induces a decomposition of the complete tensor product into mutually orthogonal subspaces. Any weak-equivalence class $\mathfrak{C}_{\mathfrak{W}}(\otimes\varphi_\alpha)$ contains the whole equivalence class $\mathfrak{C}(\otimes\varphi_\alpha)$.

Partial-tensor products are a simple generalization of ITP. Decompose the index set I into finite subsets I_r, such that $\bigcup_r I_r = I$. For every r form the usual finite tensor product

$$H(I_r) = \bigotimes_{\alpha \in I_r} H_\alpha; \tag{1.12}$$

choose some unit vector ψ_r^0 from each $H(I_r)$, and form the ITP of the $H(I_r)$ with respect to the reference vector $\psi^0 = \otimes\psi_r^0$,

$$H_{\psi^0} = \bigotimes_{r}^{(\otimes\psi_r^0)} H(I_r). \tag{1.13}$$

The resulting Hilbert space H_{ψ^0} is called a partial-tensor product (PTP). It differs (possibly) from an ITP because the reference vector need not be a product vector with respect to the original H_α.

The corresponding representations of the CCR are defined as follows: Let $h_1, h_2, \cdots$ be an orthonormal basis of the test-function space $\mathfrak{U}$, and let every element of $\mathfrak{U}$ be a finite linear combination of the h_i. Let I be the set of natural numbers and let H_α be

isomorphic to $L^2(R^1)$, the space of square-integrable functions on R^1, for all $\alpha \in I$. Let a Schrödinger representation of $[Q, P] = i$ be given in each H_α and denote the corresponding Weyl operators by $\tilde{U}_\alpha(p)$ and $\tilde{V}_\alpha(q)$, i.e., $\tilde{U}_\alpha(p) = e^{ipQ}$ and $\tilde{V}_\alpha(q) = e^{iqP}$. Decompose the set I of natural numbers into finite subsets I_r, $r = 1, 2, \cdots$, and form a PTP H_{φ^0} as in Eq. (1.13). Let $g(r)$ be the number of elements of I_r. In each $H(I_r)$, define a Schrödinger representation for $g(r)$ degrees of freedom; i.e., if $n \in I_r$, take

$$\hat{U}_n(p) = \tilde{U}_n(p) \otimes \left(\bigotimes_{\substack{\alpha \in I_r \\ \alpha \neq n}} \mathbf{1}_\alpha \right),$$

$$\hat{V}_n(q) = \tilde{V}_n(q) \otimes \left(\bigotimes_{\substack{\alpha \in I_r \\ \alpha \neq n}} \mathbf{1}_\alpha \right), \tag{1.14}$$

as operators in $H(I_r)$. In $\otimes_r H(I_r)$ one defines unitary operators $U_n(p)$ and $V_n(q)$ by

$$U_n(p) = \hat{U}_n(p) \otimes \left(\bigotimes_{r' \neq r} \mathbf{1}_{r'} \right),$$

$$V_n(q) = \hat{V}_n(q) \otimes \left(\bigotimes_{r' \neq r} \mathbf{1}_{r'} \right). \tag{1.15}$$

Now let $f, g \in \mathfrak{U}$; then

$$f = \sum_1^N p_n h_n, \quad g = \sum_1^M q_n h_n.$$

We define

$$U(f) \equiv \prod_1^N U_n(p_n), \quad V(g) \equiv \prod_1^M V_n(q_n). \tag{1.16}$$

This is, obviously, a representation of the CCR and in this form it was given by Hegerfeldt.[4] It is called a partial-tensor-product representation (PTPR) with respect to the basis h_i of $\mathfrak{U}$. The irreducibility of the Schrödinger representation in each $H(I_r)$ implies that every PTP H_{φ^0} is irreducible under[4] $U(f, g)$. By a renumbering of the basis vectors h_i and of the index set I, one can transform the subsets I_r into intervals

$$I_1 = (1, \cdots, i_1), \quad I_2 = (i_1 + 1, \cdots, i_2), \cdots. \tag{1.17}$$

In the following, we always assume this kind of order.

The special case with all I_r 1-point sets, i.e., $I_r = \{r\}$ for all r, is called a direct- or tensor-product representation, and it has been investigated by Klauder, McKenna, and Woods.[5,6]

In Sec. 2, we consider one partition and two Hilbert spaces belonging to different reference vectors. We get a criterion for the corresponding representations to be equivalent or not. In Sec. 3, we assume two different partitions which are comparable in a certain sense. Section 4 serves to discuss the general case with two different partitions which are not comparable in the sense of Sec. 3.

2. DIRECTLY COMPARABLE REPRESENTATIONS

Let I_r, $r = 1, 2, \cdots$, be a partition of the index set I into finite intervals [cf. Eq. (1.17)]. Let

$$H_1 \equiv H_{\varphi^0} \equiv \bigotimes_r^{(\otimes \varphi_r^0)} H(I_r),$$

$$H_2 \equiv H_{\psi^0} \equiv \bigotimes_r^{(\otimes \psi_r^0)} H(I_r)$$

be two PTP with respect to the reference vectors $\varphi^0 = \otimes \varphi_r^0$ and $\psi^0 = \otimes \psi_r^0$. Let $U(f, g)$ be the PTPR with respect to the basis h_i of $\mathfrak{U}$ as defined in Eqs. (1.14), (1.15), (1.16). By $U_1(f, g)$ and $U_2(f, g)$, we denote the restriction of $U(f, g)$ to H_1 and H_2, respectively. To derive a criterion for the equivalence of $U_1(f, g)$ and $U_2(f, g)$, we need some facts about von Neumann algebras in connection with infinite tensor products and these representations of the CCR.

The algebra $B(H(I_r))$ of all bounded linear operators in $H(I_r)$ is extended to an algebra $\bar{B}(H(I_r))$ in $\otimes_r H(I_r)$,

$$\bar{B}(H(I_r)) = B(H(I_r)) \otimes \left(\bigotimes_{r' \neq r} \mathbf{1}_{r'} \right).$$

The set of all $\bar{B}(H(I_r))$ generates the algebra of extended operators $B^\#$,

$$B^\# = \left\{ \bigcup_r \bar{B}(H(I_r)) \right\}''.$$

Let $W(I_r)$ be the finite-dimensional subspace of $\mathfrak{U}$ spanned by the basis vectors h_i with $i \in I_r$, i.e.,

$$W(I_r) = \{h_i : i \in I_r\}^L. \tag{2.1}$$

Because of the irreducibility of the Schrödinger representation in each $H(I_r)$, we have

$$\bar{B}(H(I_r)) = \{U(f, g) : f, g \in W(I_r)\}'',$$

and, furthermore,

$$\left\{ \bigcup_r \bar{B}(H(I_r)) \right\}'' = \left\{ \bigcup_r \{U(f, g) : f, g \in W(I_r)\}'' \right\}''$$

$$= \left\{ \bigcup_r \{U(f, g) : f, g \in W(I_r)\} \right\}''$$

$$= \left\{ U(f, g) : f, g \in \bigcup_r W(I_r) \right\}''$$

Thus,

$$B^\# = \{U(f, g) : f, g \in \mathfrak{U}\}''. \tag{2.2}$$

As a consequence of a theorem given by von Neumann,[3] we know that the projection onto a given weak-equivalence class is an element of $B^\#$. Thus,

$$P = P\{\mathfrak{C}_{\mathfrak{W}}(\otimes \varphi_r^0)\} \in B^\# \tag{2.3}$$

Theorem 2.1: The representations $U_1(f, g)$ and $U_2(f, g)$ are unitarily equivalent if and only if

$$\sum_r \left| |\langle \varphi_r^0, \psi_r^0 \rangle| - 1 \right| < \infty.$$

Proof: (Sufficiency): $\sum_r \left| |\langle \varphi_r^0, \psi_r^0 \rangle| - 1 \right| < \infty$, that is, $\otimes \varphi_r^0 \underset{\mathfrak{W}}{\sim} \otimes \psi_r^0$, implies the existence of a sequence of complex numbers $\{z_r : |z_r| = 1, r = 1, 2, \cdots\}$ such that [cf. Eq. (1.10)] $\otimes z_r \varphi_r^0 \sim \otimes \psi_r^0$. The sequence $\{z_r\}$ gives rise to a unitary operator $T \equiv T(\{z_r\})$ in $\otimes_r H(I_r)$ mapping H_1 onto H_2 such that

$$T \otimes \varphi_r = \otimes z_r \varphi_r \tag{2.4}$$

for all C_0-sequences[3] $\{\varphi_r\}$. Let

$$f = \sum_1^N p_n h_n, \quad g = \sum_1^M q_n h_n.$$

Then, we have, for all $\otimes \varphi_r \in H_1$ [cf. Eqs. (1.13)–(1.15)],

$$\begin{aligned} U_2(f, g)T \otimes \varphi_r &= U_2(f, g) \otimes z_r \varphi_r \\ &= \otimes \prod_{n \in I_r} \hat{U}_n(p_n) \hat{V}_n(q_n) z_r \varphi_r \\ &= \otimes z_r \prod_{n \in I_r} \hat{U}_n(p_n) \hat{V}_n(q_n) \varphi_r \\ &= T \otimes \prod_{n \in I_r} \hat{U}_n(p_n) \hat{V}_n(q_n) \varphi_r \\ &= T U_1(f, g) \otimes \varphi_r. \end{aligned}$$

That is,

$$U_2(f, g)T = T U_1(f, g) \tag{2.5}$$

for a total set in H_1. Because U_1, U_2, and T are linear and continuous Eq. (2.5) holds everywhere in H_1.

(Necessity): Suppose that the reference vectors φ^0 and ψ^0 are not weakly equivalent. This means that the corresponding weak-equivalence classes $\mathfrak{C}_{\mathfrak{W}}(\varphi^0)$ and $\mathfrak{C}_{\mathfrak{W}}(\psi^0)$ are orthogonal. Equivalence of the representations implies the existence of a one-to-one and isometric (and, therefore, linear and continuous) transformation T, such that

$$T W_1 T^* = W_2, \quad \text{for all} \quad W \in \{U(f, g) : f, g \in \mathfrak{U}\},$$

and, consequently,

$$T W_1 T^* = W_2, \quad \text{for all}$$
$$W \in \{U(f, g) : f, g \in \mathfrak{U}\}'' = B^{\#} \tag{2.6}$$

[cf. Eq. (2.2)]. But the above mentioned $P\{\mathfrak{C}_{\mathfrak{W}}(\varphi^0)\}$ [Eq. (2.3)] when restricted to H_1 gives **1** in H_1, and the restriction of P to H_2 is **0** in H_2, contradicting Eq. (2.6).

This is a slight modification of a proof presented by Streit.[7] Choosing each I_r to consist of a single point, we have reproduced a theorem of Klauder, McKenna, and Woods.[6]

3. COMPARABLE REPRESENTATIONS

Let $\{I_r : r = 1, 2, \cdots\}$ and $\{K_s : s = 1, 2, \cdots\}$ be partitions of I into finite intervals such that there is another partition $\{L_t : t = 1, 2, \cdots\}$ of I into finite intervals and both $\{I_r\}$ and $\{K_s\}$ are refinements of $\{L_t\}$; i.e., for each t there are (finite) index sets $R(t)$, $S(t)$ with

$$\bigcup_{r \in R(t)} I_r = L_t = \bigcup_{s \in S(t)} K_s.$$

We call this comparable partitions. Let

$$H_1 = \bigotimes_r^{(\otimes \varphi_r^0)} H(I_r) \quad \text{and} \quad H_2 = \bigotimes_s^{(\otimes \psi_s^0)} H(K_s)$$

be PTP with reference vectors $\varphi^0 = \otimes \varphi_r^0$ and $\psi^0 = \otimes \psi_s^0$. Let $U_1(f, g)$ and $U_2(f, g)$ be PTPR of the CCR in H_1 and H_2, respectively, with respect to the basis, $h_1, h_2, \cdots$ of $\mathfrak{U}$. For all product vectors $\varphi = \otimes_r \varphi_r \in H_1$ and $\psi = \otimes_s \psi_s \in H_2$, we define

$$T_1 \varphi = \bigotimes_t \left(\bigotimes_{r \in R(t)} \varphi_r \right), \quad T_2 \psi = \bigotimes_t \left(\bigotimes_{s \in S(t)} \psi_s \right). \tag{3.1}$$

By a theorem of von Neumann,[3] T_1 and T_2 extend in a unique way to isometric isomorphisms, with T mapping

$$H_1 \text{ onto } \mathcal{H}_1 = \bigotimes_t^{(\otimes_t (\otimes_{r \in R(t)} \varphi_r^0))} H(L_t),$$

and T_2 mapping

$$H_2 \text{ onto } \mathcal{H}_2 = \bigotimes_t^{(\otimes_t (\otimes_{s \in S(t)} \psi_s^0))} H(L_t).$$

We define

$$\hat{U}_1(f, g) = T_1 U_1(f, g) T_1^*$$

and

$$\hat{U}_2(f, g) = T_2 U_2(f, g) T_2^*,$$

in $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. $\hat{U}_1$ and $\hat{U}_2$ are obviously PTPR. By construction, $\hat{U}_1$ and U_1 are unitarily equivalent, and also $\hat{U}_2$ and U_2. This implies that U_1 and U_2 are unitarily equivalent if and only if $\hat{U}_1$ and $\hat{U}_2$ are so. Applying Theorem 2.1 to $\hat{U}_1$ and $\hat{U}_2$, we have the following theorem.

Theorem 3.1: $U_1(f, g)$ and $U_2(f, g)$ are unitarily equivalent if and only if

$$\sum_t \left| \left| \left\langle \bigotimes_{r \in R(t)} \varphi_r^0, \bigotimes_{s \in S(t)} \psi_s^0 \right\rangle \right| - 1 \right| < \infty.$$

4. THE NONCOMPARABLE CASE

Let $\{I_r\}$ and $\{K_s\}$ be partitions of I into finite intervals, but not comparable in the sense of Sec. 3. Let

$$H_1 = \bigotimes_r^{(\otimes \varphi_r^0)} H(I_r) \quad \text{and} \quad H_2 = \bigotimes_s^{(\otimes \psi_s^0)} H(K_s) \tag{4.1}$$

be PTP with reference vectors $\varphi^0 = \otimes\varphi_r^0$ and $\psi^0 = \otimes\psi_s^0$. Let $U_1(f, g)$ and $U_2(f, g)$, respectively, be the correlated PTPR with respect to the basis h_i of $\mathfrak{U}$. Furthermore, we need some auxiliary theorems.

Consider a representation of the CCR on a finite-(n-) dimensional test-function space $\mathfrak{U}'$. Let d^nf denote the Lebesgue measure defined by the scalar product in $\mathfrak{U}'$. With any given orthonormal basis $\{h_i' : i = 1, 2, \cdots, n\}$ and $f = \sum_1^n \alpha_i h_i'$, one can write $d^nf = d\alpha_1 \cdots d\alpha_n$. Klauder and McKenna have shown[5,6] the following result.

Lemma 4.1: If $U(f, g), f, g \in \mathfrak{U}'$ is an irreducible representation of the CCR in a Hilbert space H, one has, for all $\psi_1, \varphi_1, \varphi_2, \psi_2 \in H$,

$$\int_{\mathfrak{U}'\times\mathfrak{U}'} d^nf d^ng(2\pi)^{-n}\langle\psi_1, U(f, g)\varphi_1\rangle\langle U(f, g)\varphi_2, \psi_2\rangle = \langle\psi_1, \psi_2\rangle\langle\varphi_2, \varphi_1\rangle.$$

A generalization of this kind of kernel integral formula is possible for PTPR as shown by Hegerfeldt.[8] Consider, e.g., the PTP H_1 [Eq. (4.1)] and the corresponding PTPR $U_1(f, g)$. Let

$$J_r = \bigcup_{r'=1}^{r} I_{r'}, \tag{4.2}$$

and let $W_r \equiv W(J_r)$ be the subspace of $\mathfrak{U}$ as defined in Eq. (2.1), with $\dim W_r = N(r)$, say. By d^Nf we denote the Lebesgue measure in W_r induced by the scalar product (f, g). For any $\psi_1, \varphi_1, \varphi_2, \psi_2 \in H_1$, we put

$$\mathbf{I}_r(\psi_1, \varphi_1, \varphi_2, \psi_2) \equiv \int_{W_r\times W_r} d^Nf d^Ng(2\pi)^{-N}\langle\psi_1, U_1(f, g)\varphi_1\rangle \times \langle U_1(f, g)\varphi_2, \varphi_1\rangle.$$

Lemma 4.2: We have

$$\lim_{r\to\infty} \mathbf{I}_r(\psi_1, \varphi_1, \varphi_2, \psi_2) = \langle\psi_1, \psi_2\rangle\langle\varphi_2, \varphi_1\rangle$$

for all $\psi_1, \varphi_1, \varphi_2, \psi_2 \in H_1$.

For a proof cf. Ref. 8.

As an abbreviation, we put $\mathbf{I}_r(\varphi, \varphi, \varphi, \varphi) \equiv \mathbf{I}_r(\varphi)$. Let H be the tensor product of two Hilbert spaces H_1 and H_2,

$$H = H_1 \otimes H_2.$$

For any vector $\psi \in H$ one can choose sets of orthonormal vectors $\psi_i^{(1)} \in H_1$ and $\psi_i^{(2)} \in H_2$, $i = 1, 2, \cdots$, such that

$$\psi = \sum_i \lambda_i \psi_i^{(1)} \otimes \psi_i^{(2)}, \quad \lambda_1 \geq \lambda_2 \geq \cdots \geq 0. \tag{4.3}$$

This decomposition is called a standard diagonal expansion[9] of ψ with respect to $H_1 \otimes H_2$.

Now suppose that the representations $U_1(f, g)$ and $U_2(f, g)$ are unitarily equivalent. Let T be the (isometric) transformation establishing the equivalence

$$U_1(f, g)T = TU_2(f, g). \tag{4.4}$$

Application of Lemma 4.2 to $T\psi^0$ (where ψ^0 reference vector of H_2 and $\|\psi^0\| = 1$) yields

$$\lim_{r\to\infty} \mathbf{I}_r(T\psi^0) = \|T\psi^0\|^4 = \|\psi^0\|^4 = 1. \tag{4.5}$$

On the other hand, with Eq. (4.4), we have

$$\begin{aligned}\mathbf{I}_r(T\psi^0) &= \int_{W_r\times W_r} d^Nf d^Ng(2\pi)^{-N}\,|\langle T\psi^0, U_1(f, g)T\psi^0\rangle|^2 \\ &= \int_{W_r\times W_r} d^Nf d^Ng(2\pi)^{-N}\,|\langle T\psi^0, TU_2(f, g)\psi^0\rangle|^2 \\ &= \int_{W_r\times W_r} d^Nf d^Ng(2\pi)^{-N}\,|\langle\psi^0, U_2(f, g)\psi^0\rangle|^2.\end{aligned} \tag{4.6}$$

The restriction of $U_2(f, g)$ to $f, g \in W_r$ is a representation of the CCR for $N(r)$ degrees of freedom. Therefore,[1] one can decompose H_2 as

$$H_2 = H(J_r) \otimes H'(J_r)$$

and

$$U_2(f, g) = U_r(f, g) \otimes \mathbf{1}';$$

such that, for $f, g \in W_r$, $U_r(f, g)$ is irreducible in $H(J_r)$. In the standard diagonal expansion [cf. Eq. (4.3)] of ψ^0, with respect to $H(J_r) \otimes H'(J_r)$,

$$\psi^0 = \sum_i \lambda_i^{(r)}\psi_i(J_r) \otimes \psi_i'(J_r), \quad \lambda_1^{(r)} \geq \lambda_2^{(r)} \geq \cdots \geq 0, \tag{4.7}$$

one has, due to orthonormality,

$$\sum_i \lambda_i^{(r)2} = 1. \tag{4.8}$$

Inserting Eq. (4.7) into (4.6) and noting that $\mathbf{I}_r$ is not only linear but also continuous in each argument for fixed[4] r, one can extract the (possibly infinite) sums and obtains

$$\begin{aligned}\mathbf{I}_r(T\psi^0) = \sum_{i,j,k,l} &\lambda_i^{(r)}\lambda_j^{(r)}\lambda_k^{(r)}\lambda_l^{(r)} \\ &\times \langle\psi_i'(J_r), \psi_j'(J_r)\rangle\langle\psi_k'(J_r), \psi_l'(J_r)\rangle \\ &\times \int_{W_r\times W_r} d^Nf d^Ng(2\pi)^{-N} \\ &\times \langle\psi_i(J_r), U_r(f, g)\psi_j(J_r)\rangle \\ &\times \langle U_r(f, g)\psi_k(J_r), \psi_l(J_r)\rangle.\end{aligned}$$

Applying Lemma 4.1 to the last integral, one gets

$$\mathbf{I}_r(T\psi^0) = \sum_i \lambda_i^{(r)4}.$$

Equations (4.7) and (4.8) imply

$$\mathbf{I}_r(T\psi^0) \leq \lambda_1^{(r)^2} \sum_i \lambda_i^{(r)^2} = \lambda_1^{(r)^2}.$$

Since $\lambda_1^{(r)} \leq 1$, we have the inequality

$$\mathbf{I}_r(T\psi^0) \leq \lambda_1^{(r)^2} \leq \lambda_1^{(r)} \leq 1.$$

Together with Eq. (4.5), this implies

$$\lim_{r\to\infty} \lambda_1^{(r)} = 1.$$

Hence, there exists a subsequence $\{\lambda_1^{(r_t)}\}$ converging so fast that

$$\sum_t (1 - \lambda_1^{(r_t)}) < \infty. \tag{4.9}$$

To each r_t there corresponds an interval [cf. Eq. (4.2)]

$$J_{r_t} = \{1, \cdots, j_t\}.$$

Consider the partition $\{K_s\}$ and let [cf. Eq. (1.17)]

$$K_s = \{k_{s-1} + 1, \cdots, k_s\}, \quad k_0 = 0.$$

Without affecting the convergence in Eq. (4.9), we may further require that

(a) no j_t coincides with any k_s, i.e.,

$$j_t \neq k_s \quad \text{for all } s, t, \tag{4.10}$$

(b) there falls at most one j between two successive k's, i.e.,

$$k_s < j_t < k_{s+1} \Rightarrow j_{t+1} > k_{s+1} \quad \text{for all } t. \tag{4.11}$$

Let $L_t = \{j_{t-1} + 1, \cdots, j_t\}$, $j_0 = 0$, and $\{L_t : t = 1, 2, \cdots\}$ be the resulting partition. Denote by $\{M_n\}$ the joint partition generated by $\{L_t\}$ and $\{K_s\}$, consisting of all intervals of the form $L_t \cap K_s$. Owing to Eq. (4.11) we have for each K_s either $K_s = M_n$ or $K_s = M_n \cup M_{n+1}$ with a certain $n = n(s)$. In the latter case, we can write $H(K_s) = H(M_n) \otimes H(M_{n+1})$. Consider the reference vector of H_2, $\psi^0 = \otimes\psi_s^0$, where $\psi_s^0 \in H(K_s)$, and form the standard diagonal expansion of ψ_s^0 with respect to $H(K_s) = H(M_n) \otimes H(M_{n+1})$:

$$\psi_s^0 = \sum_i \mu_i^{(n)} \psi_i(M_n) \otimes \psi_i'(M_{n+1}). \tag{4.12}$$

For each such $n(s)$ (latter case), there is a corresponding $r_t \equiv r_t(n)$ such that

$$\bigcup_{n'=1}^{n} M_{n'} = J_{r_t}. \tag{4.13}$$

Lemma 4.3: With $\lambda_i^{(r)}$, $\mu_i^{(n)}$, and $r_t(n)$ as defined in Eqs. (4.7), (4.12), (4.13), we have

$$\mu_i^{(n)} = \lambda_i^{(r_t(n))}.$$

Proof: Using Eq. (4.12), we get

$$\begin{aligned}\psi^0 = \otimes\psi_{s'}^0 &= \left(\bigotimes_{s'<s} \psi_{s'}^0\right) \\ &\otimes \left(\sum_i \mu_i^{(n)} \psi_i(M_n) \otimes \psi_i'(M_{n+1})\right) \otimes \left(\bigotimes_{s'>s} \psi_{s'}^0\right) \\ &= \sum_i \mu_i^{(n)} \left\{\left(\bigotimes_{s'<s} \psi_{s'}^0\right) \otimes \psi_i(M_n)\right\} \\ &\otimes \left\{\psi_i'(M_{n+1}) \otimes \left(\bigotimes_{s'>s} \psi_{s'}^0\right)\right\}.\end{aligned}$$

This is the standard diagonal expansion of ψ^0 with respect to $H_2 = H(J_{r_t(n)}) \otimes H'(J_{r_t(n)})$. Comparing with Eq. (4.7), and noting that the standard diagonal expansion is (essentially) unique,[9] we get the desired result. Certainly, we may write as well

$$\mu_i^{(n(r_t))} = \lambda_i^{(r_t)}, \tag{4.14}$$

because the correspondence is 1-to-1.

Let us fix a certain unit vector from each $H(M_n)$ [cf. Eq. (4.12)]:

$$\begin{aligned}\tilde{\psi}_n^0 &= \psi_{s(n)}^0, \quad \text{if} \quad M_n = K_{s(n)}, \\ &= \psi_1(M_n), \quad \text{if} \quad M_n \cup M_{n+1} = K_{s(n)}, \\ &= \psi_1'(M_n), \quad \text{if} \quad M_{n-1} \cup M_n = K_{s(n)}.\end{aligned} \tag{4.15}$$

Let $\nu(s)$ be the set of those n for which M_n is contained in K_s [$\nu(s)$ consists of one or two n's], i.e.,

$$\nu(s) = \{n : M_n \subseteq K_s\}.$$

Define

$$\tilde{\psi}^0 = \bigotimes_s \left(\bigotimes_{n\in\nu(s)} \tilde{\psi}_n^0\right) \in \bigotimes_s H(K_s). \tag{4.16}$$

Lemma 4.4: $\tilde{\psi}^0$, as defined in Eq. (4.16), is equivalent to the reference vector ψ^0.

Proof: Whenever $\nu(s)$ consists of one n only, we have

$$\left\langle \psi_s^0, \bigotimes_{n\in\nu(s)} \tilde{\psi}_n^0 \right\rangle = 1;$$

and if $\nu(s)$ contains two elements [cf. Eqs. (4.12) and (4.15)],

$$\left\langle \psi_s^0, \bigotimes_{n\in\nu(s)} \tilde{\psi}_n^0 \right\rangle = \mu_1^{(n(s))}.$$

Lemma 4.3 [Eq. (4.14)] and Eq. (4.9) then imply

$$\begin{aligned}\sum_s \left| \left\langle \psi_s^0, \bigotimes_{n\in\nu(s)} \tilde{\psi}_n^0 \right\rangle - 1 \right| &= \sum_t (1 - \mu_1^{(n(r_t))}) \\ &= \sum_t (1 - \lambda_1^{(r_t)}) < \infty.\end{aligned}$$

That is the equivalence of $\tilde{\psi}^0$ and ψ^0, hence $\tilde{\psi}^0 \in H_2$.

Owing to the irreducibility of $U_2(f, g)$,

$$M = \{\psi' : \psi' = U_2(f, g)\tilde{\psi}^0, f, g \in \mathfrak{U}\}$$

is a total set in H_2, and all $\psi' \in M$ are factorizable in a certain way

$$\psi' = \bigotimes_s \left(\bigotimes_{n \in \nu(s)} \psi'_n \right), \quad \psi'_n \in H(M_n), \quad \text{for all} \quad \psi' \in M.$$

Thus, we can define

$$T\psi' \equiv T \bigotimes_s \left(\bigotimes_{n \in \nu(s)} \psi'_n \right) = \bigotimes_n \psi'_n, \quad \text{for all} \quad \psi' \in M. \tag{4.17}$$

This T extends by linearity and continuity to an isometric isomorphism,[3] mapping H_2 onto

$$\mathcal{H}_2 = \bigotimes_n^{(\otimes \tilde{\psi}_n^0)} H(M_n).$$

$U_2'(f, g) = TU_2(f, g)T^*$ is obviously a PTPR and unitary equivalent to $U_2(f, g)$. Let

$$N(t) = \{n : M_n \subseteq L_t\},$$
$$R(t) = \{r : I_r \subseteq L_t\}. \tag{4.18}$$

With these notations, Theorem 3.1 applies and yields

$$\sum \left| \left\langle \bigotimes_{r \in R(t)} \varphi_r^0, \bigotimes_{n \in N(t)} \tilde{\psi}_n^0 \right\rangle - 1 \right| < \infty. \tag{4.19}$$

If, on the other hand (without assuming unitary equivalence of U_1 and U_2),

$$\lim_{r \to \infty} \lambda_1^{(r)} = 1$$

holds, where $\lambda_i^{(r)}$ is defined as in Eq. (4.7), we can choose a subsequence satisfying Eqs. (4.9)–(4.11). So we may construct a new reference vector as defined in Eqs. (4.15) and (4.16) (cf. Lemma 4.4). Furthermore, if Eq. (4.19) holds, we know by Theorem 3.1 that $U_1(f, g)$ and $U_2(f, g)$ are unitary equivalent. We summarize these results as follows.

Theorem 4.1: Let H_1 and H_2 be PTP as defined in Eq. (4.1) and $U_1(f, g)$, $U_2(f, g)$, respectively, the corresponding PTPR. Let $\lambda_i^{(r)}$ be defined by Eq. (4.7). $U_1(f, g)$ and $U_2(f, g)$ are unitarily equivalent if and only if

$$\lim_{r \to \infty} \lambda_1^{(r)} = 1,$$

and [$\tilde{\psi}^0$ defined in (4.15) and (4.16), and $N(t)$ and $R(t)$ in (4.18)]

$$\sum_t \left| \left| \left\langle \bigotimes_{r \in R(t)} \varphi_r^0, \bigotimes_{n \in N(t)} \tilde{\psi}_n^0 \right\rangle \right| - 1 \right| < \infty.$$

5. CONCLUSION

It turned out that the only operators needed to transform one PTPR into another unitary equivalent one were

(a) the unitary operator depending on a sequence of complex numbers [cf. Eq. (2.4)],

(b) the isomorphisms generated by

(1) setting parentheses [cf. Eq. (3.1)],

(2) omitting parentheses [cf. Eq. (4.17)].

If we call them "trivial transformations," we may summarize as follows. If two PTPR with respect to the same basis of the test-function space are unitary equivalent, then the operator establishing the unitary equivalence is a product of trivial transformations. Needless to say, all representations obtained by applying these trivial transformations are unitary equivalent.

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Scattering of Electromagnetic Waves in Uniformly Moving Media

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Various representations are considered for 2- and 3-dimensional electromagnetic wavefunctions in uniformly moving media. Rather than solving the relevant wave equation for the fields, the present formalism exploits the transformation formulas for plane waves in moving media, and as a starting point a spectral (plane-wave) representation is constructed. The procedure applies to arbitrary orders of β, but for simplicity only first-order velocity effects are considered in detail. Then, similarly to the velocity-independent problem, waves in uniformly moving media are represented in terms of complex integrals, special function series, inverse-distance differential-operator series, and surface integrals. Since familiar forms and functions are used, the present representations are extensions of the corresponding velocity-independent expressions. The latter are available at any given stage by letting the velocity vanish or by replacing the moving medium by free space. Scattering by circular cylinders and spheres is considered, and results are specialized to the case of thin cylinders; the new velocity effects introduce additional multipole terms. The original wavefunctions are transformed into the frame of reference of the medium at rest. Scattering by arbitrary objects moving in free space follows as a special case.

1. INTRODUCTION AND PRELIMINARY CONSIDERATIONS

The problem of scattering of a plane wave at a plane interface has been discussed[1] recently. Thus, as one logical extension of the plane interface problem, Censor[2] considers the problem of a cylinder of arbitrary cross section moving along its axis. A similar problem is discussed by Kong and Cheng.[3] Another relevant case is scattering by a rotating cylinder, which has been investigated to the first order in the velocity by Censor and Nathan.[4] Recently, the author was informed that similar results were previously derived by Tai.[5] Another class of problems, corresponding to the moving half-space, involves objects at rest with respect to the surrounding medium, moving relative to the observer. The limiting case of objects moving in free space has been discussed previously.[6] The far-field cases for moving cylinders and conducting spheres have been studied by Lee and Mittra[7] and Restrick,[8] respectively. For this class of problems, Einstein's[9] prescription can be used: the incident wave is transformed into the scatterer's frame of reference, the problem is solved there, and the results are transformed back into the observer's frame.

Presently, we consider the 2- and 3-dimensional problems of scattering in moving media. In general, such a problem consists of two interdependent parts, one being the fluid-dynamical interaction of the scatterer with the medium and the other the electromagnetic problem. An exact treatment would involve regions in the vicinity of the object where the motion of the medium is nonuniform. Special cases involving nonuniform motion, to the first order in the velocity, have been discussed earlier by Censor and Nathan,[4] and Censor.[10,11] The present formalism, which does not take general relativity into account, is adequate for scattering and propagation problems in regions of uniform velocity only. The first-order analysis of this formalism has been introduced before.[12] Note that, for problems of objects moving relative to the medium, Einstein's method fails, since it is not feasible to define a frame of reference in which both the medium and the object are at rest. Seto[13] discusses the wave equation in moving media and cites earlier references. Since it is shown there that the separability of this equation is very poor, the present approach is different. Rather than trying to solve the equation for the cases at hand, a solution is constructed as a spectral (plane-wave) representation, in a manner similar to that described by Stratton,[14] and then recast in terms of applicable forms, e.g., special-functions series, or inverse-distance power series.

In order to extend velocity-independent results to the problem of moving media, the relativistic transformation formulas for the various parameters of a plane electromagnetic wave are given. See Ref. 1 for a more detailed derivation and references. A plane electromagnetic wave

$$\boldsymbol{\phi} = \mathbf{f}e^{iA},$$
$$A = \mathbf{k}\cdot\mathbf{r} - \omega t \tag{1}$$

is defined in Γ, the frame of reference of the medium at rest, where $\boldsymbol{\phi}$ stands for an $\mathbf{E}$ or $\mathbf{H}$ field, $f = |\mathbf{f}|$ and $\hat{\mathbf{f}} = \mathbf{f}/f$ are the amplitude and direction of polarization, respectively, and A is the phase. Consider a

second frame Γ'. Viewed from Γ, the origin of Γ' is seen to move with a velocity $\mathbf{v} = \hat{\mathbf{v}}\beta c$, where c is the velocity of light in free space. For an observer in Γ', the relativistic transformation formulas yield

$$\begin{aligned} \Phi' &= \mathbf{f}' e^{iA'}, \\ \mathbf{f}' &= \mathsf{F} \cdot \mathbf{f}, \\ \mathsf{F} &= [(1-\gamma)\hat{\mathbf{v}} + \gamma B\hat{\mathbf{k}}]\hat{\mathbf{v}} + \gamma(1 - B\hat{\mathbf{v}} \cdot \hat{\mathbf{k}})\mathsf{I}, \\ B &= v/C, \quad \gamma = (1-\beta^2)^{-\frac{1}{2}}. \end{aligned} \tag{2}$$

Substituting the Lorentz transformation in A and collecting terms, we get

$$\begin{aligned} A' &= A = \mathbf{k}' \cdot \mathbf{r}' - \omega' t', \\ \omega' &= \gamma\omega(1 - B\hat{\mathbf{v}} \cdot \hat{\mathbf{k}}) \equiv \gamma\omega(1 - B\cos\alpha), \\ \mathbf{k}' &= \mathsf{K} \cdot \mathbf{k} = \{\mathsf{I} - \hat{\mathbf{v}}[(1-\gamma)\hat{\mathbf{v}} + \gamma v\hat{\mathbf{k}}C/c^2]\} \cdot \mathbf{k}, \\ k' &= |\mathbf{k}'| = k\gamma(1 - \beta^2 \sin^2\alpha - 2\beta C\cos\alpha/c \\ &\quad + \beta^2 C^2/c^2)^{\frac{1}{2}}. \end{aligned} \tag{3}$$

The direction of propagation transforms according to

$$\tan\alpha' = (\sin\alpha)/\gamma(\cos\alpha - vC/c^2). \tag{4}$$

Writing $k' = \omega'/C'$ specifies a transformation for the phase velocity, namely,

$$C' = (C - v\cos\alpha)/(1 - \beta^2\sin^2\alpha - 2\beta C\cos\alpha/c + \beta^2C^2/c^2)^{\frac{1}{2}}. \tag{5}$$

By means of (5), the relation for the direction of propagation may be written in a form needed in the sequel

$$\cos\alpha' = C'(\cos\alpha - \beta C/c)/(C - v\cos\alpha). \tag{6}$$

In free space there is no preferred frame of reference; hence, inverse transformation formulas are obtained simply by exchanging primed and unprimed symbols and replacing $\mathbf{v}$ by $-\mathbf{v}$, but in the present case this is not self-evident. Because of the symmetry of A [Eqs. (1) and (3) with respect to primed and unprimed quantities], the inverse transformations must have the same structure and follow from (3)–(6) according to the above prescription. Similarly to (2), for the amplitude we define

$$\begin{aligned} &\mathbf{f} = \mathsf{F}' \cdot \mathbf{f}', \ \mathsf{F} \cdot \mathsf{F}' = \mathsf{I}, \\ &\mathsf{F}' = \mathsf{F}^{-1} = [(\gamma-1)\hat{\mathbf{v}}\hat{\mathbf{v}} - \gamma B\hat{\mathbf{k}}\hat{\mathbf{v}} + \mathsf{I}]/\gamma(1 - B\hat{\mathbf{v}} \cdot \hat{\mathbf{k}}) \\ &\quad = [(1-\gamma)\hat{\mathbf{v}} - \gamma v\hat{\mathbf{k}}'/C']\hat{\mathbf{v}} + \gamma(1 + \mathbf{v} \cdot \hat{\mathbf{k}}'/C')\mathsf{I}. \end{aligned} \tag{7}$$

2. WAVES IN MOVING MEDIA

Two Dimensions

The general 2-dimensional solution for time-harmonic waves in moving media is constructed by superposing plane electromagnetic waves (2) polarized in the $\hat{\mathbf{z}}$ direction such that in Γ' they possess a frequency ω'. An amplitude $g(\alpha)$ is associated with each component wave propagating in direction α. The reference direction is taken as $\hat{\mathbf{v}}$. This yields, in Γ',

$$\psi' = \int e^{ik'(\tau')r'\cos(\theta'-\tau') - i\omega' t'} g(\tau') \frac{d\tau'}{\pi}, \tag{8}$$

where the contour of integration will be determined subsequently. In order that the integrand be a solution in Γ, the propagation constant must satisfy

$$k'(\tau') = \omega'/C'(\tau'), \tag{9}$$

where $C'(\tau')$ is given by (5). The inverse transformation formula of (5), with α, C, and $\mathbf{v}$ replaced by α', C', and $-\mathbf{v}$, yields $1/C'(\tau')$ as a solution of a second-order algebraic equation

$$\begin{aligned} 1/C'(\tau') &= \{A_1 \pm [A_1^2 + (1 - \beta^2C^2/c^2)A_2]^{\frac{1}{2}}\}/A_2, \\ A_1 &= \beta(c - C^2/c)\cos\tau', \\ A_2 &= \beta^2(C^2 - c^2)\cos^2\tau' + C^2/\gamma^2. \end{aligned} \tag{10}$$

By substituting $\beta = 0$, it becomes clear that the positive sign of the square root should be retained, leading to $C' = C$. In order to recast (8) in terms of previously given forms, we proceed by expanding (10) as a Taylor series in powers of β:

$$\begin{aligned} \psi' &= \int \exp\{iKr'\cos(\theta' - \tau') \\ &\quad \times [\exp(\beta\partial_\beta)C/C'|_{\beta=0}] - i\omega' t'\} g(\tau')\, d\tau'/\pi, \\ K &= \omega'/C, \\ &\exp(\beta\partial_\beta) = 1 + \beta\partial_\beta + (1/2!)\beta^2\partial_\beta^2 + \cdots, \\ &\beta\partial_\beta\left(\frac{C}{C'}\right)\bigg|_{\beta=0} = \beta\left(\frac{c}{C} - \frac{C}{c}\right)\cos\tau' \equiv V\cos\tau', \\ &\partial_\beta^2\left(\frac{C}{C'}\right)\bigg|_{\beta=0} = 1 - \frac{C^2}{c^2} \\ &\qquad - \cos^2\tau'\left(1 - \frac{2c^2}{C^2} + \frac{C^2}{c^2}\right), \quad \text{etc.} \end{aligned} \tag{11}$$

In the sequel, only the first-order velocity effects will be considered in detail. Higher-order terms are available by means of the same procedures; however, the expressions become cumbersome. Equation (11) now contains

$$\cos(\theta' - \tau')\cos\tau' = \tfrac{1}{2}[\cos\theta' + \cos(\theta' - 2\tau')] \tag{12}$$

in the exponent. Exploiting the representation of a plane wave in terms of cylindrical wavefunctions, we continue in a manner similar to Stratton.[15] This yields

$$\psi' = e^{\frac{1}{2}iKr'V\cos\theta' - i\omega' t'} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} i^{n-m} a_n e^{i(n-m)\theta'} \times H_{n-2m}(Kr')J_m(\tfrac{1}{2}Kr'V). \tag{13}$$

At large distances $r' \sim \infty$, Eq. (13) yields

$$\psi' \sim \mathcal{K}(Kr')e^{iKr'V\cos\theta'-i\omega' t'}g(\theta'), \tag{14}$$

where $\mathcal{K}(Kr') = (2/i\pi Kr')^{\frac{1}{2}}e^{iKr'}$. The same result can be obtained from (11) to the first order in β by using the method of stationary phase, assuming that $e^{iKr'V\cos\tau'}$ is a slowly varying function. Consequently, if $'\varphi$ is measured in the far field and only first-order velocity effects are of importance, $g(\theta')$ can be derived from (14), and a Fourier analysis yields the coefficients a_n. Since (13) is adequate for low velocities, it is expected that, for scatterers not too large with respect to wavelength, $Kr'V$ will be a small number. Hence, $J_m(\frac{1}{2}Kr'V)$ is expanded near the origin and only first-order velocity effects are retained. This implies that only the leading terms of J_0, J_1, and J_{-1} are significant. Alternatively, the same results are obtained by recasting the exponential (11) as a Taylor series in powers of β and keeping only the first-order velocity-dependent term:

$$\begin{aligned}\psi' &= \int e^{iKr'\cos(\theta'-\tau')-i\omega' t'} \\ &\quad\times [1 + iKr'V\cos(\theta'-\tau')\cos\tau']g(\tau')\frac{d\tau'}{\pi} \\ &= \int g(1 + r'V\cos\tau'\partial_{r'})e^{iKr'\cos(\theta'-\tau')-i\omega' t'}\frac{d\tau'}{\pi} \\ &= \sum_{n=-\infty}^{\infty} i^n a_n e^{in\theta'}[H_n + \tfrac{1}{2}iKr'V(e^{i\theta'}H'_{n+1} - e^{-i\theta'}H'_{n-1})] \\ &= \sum_{n=-\infty}^{\infty} i^n e^{in\theta'}[a_n H_n + \tfrac{1}{2}(a_{n-1} + a_{n+1})Kr'VH'_n],\end{aligned} \tag{15}$$

where the primed Hankel functions are differentiated with respect to the argument Kr'. For $\beta = 0$, the coefficients a_n are presumably known. Here, they are expected to be velocity dependent (as shown for special cases subsequently). Another complication results from the coupling of the different terms of the series, i.e., the fact that the term containing $e^{in\theta'}$ involves a_n, a_{n-1}, and a_{n+1}. However, as long as the first order of $Kr'V$ is considered, the effect is limited to adjacent terms. For higher-order velocity effects, the coupling will be stronger.

In (13), $i^{n-2m}H_{n-2m}$ can be replaced by the operator $\mathcal{K}(Kr')\mathfrak{D}$, given by Twersky,[16] acting on $\sum_n e^{(n-2m)\theta}a_n$. This leads to

$$\begin{aligned}\psi' &\sim e^{\frac{1}{2}iKr'V\cos\theta'-i\omega' t'}\mathcal{K}(Kr') \\ &\quad\times \sum_{m=-\infty}^{\infty} i^m J_m(\tfrac{1}{2}Kr'V)e^{im\theta'}\mathfrak{D}[e^{-2im\theta'}g(\theta')],\end{aligned}$$

$$\begin{aligned}&\mathfrak{D}g(\theta') \\ &= \sum_{m=0}\frac{(1+4\partial^2)(9+4\partial^2)\cdots[(2m-1)^2+4\partial^2]}{(i8Kr')^m m!}g(\theta'), \\ &\qquad\qquad \partial \equiv \frac{\partial}{\partial\theta}.\end{aligned} \tag{16}$$

If only the first power of $Kr'V$ is of significance, then (15) or (16) yields

$$\begin{aligned}\psi' \sim \mathcal{K}(Kr')e^{-i\omega' t'}&[(1 + \tfrac{1}{2}iKr'V\cos\theta')\mathfrak{D}g(\theta') \\ &+ \tfrac{1}{2}Kr'V\cos\theta'\mathfrak{D}\cos 2\theta' g(\theta') \\ &+ \tfrac{1}{2}iKr'V\sin\theta'\mathfrak{D}\sin 2\theta' g(\theta')].\end{aligned} \tag{17}$$

The exact (with respect to $\mathbf{r}'$) 2-dimensional representation[17] follows from (17) in a straightforward way, since $\cos 2\theta'$ and $\sin 2\theta'$ are periodic in π.

Equation (13) may be rewritten in terms of the surface-integral representation.[16] Since

$$e^{i(n-2m)\theta}H_{n-2m}(Kr)$$

is a formal solution in Γ, to the first order in the velocity, (13) yields

$$\begin{aligned}\psi' &= e^{\frac{1}{2}iKr'V\cos\theta'-i\omega' t'}\sum_{m=-\infty}^{\infty} i^m J_m(\tfrac{1}{2}KVr') \\ &\quad\times e^{im\theta'}\{H_0(K|\mathbf{r}'-\boldsymbol{\rho}'|);\psi'_m(\boldsymbol{\rho}')\}, \\ \psi'_m &= \sum_n a_n i^{n-2m}e^{i\theta'(n-2m)}H_{n-2m}(Kr'), \\ &\{H_0(K|\mathbf{r}'-\boldsymbol{\rho}'|);\psi(\boldsymbol{\rho})\} \\ &= \frac{1}{4i}\oint[H_0(K|\mathbf{r}'-\boldsymbol{\rho}'|)\partial_n\psi(\boldsymbol{\rho}') \\ &\quad - \psi(\boldsymbol{\rho})\partial_n H_0(K|\mathbf{r}'-\boldsymbol{\rho}'|)]\,ds(\boldsymbol{\rho}').\end{aligned} \tag{18}$$

Each term in braces satisfies the Sommerfeld[18] radiation condition. Therefore, the problem is determined uniquely by the tangential $\mathbf{E}$ and $\mathbf{H}$ fields on an arbitrary surface enclosing the scatterer, as in the velocity-independent case. Again, if $Kr'V$ is small enough for a given surface, only the leading terms of J_0, J_{-1}, and J_1 are retained.

Three Dimensions

In three dimensions we start with the analog of (8):

$$\begin{aligned}\Psi' &= \int e^{ik'(\hat{\mathbf{p}}')\hat{\mathbf{p}}'\cdot\mathbf{r}'-i\omega' t'}\mathbf{g}(\hat{\mathbf{p}}')\frac{d\Omega_{p'}}{2\pi}, \\ \int d\Omega p &\equiv \int_{-\pi}^{\pi}d\beta\int_0^{\frac{1}{2}\pi-i\infty}\sin\tau\,d\tau,\end{aligned} \tag{19}$$

where $\hat{\mathbf{p}}(\beta,\tau)$ is a complex unit vector specified by β and τ.

By taking the velocity along the polar axis, (9) and (10) are valid; hence, $k'(\hat{\mathbf{p}}') = k'(\tau')$ in (19). As in (11), $1/C'(\tau')$ is expanded in powers of β, and, for simplicity, only the first-order velocity effect is

retained. In analogy to (12), we have here

$$\begin{aligned}\cos\tau'\hat{\mathbf{p}}'\cdot\hat{\mathbf{r}}' &= \sin\tau'\cos\tau'\cos(\phi'-\beta')\\ &\quad+\cos^2\tau'\cos\theta'\\ &= \tfrac{1}{2}\cos\theta'+\tfrac{1}{2}\sin 2\tau'\sin\theta'\cos(\phi'-\beta')\\ &\quad+\tfrac{1}{2}\cos 2\tau'\cos\theta'. \qquad (20)\end{aligned}$$

The representation of a scalar plane wave in terms of spherical wavefunctions (see Stratton[19]) yields

$$\begin{aligned}\psi &= e^{\frac{1}{2}iKr'V\cos\theta'-i\omega't'}\sum_{n=0}^{\infty}\sum_{m=-n}^{n} i^n j_n(\tfrac{1}{2}Kr'V)\\ &\quad\times\{n,|m|\}P_n^{|m|}(\cos\theta')e^{im\phi'}\\ &\quad\times\int e^{iK\hat{\mathbf{p}}'\cdot\mathbf{r}'}P_n^{|m|}(\cos 2\tau')e^{-im\beta'}\mathbf{g}(\hat{\mathbf{p}}')\frac{d\Omega_{p'}}{2\pi},\\ \{n,m\} &= (n-m)!/(n+m)!. \qquad (21)\end{aligned}$$

For the 2-dimensional case, a new scattering amplitude has been defined so that (13) could be derived. Using forms given by Friedman and Russek,[20] one could work with the Cartesian components of $\mathbf{g}$, noting that the Cartesian components of ψ' satisfy the scalar wave equation. The complex-integral representation can then be replaced by series representation for these components. However, this would be of little value for the subsequent scattering problems. Assuming that the functions following $\exp(iK\hat{\mathbf{p}}'\cdot\mathbf{r}')$ in (21) are slowly varying, the method of stationary phase yields for the far field the analog of (14):

$$\psi'\sim h(Kr')e^{iKr'V\cos\theta'-i\omega't'}\mathbf{g}(\hat{\mathbf{r}}'), \qquad (22)$$

where $h(Kr')=e^{iKr'}/iKr'=h_0^{(1)}(Kr')$. Similarly to the 2-dimensional case, there is a first-order velocity effect in the phase at large distances. $\mathbf{g}(\hat{\mathbf{r}}')$ can be decided from far-field measurements.

Similarly to the 2-dimensional case, we expect $Kr'V$ to be small enough on the surface of the scatterers, such that terms of order $(Kr'V)^2$ are negligible. Thus, for the analog of (15), we start with

$$\psi'=\int\mathbf{g}(1+r'V\cos\tau'\partial_{r'})e^{iK\hat{\mathbf{p}}'\cdot\mathbf{r}'-i\omega't'}\frac{d\Omega_{p'}}{2\pi}. \qquad (23)$$

In order to derive the special-functions series representation analogous to (15), $\mathbf{g}^*=\cos\theta\mathbf{g}(\hat{\mathbf{r}})$ must be recast in terms of vector spherical harmonics $\mathbf{C}_n^m$, $\mathbf{B}_n^m$, $\mathbf{P}_n^m$.[21] This has been derived[6,12] in connection with objects moving in free space:

$$\begin{aligned}\mathbf{g}^* &= \sum_{n,m}(\mathbf{C}_n^m c_{nm}^*+\mathbf{B}_n^m b_{nm}^*+\mathbf{P}_n^m p_{nm}^*),\\ c_{nm}^* &= [A_1(m,n-1)+A_3(m,n-1)]c_{n-1,m}\\ &\quad+[A_2(m,n+1)+A_4(m,n+1)]c_{n+1,m}\\ &\quad+A_5(m,n)b_{nm},\\ b_{nm}^* &= [A_1(m,n-1)+A_3(m,n-1)]b_{n-1,m}\\ &\quad+[A_2(m,n+1)+A_4(m,n+1)]b_{n+1,m}\\ &\quad+A_5(m,n)c_{nm},\\ p_{nm}^* &= A_1(m,n-1)p_{n-1,m}+A_2(m,n+1)p_{n+1,m},\end{aligned}$$

$$\begin{aligned}A_1(m,n) &= \frac{n-m+1}{2n+1}, \qquad (24)\\ A_2(m,n) &= \frac{n+m}{2n+1},\\ A_3(m,n) &= -\frac{n+1-m}{(2n+1)(n+1)},\\ A_4(m,n) &= \frac{n+m}{n(2n+1)},\\ A_5(m,n) &= \frac{im}{n(n+1)}.\end{aligned}$$

Hence, the analog of (15) for the 3-dimensional case is

$$\begin{aligned}\psi' &= e^{-i\omega't'}\sum_{n,m} i^n[(c_{nm}+c_{nm}^*Vr'\partial_{r'})\mathbf{M}_{nm}\\ &\quad-i(b_{nm}+b_{nm}^*Vr'\partial_{r'})\mathbf{N}_{nm}\\ &\quad-i(p_{nm}+p_{nm}^*Vr'\partial_{r'})\mathbf{L}_{nm}]\\ &\equiv(\psi_1'+Vr'\partial_{r'}\psi_2'), \qquad (25)\end{aligned}$$

which involves the propagation constant $K=\omega'/C$. The analog of (16) is

$$\begin{aligned}\psi' &= e^{\frac{1}{2}iKr'V\cos\theta'-i\omega't'}h(Kr')\\ &\quad\times\sum_{n,m} i^n j_n(\tfrac{1}{2}Kr'V)\{n,|m|\}P_n^{|m|}(\cos\theta')\\ &\quad\times e^{im\phi'}\tilde{\mathfrak{D}}\cdot P_n^{|m|}(\cos 2\theta')e^{-im\phi}\mathbf{g}(\hat{\mathbf{r}}'), \qquad (26)\end{aligned}$$

where $\tilde{\mathfrak{D}}$ is the operator given by Twersky.[21] Similarly to (17), for small values of $Kr'V$ only $n=-1$, 0, and 1 are significant in (26). In (25), ψ_1' and ψ_2' are both solutions of the conventional vector wave equation. This implies the argument following Eq. (18), to the first order in KVr'.

3. SCATTERING PROBLEMS IN MOVING MEDIA

It was pointed out in the Introduction that the present formalism is valid in regions of uniformly moving media only. Hence, in the case of objects immersed in moving media and perturbing their uniform flow, the method fails. In many cases, the regions of nonuniform motion are localized in the vicinity of the objects, and for all practical purposes the velocity is uniform for $|\mathbf{r}'|>|\mathbf{r}_1'|$. If the velocity $\mathbf{v}=\mathbf{v}(\mathbf{r}')$ in the region $|\mathbf{r}'|<|\mathbf{r}_1'|$ is time independent, but otherwise arbitrary, then there are no moving boundary surfaces present; hence there are no Doppler

frequency shifts and the frequency is preserved everywhere. For such a case it is heuristically assumed that at large distances the fields reduce to (14) and (22) for the 2- and 3-dimensional cases, respectively. The following argument is used. The region internal with respect to the surface $|\mathbf{r}_1'|$ is assumed to be an arbitrary time-invariant "object," immersed in a uniformly moving medium. The boundary conditions, namely, the continuity of the tangential electric and magnetic field across the surface, are derived from Maxwell's equations without reference to the constitutive relations. Therefore, in principle, the solution of the boundary-value problem at an arbitrary surface $|\mathbf{r}'| > |\mathbf{r}_1'|$ would yield the coefficients a_n [Eq. (15)] or the corresponding c_{nm}, c_{nm}^*, etc. [Eq. (25)]. If $g(\theta')$ [Eq. (14)] or $\mathbf{g}(\hat{\mathbf{r}}')$ [Eq. (22)] are found from far-field measurements, orthogonality relations can be exploited to find the coefficients. Knowing the scattering amplitude, we can use the various representations, e.g., (15) and (17), and the corresponding equations (25) and (26) in three dimensions to describe the field everywhere in the region $|\mathbf{r}'| > |\mathbf{r}_1'|$.

Furthermore, there exists a class of problems involving scattering by objects immersed in uniformly moving media which might be of importance for applications. One such problem has been considered before,[1] and deals with the performance of a parabolic reflector immersed in a moving medium. More generally, one may consider scatterers made of artificial dielectrics (see, for example, Collin,[22] and Golden and Smith[23]). In this case, the artificial medium of the scatterers is made of a large number of conducting obstacles, with spacing and dimensions small with respect to wavelength. If the number of obstacles per unit volume is large, it will be assumed that the supporting medium has little effect, and the constitutive relations are determined by the configuration of obstacles only. If the artificial medium offers little resistance to the flow of the external medium, then, as far as the electromagnetic problem is concerned, we deal with a uniformly moving medium terminating on the surface of a homogeneous isotropic scatterer. For example, consider a metallic mesh with holes small with respect to wavelength. For the electromagnetic problem, if the holes are small enough, the surface will act as a "Faraday cage," i.e., as a perfect-conductor shielding. At the same time, the medium may flow through it; hence, the electromagnetic problem involves a uniformly moving medium terminating on the surface of the scatterer. In view of the above arguments, we subsequently consider the general problem of homogeneous and isotropic scatterers immersed in simple uniformly moving media.

Scattering by a Circular Cylinder

For the 2-dimensional scattering problem, consider a circular cylinder at rest in Γ', its axis oriented in the $\hat{\mathbf{z}}$ direction, perpendicular to the velocity $\mathbf{v} = v\hat{\mathbf{x}}$. The incident wave is a proper plane wave in Γ of the medium at rest. For simplicity, its direction of propagation is taken as $\hat{\mathbf{k}} = \hat{\mathbf{k}}' = \hat{\mathbf{v}}$. It follows from (2) that a plane wave, propagating perpendicularly to $\hat{\mathbf{z}}$ polarized transverse magnetic or transverse electric with respect to $\hat{\mathbf{v}}$, retains these properties both in Γ and Γ'. Hence, the incident wave is given by (2), with $\hat{\mathbf{f}}' = \hat{\mathbf{z}}$,

$$\Phi' = \phi'\hat{\mathbf{z}} = \hat{\mathbf{z}}e^{ik'x'-i\omega't'} = \hat{\mathbf{z}}\sum_{n=-\infty}^{\infty} i^n J_n(k'r')e^{in\theta'-i\omega't'}. \tag{27}$$

The wave inside the scatterer is

$$\Psi = \sum_{n=-\infty}^{\infty} i^n b_n J_n(\kappa r')e^{in\theta'-i\omega't'},$$
$$\kappa = \omega'/C_i, \quad C_i = (\mu_i\epsilon_i)^{-\frac{1}{2}}, \tag{28}$$

where κ, C_i, etc., apply inside the scatterer. The scattered field is specified by (15), exact to the first order in the velocity. The associated fields perpendicular to $\hat{\mathbf{z}}$ are found by application of Maxwell's equation to (15), (27), and (28) and substitution of the Minkowski constitutive relations (for theory and references see Sommerfeld[24] and Tai[25]). To the first order in β, this yields

$$\nabla^* \times \mathbf{E}' = i\omega'\mu\mathbf{H}',$$
$$\nabla^* \times \mathbf{H}' = -i\omega\epsilon\mathbf{E}',$$
$$\nabla^* = \nabla + i\omega'\mathbf{\Lambda}, \quad \mathbf{\Lambda} = (C_e^{-2} - c^{-2})\mathbf{v}, \tag{29}$$
$$\Lambda = |\mathbf{\Lambda}| = V/C_e,$$
$$C_e = (\mu_e\epsilon_e)^{-\frac{1}{2}}, \quad c = (\mu_0\epsilon_0)^{-\frac{1}{2}},$$

where μ_e and ϵ_e are measured in the external region in Γ and ∇^* is a special case of the extended ∇ operator investigated by Nathan and Censor.[26] In the sequel, V and Λ are distinguished [although they are related in a simple manner by (29)] in order to be able to trace back the effect of V, resulting from the wavefunction (15), and the one introduced via the boundary conditions by means of Λ. Consequently, the continuity of the tangential electric and magnetic fields prescribes the following boundary conditions at $r' = \rho$, the surface of the circular cylinder:

$$\phi' + \psi' = \Psi,$$
$$(\partial_{r'} - i\omega'\Lambda\cos\theta')(\phi' + \psi') = a\partial_{r'}\Psi, \tag{30}$$

where $a = \mu_e/\mu_i$, ϵ_e/ϵ_i for E', H' polarization, respectively. Keeping first-order β terms only, Eq. (30) and the orthogonality of (15), (27), and (28) with respect

to $e^{in\theta'}$ yield

$$J_n(k'\rho) + a_nH_n(K\rho) + \tfrac{1}{2}(a_{n-1} + a_{n+1})KV\rho H_n'(K\rho) = b_nJ_n(\kappa\rho), \tag{31a}$$

$$J_n'(k'\rho)(k' - 2\omega'\Lambda) + a_nKH_n'(K\rho) + \tfrac{1}{2}a_{n-1}\{[K^2\rho VH_n'(K\rho)]' + 2\omega'\Lambda H_{n-1}(K\rho)\} + \tfrac{1}{2}a_{n+1}\{[K^2\rho VH_n'(K\rho)]' - 2\omega'\Lambda H_{n+1}(K\rho)\} = \kappa ab_nJ_n'(\kappa\rho). \tag{31b}$$

Now, if we eliminate b_n, this yields a_n in terms of a_{n+1}, a_{n-1}. Increasing and decreasing index n by one, we can calculate the velocity-independent part of a_{n+1}, a_{n-1}. This yields

$$a_n = \frac{J_n(\kappa\rho)J_n'(k'\rho)(k' - 2\omega'\Lambda) - J_n(k'\rho)\kappa aJ_n'(\kappa\rho)}{\kappa aJ_n'(\kappa\rho)H_n(K\rho)} \times \frac{+\tfrac{1}{2}A_{n\pm1}(J_n(\kappa\rho)\{[K^2\rho VH_n'(K\rho)]' \pm 2\omega'\Lambda H_{n\pm1}(K\rho)\} - \kappa aJ_n'(\kappa\rho)KV\rho H_n'(K\rho))}{-KJ_n(\kappa\rho)H_n'(K\rho)},$$

$$A_{n\pm1} = \frac{J_{n\pm1}(\kappa\rho)J_{n\pm1}'(K\rho)K - \kappa aJ_{n\pm1}(K\rho)J_{n\pm1}'(\kappa\rho)}{\kappa aJ_{n\pm1}'(\kappa\rho)H_{n\pm1}(K\rho) - J_{n\pm1}(\kappa\rho)KH_{n\pm1}'(K\rho)}, \tag{32}$$

where in the numerator of a_n both A_{n+1} and $-$ and A_{n-1} and $+$ appear; A_{n+1} and A_{n-1} are given in the second expression with the top or bottom signs, respectively. For $\beta = 0$, $K = k'$, or for $C = c$, i.e., free space, $V = 0$, and $\Lambda = 0$, Eq. (32) reduces to the velocity-independent case of scattering by a cylinder. Clear-air scattering, i.e., the case of the scatterer and the external moving medium having the same constitutive constants in their proper frames of reference, has been considered by Censor and Nathan,[4] and Censor.[1,2,11] For completeness, consider the present case: (32) yields

$$a_n = \frac{-2\omega'\Lambda J_n'(K\rho)J_n(K\rho)}{K[J_n'(K\rho)H_n(K\rho) - J_n(K\rho)H_n'(K\rho)]} = -\tfrac{1}{4}i\rho\omega'\Lambda[J_n^2(K\rho)]'. \tag{33}$$

The case of a perfect conducting cylinder and E polarization is provided by $\phi' + \psi' = 0$; hence, Eq. (31a) is considered with $b_n = 0$, yielding

$$a_n = -[J_n(k'\rho) - \tfrac{1}{2}(A_{n-1} + A_{n+1})KV\rho H_n'(K\rho)]/H_n(K\rho),$$
$$A_{n\pm1} = -J_{n\pm1}(K\rho)/H_{n\pm1}(K\rho). \tag{34}$$

For H polarization, consider Eq. (31b) with $b_n = 0$. Then

$$a_n = -(J_n'(k'\rho)(k' - 2\omega'\Lambda) + \tfrac{1}{2}A_{n-1}\{[K^2\rho VH_n'(K\rho)]' + 2\omega'\Lambda H_{n-1}(K\rho)\} + \tfrac{1}{2}A_{n+1}\{[K^2\rho VH_n'(K\rho)]' - 2\omega'\Lambda H_{n+1}(K\rho)\})/KH_n'(K\rho),$$
$$A_{n\pm1} = -J_{n\pm1}'(K\rho)/H_{n\pm1}'(K\rho). \tag{35}$$

Again, either $C_e = c$ or $\beta = 0$ reduces (34)–(35) to the velocity-independent result of scattering by a perfectly conducting cylinder. Thin scatterers have been considered by Twersky[27] for the velocity-independent case, by expanding the forms corresponding to (32), (34), and (35), near the origin $\rho \sim 0$ (Twersky develops a 2-space formalism, and the following forms are specialized to the conventional 1-space problems). Thus, for perfectly conducting thin cylinders and E polarization,

$$a_0 = -i\pi[2 \ln (2/\delta k\rho)], \quad \delta = 1.781\cdots,$$
$$a_n = i\pi n(\tfrac{1}{2}k\rho)^{2n}/(n!)^2, \quad n = 1, 2, \cdots. \tag{36}$$

For H polarization,

$$a_0 = -i\pi(\tfrac{1}{2}k\rho)^2,$$
$$a_n = i\pi(\tfrac{1}{2}k\rho)^{2n}/(n!)^2, \quad n = 1, 2, \cdots. \tag{37}$$

Hence, for E polarization the monopole term is predominant, and for H polarization a_0 and a_1 are of the same power in ρ. Therefore, the monopole and dipole terms are predominant. For thin dielectric circular cylinders, the E polarized wave produces

$$a_0 = i\pi(\tfrac{1}{2}k\rho)^2[(\epsilon_i/\epsilon_e) - 1],$$
$$a_1 \propto \rho^4, \quad a_n \propto \rho^{2n}, \quad n = 2, 3, \cdots. \tag{38}$$

For H polarization,

$$a_1 = i\pi(\tfrac{1}{2}k\rho)^2[(\epsilon_i/\epsilon_e) - 1]/[(\epsilon_i/\epsilon_e) + 1],$$
$$a_0 \propto \rho^4, \quad a_n \propto \rho^{2n}, \quad n = 2, 3, \cdots. \tag{39}$$

Therefore, in (38) and (39), the monopole and dipole terms, respectively, predominate. Near the origin, (35) becomes

$$a_0 = \tfrac{1}{4}i\rho^2\omega'\Lambda K,$$
$$a_1 = -a_0, \tag{40}$$
$$a_n \propto \rho^{2n}, \quad n = 1, 2, \cdots,$$

regardless of polarization. Hence, in (15), $n = -1, 0,$ and 1 terms must be taken into account, and we have a monopole plus dipole field. In (34), the $A_{n\pm1}$ are the forms obtained for a medium at rest; hence, they are given by inspection of (36). Consequently, (34) yields

$$a_0 = -i\pi[2 \ln (2/\delta K\rho)],$$
$$a_1 = -\tfrac{1}{2}a_0 KV, \tag{41}$$

where the a_n, $n \geq 2$, are negligible. Therefore, the effect of the velocity is to introduce a dipole term of the first order in β, similarly to (40), but in (40) the zero-order velocity effect vanishes. Now consider (35) for the H polarization and thin cylinders. Note that $A_{n\pm1}$ [Eq. (35)] is the expression obtained for the corresponding velocity independent problem. Therefore, $\rho \sim 0$ is given by (37). Thus, (35) yields

$$a_0 = -i\pi(\tfrac{1}{2}k'\rho)^2,$$
$$a_1 = i\pi(\tfrac{1}{2}K\rho)^2[(1/K)(k' - 2\omega'\Lambda) - \tfrac{1}{2}V], \tag{42}$$
$$a_2 = Vi\pi(\tfrac{1}{2}K\rho)^2,$$

and the higher multipoles are negligible. Equation (32) may be subjected to a similar treatment, noting that $A_{n\pm1}$ are given by (38) and (39) for dielectric cylinders and E and H polarization, respectively. Again, velocity effects appear and produce higher multipoles of first order in the velocity.

The significance of these results is that they are expected to be relevant for arbitrary thin cylinders in moving media which are not uniform in the vicinity of the scatterer. The velocity effects are introduced via V and Λ: The first is part of the wavefunction, e.g., (15), and the latter results from the boundary conditions at the surface of the scatterer. For an arbitrary scatterer perturbing the flow in its vicinity, we still expect V type effects to be present, in addition to other effects that might be present because of the velocity at the surface. For an impenetrable object, where the medium at the surface must move tangentially, we expect velocity effects introduced by the boundary conditions. The effect of the direction of the flow with respect to the surface has been discussed before.[11,1] For a medium moving tangent to the surface, we expect the largest boundary-condition-type velocity effects.

Scattering by a Sphere

Theory and references for scattering of a plane electromagnetic wave by an arbitrary refractive sphere are given by Stratton.[28] For simplicity, the direction of propagation of the incident plane wave is taken parallel to the velocity, $\hat{\mathbf{z}} = \hat{\mathbf{v}}$. However, there is some loss of generality, since this is the only case where a plane wave is transversal both in Γ and Γ'. [See Eq. (2).] Thus, for an arbitrary plane wave in Γ' we have longitudinal field components. Similarly to Stratton,[28] the incident plane wave is recast in terms of vector spherical waves:

$$\begin{aligned}\phi'_E &= \hat{\mathbf{x}}e^{ik'z'-i\omega't'} \\ &= e^{-i\omega't'}\sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} \\ &\quad \times [\bar{\mathbf{M}}_{(o)n,1}(\mathbf{r}') - i\bar{\mathbf{N}}_{(e)n,1}(\mathbf{r}')] \\ &= e^{-i\omega't'}\sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} (\operatorname{Im} \bar{\mathbf{M}}_{n,1} - i \operatorname{Re} \bar{\mathbf{N}}_{n,1}) \\ &= \tfrac{1}{2}e^{-i\omega't'}\sum_{n=1}^{\infty} i^{n+1} \frac{2n+1}{n(n+1)} \Big(-(\bar{\mathbf{M}}_{n,1} + \bar{\mathbf{N}}_{n,1}) \\ &\quad + \frac{(n+1)!}{(n-1)!}(\bar{\mathbf{N}}_{n,-1} - \bar{\mathbf{M}}_{n,-1})\Big),\end{aligned} \tag{43}$$

where the indices (e) and (o) denote the even and odd functions, respectively, Im and Re denote the imaginary and real parts (this applies to real arguments only), and the bar signifies the $j_n(k'r')$ nonsingular spherical Bessel functions. The reason for keeping the $m = 1$ and $m = -1$ terms in (43) and subsequently is due to the fact that, in (24), c_{nm} and b_{nm} are coupled, i.e., both the even and odd functions are needed for both $\mathbf{M}$ and $\mathbf{N}$ waves, in contradistinction to the velocity-independent case. In view of (43), the internal field Ψ_E is given by

$$\Psi_E = e^{-i\omega't'}\sum_{n=1}^{\infty} i^n(c_{nm}^{(i)}\bar{\mathbf{M}}_{nm} - ib_{nm}^{(i)}\bar{\mathbf{N}}_{nm}), \quad m = \pm 1, \tag{44}$$

where (i) designates coefficients relevant to the internal region and the bar signifies the $j_n(\kappa r')$ functions, with propagation constant κ. The scattered field is given by (25) with $m = \pm 1$ and $\mathbf{L}_{nm} = 0$. Exploiting (29), we derive the boundary conditions similar to (30):

$$\hat{\mathbf{r}}' \times (\boldsymbol{\phi}' + \boldsymbol{\psi}') = \hat{\mathbf{r}}' \times \boldsymbol{\Psi}, \tag{45a}$$

$$\hat{\mathbf{r}}' \times [(\nabla + i\omega'\Lambda\hat{\mathbf{r}}' \cos\theta') \times (\boldsymbol{\phi}' + \boldsymbol{\psi}')] = a\hat{\mathbf{r}}' \times \nabla \times \boldsymbol{\Psi}, \tag{45b}$$

at the surface of the sphere $r' = \rho$. The $\nabla \times$ operation has the effect of turning the $\mathbf{M}_{nm}$ and $\mathbf{N}_{nm}$ functions into $k\mathbf{N}_{nm}$ and $k\mathbf{M}_{nm}$, respectively. Multiplying $\boldsymbol{\phi}'$ by $\cos\theta'$ is equivalent to differentiating (43) with respect to $ik'r'$. Multiplying $\boldsymbol{\psi}'$ by $\cos\theta'$ affects only the parts independent of V and is prescribed by (24). The effect of the $\hat{\mathbf{r}}' \times [\hat{\mathbf{r}}' \times \cdots]$ operation is to eliminate the $\mathbf{p}_n^m$ functions and to invert the sign. Consequently, (45) and the orthogonality relations lead to the following

set of algebraic equations for the coefficients: Eq. (45a) yields

$$-\begin{Bmatrix} 1 \\ (n+1)!/(n-1)! \end{Bmatrix} \frac{i(2n+1)}{2n(n+1)} j_n(k'\rho) + (c_{n,\pm1} + c^*_{n,\pm1} V\rho\partial_\rho) h_n(K\rho) = c^{(i)}_{n,\pm1} j_n(\kappa\rho), \quad (46a)$$

$$\begin{Bmatrix} 1 \\ (n+1)!/(n-1)! \end{Bmatrix} \frac{(2n+1)}{2n(n+1)} \frac{\partial_{k'\rho}}{k'\rho} [k'\rho j_n(k'\rho)] + (b_{n,\pm1} + b^*_{n,\pm1} V\rho\partial_\rho) \frac{\partial_{K\rho}}{K\rho} [K\rho h_n(K\rho)] = b^{(i)}_{n,\pm1} \frac{\partial_{\kappa\rho}}{\kappa\rho} [\kappa\rho j_n(\kappa\rho)], \quad (46b)$$

where the top or bottom expression in braces is considered with the corresponding $m = 1$ or $m = -1$, respectively. Equation (45b) prescribes

$$\begin{Bmatrix} 1 \\ (n+1)!/(n-1)! \end{Bmatrix} \frac{i(2n+1)}{2n(n+1)} (k' \mp \omega'\Lambda\partial_{k'\rho}) \frac{\partial_{k'\rho}}{k'\rho} \times [k'\rho j_n(k'\rho)] - \omega'\Lambda\Big(c_{n-1,\pm1} h_{n-1}(K\rho) \times [A_1(\pm1, n-1) + A_3(\pm1, n-1)] - c_{n+1,\pm1} h_{n+1}(K\rho)[A_2(\pm1, n+1) + A_4(\pm1, n+1)] + b_{n,\pm1} \frac{\partial_{K\rho}}{K\rho} [K\rho h_n(K\rho)] A_5(\pm1, n) \Big) - K(c_{n,\pm1} + c^*_{n,\pm1} V\rho\partial_\rho) \frac{\partial_{K\rho}}{K\rho} [K\rho h_n(k\rho)] - \partial_\rho (c_{n,\pm1} + c^*_{n,\pm1} V\rho\partial_\rho) h_n(K\rho) = -\kappa a c^{(i)}_{n,\pm1} \frac{\partial_{\kappa\rho}}{\kappa\rho} [\kappa\rho j_n(\kappa\rho)],$$

$$\begin{Bmatrix} -1 \\ (n+1)!/(n-1)! \end{Bmatrix} \frac{i(2n+1)}{2n(n+1)} (k' \mp \omega'\Lambda\partial_{k'\rho}) j_n(k'\rho) - i\omega'\Lambda\Big(-b_{n-1,\pm1} \frac{\partial_{K\rho}}{K\rho} [K\rho h_{n-1}(K\rho)](A_1 + A_3) + b_{n-1,\pm1} \frac{\partial_{K\rho}}{K\rho} [K\rho h_{n+1}(K\rho)](A_2 + A_4) + c_{nm} h_n(K\rho) A_5 \Big) - iK(b_{n,\pm1} + b^*_{n,\pm1} V\rho\partial_\rho) h_n(K\rho) + i\partial_\rho (b_{n,\pm1} + b^*_{n,\pm1} V\rho\partial_\rho) \frac{\partial_{K\rho}}{K\rho} [K\rho h_n(K\rho)] = -i\kappa a b^{(i)}_{n,\pm1} j_n(\kappa\rho), \quad (47)$$

where m and n in A_1, etc., are the same in the two expressions (47). The solution of (46) and (47) for the coefficients is cumbersome, although straightforward. As for the cylinder case, coupling of coefficients is eliminated by substituting adjacent terms. The case of a perfectly conducting sphere is given by (46) with $c^{(i)}$, $b^{(i)} = 0$. This is a relatively simple case. Equations (46a) and (46b) yield $c_{n,\pm1}$ and $b_{n,\pm1}$ in terms of velocity-dependent $c_{n-1,\pm1}$, $c_{n+1,\pm1}$, $b_{n,\pm1}$, and $b_{n-1,\pm1}$, $b_{n+1,\pm1}$, $c_{n,\pm1}$, respectively. The velocity-dependent coefficients are eliminated by substituting the zeroth-order terms of the relevant adjacent terms.

4. MOVING OBJECTS

The results obtained in Γ', at rest with respect to the object, may be transformed into an arbitrary frame of reference, giving account of scattering by moving objects. Two cases of interest are discussed using essentially the same procedure. First, consider the external medium in Γ' to be at rest with respect to the scatterer. Then for an arbitrary observer we deal with a scatterer moving together with the surrounding medium. Secondly, we consider the problems of a scatterer moving in a medium at rest. The two problems are combined by transforming (8) and (19) into an arbitrary frame of reference, moving with a velocity $\mathbf{v}''$ with respect to Γ. The case $v = 0$ and arbitrary $\mathbf{v}''$ yields the results for the first problem; $\mathbf{v}'' = -\mathbf{v}$ leads to the solution of the second one. In free space, the two problems lead to the same results obtained previously.[6]

Two Dimensions

According to (31), the phase is an invariant, and is left in (8) in terms of Γ' coordinates. The amplitude is transformed by applying F'', given by (2), with γ'', $\mathbf{v}''$, and $\mathbf{k}'$. For a field polarized normal to $\mathbf{v}''$ this yields

$$\psi'' = \gamma'' \int e^{ik'(\tau')r' \cos(\theta' - \tau') - i\omega' t'} \left(1 - \frac{v''}{C'} \cos\tau'\right) g(\tau') \frac{d\tau'}{\pi}. \quad (48)$$

For the first problem, i.e., $v = 0$ and arbitrary v'', we get

$$\psi'' = \sum_{n=-\infty}^{\infty} i^n b_n H_n(k'r') e^{in\theta' - i\omega' t'},$$
$$b_n = \gamma''[a_n - (v''/C)(a_{n-1} + a_{n+1})], \quad (49)$$

where the a_n are the coefficients of $g(\theta')$. This is a relativistically exact form. Since it has the same structure as (28), other representations follow by inspection. Results can be obtained in terms of Γ'' coordinates by substituting the Lorentz transformation. In free space, $C = c$ in (49). The second problem $v'' = -v$, similarly to (1), to first order in β yields

$$\psi \sim \mathcal{H}(Kr') e^{ikr'V \cos\theta' - i\omega' t'} (1 + B \cos\theta') g(\theta'), \quad (50)$$

where ψ is measured in Γ of the medium at rest, B is

defined in (2). For free space $C = c$ and $V = 0$ and, to first order in β, Eq. (50) and the far-field form of (49) coincide. The special-function series representation is obtained from (15) by multiplying g by $(1 + B\cos\tau')$. Thus in Γ one gets

$$\psi = \sum_{n=-\infty}^{\infty} i^n e^{in\theta'}[b_n H_n + \tfrac{1}{2}(b_{n-1} + b_{n+1})kr'VH_n'],$$
$$b_n = a_n - \tfrac{1}{2}B(a_{n+1} + a_{n-1}). \quad (51)$$

Again, for free space and first order in the velocity, (51) coincides with (49).

Three Dimensions

In three dimensions $\mathsf{F}''[(2)]$ with $\mathbf{k}'$ and $\mathbf{v}''$ is applied to $\mathbf{g}$ in (19). For the first problem, this leads to

$$\boldsymbol{\psi}'' = \mathsf{A}\cdot\boldsymbol{\psi}' + \gamma''B'' \times \int e^{ik'\hat{\mathbf{p}}'\cdot\mathbf{r}'-i\omega' t'}[\hat{\mathbf{p}}'(\hat{\mathbf{v}}''\cdot\mathbf{g}) - (\hat{\mathbf{v}}''\cdot\hat{\mathbf{p}}')\mathbf{g}]\frac{d\Omega_{p'}}{2\pi},$$
$$B'' = v''/C, \quad \mathsf{A} \equiv (1-\gamma'')\hat{\mathbf{v}}''\hat{\mathbf{v}}'' + \gamma''\mathsf{I}. \quad (52)$$

The first dyadic has been taken out of the integral sign, and acts on $\boldsymbol{\psi}'$, the field measured in Γ'. Since $\hat{\mathbf{v}}''\cdot\hat{\mathbf{p}}' = \cos\tau'$, according to (24), we conclude

$$(\hat{\mathbf{v}}''\cdot\hat{\mathbf{p}}')\mathbf{g} = \mathbf{g}^*. \quad (53)$$

Exploiting the recurrence relation

$$-\sin\theta\partial_\theta P_n^m(\cos\theta) = [(n+m)(n+1)P_{n-1}^m - n(n-m+1)P_{n+1}^m]/(2n+1), \quad (54)$$

we find that

$$\hat{\mathbf{f}}'(\hat{\mathbf{v}}''\cdot\mathbf{B}_n^m) = A_6\mathbf{P}_{n-1}^m + A_7\mathbf{P}_{n+1}^m,$$
$$A_6(m,n) = (n+m)(n+1)/(2n+1),$$
$$A_7(m,n) = -n(n-m+1)/(2n+1),$$
$$\hat{\mathbf{v}}'' = \hat{\mathbf{r}}'\cos\theta' - \hat{\boldsymbol{\theta}}'\sin\theta'. \quad (55)$$

From the definition of $\mathbf{C}_n^m$, we have

$$\hat{\mathbf{f}}'(\hat{\mathbf{v}}''\cdot\mathbf{C}_n^m) = -im\mathbf{P}_n^m.$$

Consequently,

$$\boldsymbol{\psi}'' = \mathsf{A}\cdot\boldsymbol{\psi}_1' - \gamma''B''\Big(\boldsymbol{\psi}_2' + i\sum_{n=1}^{\infty} i^n\mathbf{L}_{nm}[A_6(m,n+1)b_{n+1,m} - A_7(m,n-1)b_{n-1,m} - imc_{nm}]\Big), \quad (56)$$

where A is defined in (52), $\boldsymbol{\psi}_1'$ is the field involving $\mathbf{g}$, and $\boldsymbol{\psi}_2'$ involves $\mathbf{g}^*$. Therefore $\boldsymbol{\psi}''$ involves wavefunctions of the type $\mathbf{L}_{nm}$. For the second problem, to the first order in the velocity, F' [Eq. (7)] is applied to $\mathbf{g}'$ in (23), yielding

$$\boldsymbol{\psi} = \int \mathsf{F}'\cdot\mathbf{G}\exp(iK\hat{\mathbf{p}}'\cdot\mathbf{r}' - i\omega' t')\frac{d\Omega_{p'}}{2\pi},$$
$$\mathbf{G} = \mathbf{g} + g^* r' V\partial_r. \quad (57)$$

$\mathbf{g}$ and $\mathbf{g}^*$ are submitted to the same procedure used to derive $\boldsymbol{\psi}''$ above, with γ'' and v'' replaced by 1 and $-v$, respectively.

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Initial-Value Problem for the Equation $\left(\frac{\partial}{\partial t} + a(t, x, y)\frac{\partial}{\partial x} + b(t, x, y)\frac{\partial}{\partial y} + c(t, x, y) + d(t, x, y)\frac{\partial^2}{\partial x \partial y}\right)u = f(t, x, y)$ in the Complex Domain

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The initial-value problem

$$u_t + a(t, x, y)u_x + b(t, x, y)u_y + c(t, x, y)u + d(t, x, y)u_{xy} = f(t, x, y), \quad u(0, x, y) = \varphi(x, y)$$

is first considered in a complex polycylinder Q whose center is the origin. All functions appearing are holomorphic in Q. On the one hand, this problem has at most one holomorphic solution in Q, while on the other hand, the strong assumptions of holomorphy do not in general guarantee even the existence of a local holomorphic solution. We then treat the special initial-value problem of Lambropoulos [J. Math. Phys. **8**, 11 (1967)]

$$u_t + axu_x + byu_y + cxyu + u_{xy} = 0, \quad u(0, x, y) = \varphi(x, y),$$

where a, b, and c are complex constants. We are able to derive an infinite series as the formal solution, which is easy to examine. Moreover, some statements on the existence of a local holomorphic solution are given.

I. INTRODUCTION

Recently, several papers have been published which consider pseudoparabolic differential equations of the structure

$$\left(\frac{\partial^2}{\partial x \partial y} + a(t, x, y)\frac{\partial}{\partial x} + b(t, x, y)\frac{\partial}{\partial y} + c(t, x, y) + d(t, x, y)\frac{\partial}{\partial t}\right)u = f(t, x, y) \quad (1)$$

under various conditions of the unknown function $u(t, x, y)$.[1-6] Partial differential equations of type (1) are relevant for some physical problems; see for instance Refs. 2 and 5.

In Ref. 4, Eq. (1) is discussed on the complex polycylinder

$$Q \equiv \{(t, x, y): |t| < r_1, |x| < r_2, |y| < r_3\}$$

with $0 < r_i \leq \infty$, $i = 1, 2, 3$, under the conditions

$$u(t, x, 0) = \rho(t, x), \quad u(t, 0, y) = \sigma(t, y), \quad \rho(t, 0) = \sigma(t, 0), \quad (1')$$

where $\rho(t, x)$ and $\sigma(t, y)$ are given functions. For this problem, it is assumed that all functions that appear are holomorphic in Q. One can then show that the problem (1) has exactly one solution which is holomorphic in Q. The proof of this assertion is based on the consideration of a majorant problem for which the existence of a global solution may be shown by using a special series expansion.

Lambropoulos[2] studied the initial-value problem

$$\left(\frac{\partial^2}{\partial x \partial y} + ax\frac{\partial}{\partial x} + by\frac{\partial}{\partial y} + cxy + \frac{\partial}{\partial t}\right)u = 0, \quad (2)$$

$$u(0, x, y) = \varphi(x, y), \quad (2')$$

where a, b, and c are constants. He assumed that $\varphi(x, y)$ may be expanded in a Taylor series in a neighborhood of the origin and that the problem (2) has a solution which may be represented as

$$u(t, x, y) = \sum_{m,n=0}^{\infty} p_{mn}(t)\frac{x^m y^n}{(m!\, n!)^{\frac{1}{2}}}. \quad (3)$$

In Ref. 2, the coefficients $p_{mn}(t)$, $m, n = 0, 1, 2, \cdots$, were given in a representation which is, in general, fairly cumbersome. The existence of a solution of the form (3) was not studied in Ref. 2.

While Lambropoulos supposed that the initial-value problem (2) cannot be solved by using conventional methods, Neuringer gave a formal representation of the solution for (2) whose scope of validity, however, is not specified. A comparison of Lambropoulos' approach with that of Neuringer is not possible, in general, for the assumptions are of local nature in the one case, and of global nature in the other case, with respect to the spatial variables.

In the present paper, we first discuss the general equation

$$\left(\frac{\partial}{\partial t} + a(t, x, y)\frac{\partial}{\partial x} + b(t, x, y)\frac{\partial}{\partial y} + c(t, x, y) + d(t, x, y)\frac{\partial^2}{\partial x \partial y}\right)u = f(t, x, y) \quad (4)$$

under the initial condition

$$u(0, x, y) = \varphi(x, y), \tag{4'}$$

where the coefficients, the inhomogeneity f, and φ must be holomorphic in the polycylinder Q. The essential result obtained is that the initial-value problem (4) has at most one holomorphic solution under the assumptions just mentioned. On the other hand, the strong assumptions of holomorphy generally do not guarantee even the existence of a local solution. This result is surprising with respect to the attributes for the problem (1) already quoted, especially when the conditions (1') and (4') are compared with each other.

In the second part of this paper, Lambropoulos' special problem [(2)] with complex coefficients is treated. By employing a suitable substitution of the unknown function and by using a transformation of the coordinates, this problem is now transferred into a special initial-value problem (2) with $a = b = c = 0$, where the function $\varphi(x, y)$ is also slightly modified. In doing so, one obtains an infinite series as a formal solution for Lambropoulos' problem with arbitrary complex coefficients and holomorphic function φ. Further, it is possible to give sufficient criteria for the existence of a local holomorphic solution. Our representation formula is much easier to examine than Lambropoulos',[2] which already leads to a triple infinite series in the special case $a = b = c = 0$.

II. STATEMENTS ON EXISTENCE AND UNIQUENESS

Let us consider Eq. (4) under the initial condition (4'). The coefficients and the inhomogeneity of (4) may be holomorphic in Q. They can thus be expanded in Q as power series of the structure $\sum_{i,j,k=0}^{\infty} k_{ijk} t^i x^j y^k$. Henceforth, the coefficients of the series expansions of $a(t, x, y)$, $b(t, x, y)$, $c(t, x, y)$, $d(t, x, y)$, and $f(t, x, y)$ are denoted by a_{ijk}, b_{ijk}, c_{ijk}, d_{ijk}, and f_{ijk} with $i, j, k = 0, 1, 2, \cdots$. Let the given function $\varphi(x, y)$ also be holomorphic in Q. From our original initial-value problem, we derive a simpler one with a homogeneous initial condition by introducing

$$u(t, x, y) - \varphi(x, y)$$

as the new unknown function; for this substitution does not at all alter the properties of structure and holomorphy of Eq. (4). Henceforward, we study Eq. (4) under the initial condition

$$u(0, x, y) = 0. \tag{4''}$$

When using

$$u(t, x, y) \equiv \sum_{\alpha,\beta,\gamma=0}^{\infty} u_{\alpha\beta\gamma} t^\alpha x^\beta y^\gamma \tag{5}$$

as a formal expression for the unknown function and replacing the coefficients and the inhomogeneity by their series expansions, by comparison of the coefficients we obtain the recursion formula

$$\begin{aligned}(\alpha + 1)u_{(\alpha+1)\beta\gamma} &= -\sum_{i,j,k=0}^{\alpha,\beta+1,\gamma} j u_{ijk} a_{(\alpha-i)(\beta-j+1)(\gamma-k)} \\ &\quad - \sum_{i,j,k=0}^{\alpha,\beta,\gamma+1} k u_{ijk} b_{(\alpha-i)(\beta-j)(\gamma-k+1)} \\ &\quad - \sum_{i,j,k=0}^{\alpha,\beta,\gamma} u_{ijk} c_{(\alpha-i)(\beta-j)(\gamma-k)} \\ &\quad - \sum_{i,j,k=0}^{\alpha,\beta+1,\gamma+1} jk u_{ijk} d_{(\alpha-i)(\beta-j+1)(\gamma-k+1)} + f_{\alpha\beta\gamma},\end{aligned}$$

$$\alpha, \beta, \gamma = 0, 1, 2, \cdots, \tag{6}$$

under the conditions

$$u_{0\beta\gamma} = 0, \quad \beta, \gamma = 0, 1, 2, \cdots. \tag{6'}$$

The coefficients of the formal expression (5) are now uniquely determined by (6) and can thus be evaluated recursively. We have thus gained the following uniqueness theorem.

Theorem 1: The problem (4) has at most one holomorphic solution on Q.

The usual method for the proof of the existence of a solution of structure (5) is to consider a majorant problem of a particularly simple nature. This approach, however, fails in our case. The outcome of an example we will consider in the following is that, contrary to (1), it can happen that, under our assumptions of holomorphy, not even a local holomorphic solution exists for problem (4). [We mean a holomorphic solution in a neighborhood of a point $(0, x_0, y_0) \in Q$.] To verify this statement, we now study the initial-value problem

$$u_t + d(x, y) u_{xy} = f(x, y), \tag{7}$$

$$u(0, x, y) = 0, \tag{7'}$$

where the holomorphic functions $d(x, y)$ and $f(x, y)$ are made more specific later. We assume that (7) has a local holomorphic solution, at least. This can then be expressed as $\sum_{n=1}^{\infty} a^{(n)}(x, y) t^n$, for arguments on a polycylinder in Q with a center $(0, x_0, y_0)$. Here the coefficients $a^{(n)}(x, y)$, $n = 1, 2, \cdots$, are holomorphic on the considered domain, and they satisfy the simple recursion formula

$$\begin{aligned}a^{(1)}(x, y) &= f(x, y), \\ a^{(n)}(x, y) &= -\frac{1}{n} d(x, y) a_{xy}^{(n-1)}(x, y), \\ & \qquad n = 2, 3, 4, \cdots.\end{aligned} \tag{8}$$

First, we discuss the special case

$$d(x, y) \equiv -1, \quad f(x, y) \equiv [(1 - x)^2(1 - y)^2]^{-1}, \quad |x|, |y| < 1. \quad (9)$$

The recursion (8) then yields as a result

$$a^{(n)}(x, y) = n! \, [(1 - x)^{n+1}(1 - y)^{n+1}]^{-1}, \quad n = 1, 2, 3, \cdots.$$

Thus, the series under consideration is convergent only for $t = 0$. Therefore, (7) with specifications (9) has not even a local holomorphic solution. We have thus gained the following theorem containing a negative statement.

Theorem 2: The presuppositions of holomorphy assumed for the coefficients and inhomogeneity of Eq. (4) are not sufficient for the existence of a local solution of the initial-value problem (4).

The negative result for the special case (9) of problem (7) is obviously caused by the particular form of the inhomogeneity. However, we are not allowed to conclude that this inhomogeneity leads to the nonexistence of a holomorphic solution of (7) independently of the choice of the coefficient $d(x, y)$. For when we put

$$d(x, y) \equiv -\tfrac{1}{4}(1 - x)(1 - y),$$

using (8), we get

$$u(t, x, y) = [(1 - x)(1 - y)]^{-1}(e^t - 1)$$

as a global holomorphic solution.

The initial-value problem

$$u_t + du_{xy} = f(x, y), \quad d \in \mathbf{C} - \{0\}, \quad (10)$$

$$u(0, x, y) = 0, \quad (10')$$

still further simplified, has a certain importance for our following proceeding. It contains for instance the special case $a = b = c = 0$ of Lambropoulos' problem (2). Due to relation (8), a formal solution

$$u(t, x, y) \equiv -\frac{1}{d}\sum_{n=1}^{\infty}\frac{(-dt)^n}{n!}\frac{\partial^{2(n-1)}}{\partial x^{(n-1)}\partial y^{(n-1)}}f(x, y) \quad (11)$$

is easily found.

For which kind of inhomogeneity $f(x, y)$ does the series (11) converge now at least locally? This means for Lambropoulos' problem mentioned above a question upon the initial condition. By comparison with convergent series of the structure of (11), we are able to derive immediately a collection of conditions for the inhomogeneity, so that at least a local holomorphic solution of (10) exists. Two trivial sufficient conditions of that kind are obtained from the inequalities

$$\left|\frac{\partial^{2(n-1)}}{\partial x^{(n-1)}\partial y^{(n-1)}}f(x, y)\right| \leq (n!)^m k(|x|, |y|)[g(|x|, |y|)]^n, \quad n = 1, 2, 3, \cdots, \quad (12)$$

with $m = 0, 1$, where the functions k and g are continuous and positive in the considered domain. By using (11) and (12), it is not difficult to find a majorant of our solution. Estimations of type (12) are, for instance, satisfied by the inhomogeneities

$$f(x, y) \equiv e^{ax+by}, \quad a, b \in \mathbf{C},$$

for $m = 0$, and

$$f(x, y) \equiv e^{-x}/(1 - y)^2, \quad y \neq 1,$$

for $m = 1$. In both cases, we obtain for the series (11) an explicit result, namely,

$$u(t, x, y) = -(e^{ax+by}/abd)(e^{-abdt} - 1),$$

for $m = 0$, and

$$u(t, x, y) = te^{-x}/(1 - y)(1 - y + dt), \quad y \neq 1, \quad y - dt \neq 1,$$

for $m = 1$.

III. THE PROBLEM OF LAMBROPOULOS

The classical metnod of majorants is not appropriate for the special problem (2) of Lambropoulos, for (2) may be reduced directly to the simple initial-value problem (10). This will now be done. First, however, we briefly present Neuringer's procedure[6] for the treatment of (2), because we use an analogous procedure in our further considerations. Neuringer[6] defined a new unknown function

$$Q(t, x, y) \equiv e^{-\alpha xy}u(t, x, y) \quad (13)$$

and new independent variables

$$\xi \equiv xe^{-(a+\alpha)t}, \quad \eta \equiv ye^{-(b+\alpha)t}, \quad \tau \equiv t,$$

where α is given by

$$\alpha \equiv \tfrac{1}{2}\{-(a + b) + [(a + b)^2 - 4c]^{\frac{1}{2}}\}.$$

Here and in the following, we are also permitted to choose the negative root in the definition of α. A formal rearrangement leads from (2) to the following initial-value problem:

$$Q_\tau + \alpha Q + e^{-(a+b+2\alpha)\tau}Q_{\xi\eta} = 0,$$
$$Q(0, \xi, \eta) = e^{-\alpha\xi\eta}\varphi(\xi, \eta).$$

Neuringer applied to these formulas the standard Fourier-transform techniques to get a formal solution of (2).

In the following, the constants a, b, and c may also be complex. When we set, modifying (13),

$$v(t, x, y) \equiv e^{\alpha(t-xy)}u(t, x, y),$$

we obtain from (2) the problem

$$v_t + a_1 x v_x + b_1 y v_y + v_{xy} = 0, \tag{14}$$

$$v(0, x, y) = \psi(x, y) \equiv e^{-\alpha xy}\varphi(x, y), \tag{14'}$$

where $a_1 \equiv a + \alpha$ and $b_1 \equiv b + \alpha$. It is thus entirely sufficient to treat Eq. (2) for the special case $c = 0$.

Let us now introduce the new independent variables

$$\xi \equiv xe^{-a_1 t}, \quad \eta \equiv ye^{-b_1 t}, \quad \tau \equiv \beta^{-1}(e^{\beta t} - 1)$$

with

$$\beta \equiv -(a_1 + b_1) = [(a + b^2 - 4c]^{\frac{1}{2}},$$

where $\beta^{-1}(e^{\beta t} - 1)$ may be continuously continued to the value $\beta = 0$. From (14) the initial-value problem then follows:

$$v_\tau + v_{\xi\eta} = 0, \tag{15}$$

$$v(0, \xi, \eta) = \psi(\xi, \eta), \tag{15'}$$

which is equivalent to (10). The relation between the old variables and the new ones is given by

$$x \equiv \xi(\beta\tau + 1)^{a_1/\beta} \equiv \xi e^{(a_1/\beta)\ln(\beta\tau+1)},$$

$$y \equiv \eta(\beta\tau + 1)^{b_1/\beta} \equiv \eta e^{(b_1/\beta)\ln(\beta\tau+1)},$$

$$t \equiv \frac{1}{\beta}\ln(\beta\tau + 1).$$

$\beta^{-1}\ln(\beta\tau + 1)$ may be continuously continued to the value $\beta = 0$. For the logarithmic function, we choose its main branch.

It is interesting to note that the initial conditions (14') and (15') are the same. For a given function ψ, therefore, we start with the easier problem (15), where the coefficients a_1 and b_1 do not appear in the differential equation.

Theorem 3: (a) Formal solutions of (15) and (2) are given respectively as

$$v(\tau, \xi, \eta) \equiv \sum_{n=0}^{\infty} \frac{(-\tau)^n}{n!} \frac{\partial^{2n}}{\partial\xi^n \partial\eta^n} \psi(\xi, \eta), \tag{16}$$

$$u(t, x, y) \equiv e^{\alpha(xy-t)} v\left(\frac{1}{\beta}(e^{\beta t} - 1), xe^{-(a+\alpha)t}, ye^{-(b+\alpha)t}\right)$$

$$= e^{\alpha(xy-t)} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{1}{\beta}(e^{-\beta t} - 1)\right)^n$$

$$\times \frac{\partial^{2n}}{\partial x^n \partial y^n}\left[e^{-\alpha xy e^{\beta t}} \varphi(xe^{-(a+\alpha)t}, ye^{-(b+\alpha)t})\right]. \tag{17}$$

(b) If the initial-value problem (15) has a holomorphic solution in the polycylinder $\{(\tau, \xi, \eta): |\tau| < \rho_1, |\xi| < \rho_2, |\eta| < \rho_3\}$, then it may there be expressed as (16), and the function $u(t, x, y)$ defined by (17) is a holomorphic solution of (2) at least in the domain

$$\{(t, x, y): |t| < |\beta|^{-1} \ln(1 + |\beta| \rho_1),$$

$$|x| < \rho_2 |e^{a_1 t}|, |y| < \rho_3 |e^{b_1 t}|\}.$$

At $\beta = 0$, the first condition in the braces must be replaced by $|t| < \rho_1$.

Proof: The formal solution (16) follows from representation (11). By substitution of the variables, we obtain from (16) the formal solution (17). The first part of the second statement in this theorem is obtained by applying the same method which was already used to derive the recursion formula (8). Now, taking into account the relationship between the variables τ, ξ, η and t, x, y and using further a classical theorem about holomorphic functions of several complex variables, the second assertion also is proved.

Remarks:

(1) Neuringer means that Lambropoulos' method for a formal solution of (2) is very cumbersome; he also points out that, even in the simplest case $a = b = c = 0$, the formal solution involves triple infinite sums. From this point of view, our formal solution (17) is easier to examine.

(2) In general, it is difficult to determine the domain of holomorphy for our representation (17) for a given function φ. For this, our representation (16) is more suitable, because the same remarks are valid for (16) as for representation (11). According to the second statement of Theorem 3, we may also be able to determine a domain of holomorphy for the series (17).

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Fluctuation Theory for Space-Charge-Limited Currents*

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A phenomenological fluctuation theory is presented for 1-dimensional space-charge-limited currents in ideal nonmetallic solids. Notwithstanding the essential nonlinearity of the dynamical equation which governs the potential field, the theory is solved exactly for an initial statistical state that is associated with a probability measure of Gaussian form in an auxiliary field variable.

INTRODUCTION

This paper describes a phenomenological fluctuation theory for 1-dimensional space-charge-limited currents in ideal nonmetallic solids. Of special mathematical interest is the method employed here to obtain the potential field mean value (22) and equal-time 2-point correlation (26), probability averages taken over a statistical ensemble of potential fields that evolve dynamically according to the nonlinear equation (3). First, the potential field is related by the transcendental algebraic formula (4) to the field variable $\psi = \psi(x, t)$ which satisfies the linear equation (5). Then we compute the mean value and equal-time 2-point correlation for *all* even powers of ψ subject to a prescribed initial statistical state, taken here to be represented by the probability measure (10). Finally, we use some elementary properties of the gamma function to deduce the physically important mean value and equal-time 2-point correlation of the potential field, the quantities (22) and (26), from the previously obtained probability averages in ψ.

SPACE-CHARGE-LIMITED CURRENTS IN NONMETALLIC SOLIDS[1]

With trapping negligible, the 1-dimensional single-carrier current flow in an ideal nonmetallic solid is governed by the conduction-continuity and Poisson equations[2]

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(\mu n \frac{\partial \phi}{\partial x} + D\frac{\partial n}{\partial x}\right), \tag{1}$$

$$\frac{\partial^2 \phi}{\partial x^2} = -\frac{q}{\epsilon} n, \tag{2}$$

for the potential field $\phi = \phi(x, t)$ and carrier concentration $n = n(x, t)$ of particles with constant drift mobility μ, effective charge q, and diffusivity D in a medium of permittivity ϵ; by definition, μ and q have the same sign (minus for electrons, positive for holes) and the Einstein relation takes the form $D = \mu kT/q$. Combining Eqs. (1) and (2) and integrating twice with respect to x, one obtains the inhomogeneous nonlinear equation

$$\frac{\partial \phi}{\partial t} - \tfrac{1}{2}\mu\left(\frac{\partial \phi}{\partial x}\right)^2 - D\frac{\partial^2 \phi}{\partial x^2} = -\epsilon^{-1}xJ + (\text{trivial gauge function of } t \text{ alone}), \tag{3}$$

where $J = J(t)$ is the total Maxwell current (drift plus diffusion plus displacement) per unit area. Equation (3), an inhomogeneous Burgers equation[3] for $\partial\phi/\partial x$, can be integrated exactly[4]; it is satisfied by

$$\phi = -\epsilon^{-1}x\int_0^t J(t')\,dt' + \frac{D}{\mu}\ln(\psi^2) \tag{4}$$

if ψ satisfies the homogeneous linear equation

$$\frac{\partial \psi}{\partial t} + \frac{\mu}{\epsilon}\int_0^t J(t')\,dt'\frac{\partial \psi}{\partial x} - D\frac{\partial^2 \psi}{\partial x^2} = 0. \tag{5}$$

Hence, in the case of an unbounded x domain,

$$\psi = \psi(x, t) = \int_{-\infty}^{\infty} K(x - \xi, t)\psi_0(\xi)\,d\xi, \tag{6}$$

where

$$K(x, t) \equiv \tfrac{1}{2}(\pi Dt)^{-\frac{1}{2}} \times \exp\left[-(4Dt)^{-1}\left(x - \frac{\mu}{\epsilon}\int_0^t (t - t')J(t')\,dt'\right)^2\right], \tag{7}$$

and the initial value $\psi_0(x) \equiv \psi(x, 0)$ is related to a prescribed initial value of the potential field by the inverse of (4), evaluated at $t = 0$,[5]

$$\psi_0(x) = \pm\exp\left[(\mu/2D)\phi(x, 0)\right]. \tag{8}$$

PROBABILITY AVERAGES IN ψ

We now consider a statistical ensemble of space-charge-limited current dynamical systems governed by Eqs. (1)–(6). In view of formula (4), a probability measure on the potential fields at any instant of time is induced by a probability measure on the ψ fields. Whereas the dynamical evolution of the probability measure on the potential fields [implied by the nonlinear equation (3)] is complicated, the dynamical evolution of the probability measure on the ψ fields [implied by the linear equation (5)] is simple. If $dP_t[\psi(x)]$ denotes the probability measure assigned to

$\psi(x)$ at t, we have

$$dP_t[\psi(x, t)] = dP_0[\psi_0(x)], \tag{9}$$

which gives $dP_t[\psi(x)]$ in terms of $dP_0[\psi(x)]$ explicitly because of the general solution (6). Thus, for example, the initial probability measure

$$dP_0[\psi(x)] = (\text{const})\left[\exp\left(-\lambda\int_{-\infty}^{\infty}\psi(\zeta)^2\,d\zeta\right)\right] \times \prod_{\text{all } x} d\psi(x), \tag{10}$$

$\lambda \equiv$ a real positive constant parameter,

produces

$$dP_t[\psi(x)] = (\text{function of } t) \times \left[\exp\left(-\lambda\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}K^{(-2)}(\xi-\eta, t) \times \psi(\xi)\psi(\eta)\,d\xi\,d\eta\right)\right]\prod_{\text{all } x} d\psi(x), \tag{11}$$

where $K^{(-2)}(x, t)$ is the iterated inverse kernel to (7), defined implicitly by

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}K^{(-2)}(\xi-\eta, t)K(\xi-x, t)K(\eta-x', t)\,d\xi\,d\eta = \delta(x-x'), \tag{12}$$

and the prefactor function of t in (11) is fixed by the normalization condition

$$\int dP_t[\psi(x)] \equiv 1.$$

Ensemble averages of functionals of ψ at t,

$$\langle F[\psi(x, t)]\rangle \equiv \int F[\psi(x)]\,dP_t[\psi(x)] = \int F[\psi(x, t)]\,dP_0[\psi_0(x)], \tag{13}$$

can be evaluated for a prescribed initial probability measure $dP_0[\psi(x)]$ by making use of (6). Thus, for example, the characteristic functional[6]

$$\Phi = \Phi[y(x, t)] \equiv \left\langle \exp i\int_{-\infty}^{\infty}y(x, t)\psi(x, t)\,dx\right\rangle, \tag{14}$$

associated with the initial probability measure (10), is evaluated by functional integration[7] to yield

$$\Phi = \exp\left(-\frac{1}{4\lambda}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}K^{(2)}(\xi-\eta; t) \times y(\xi, t)y(\eta, t)\,d\xi\,d\eta\right), \tag{15}$$

in which the iterated kernel appears as

$$K^{(2)}(x-x', t) \equiv \int_{-\infty}^{\infty}K(x-\xi, t)K(x'-\xi, t)\,d\xi = (8\pi Dt)^{-\frac{1}{2}}\exp\left[-(x-x')^2/8Dt\right]. \tag{16}$$

It follows from the definition (14) and specific forms (15) and (16) that the probability average of any odd functional of ψ vanishes, while the basic even functionals of ψ have the probability averages[8]

$$\langle\psi(x, t)\psi(x', t)\rangle = -\frac{\delta^2\Phi}{\delta y(x, t)\delta y(x', t)}\bigg|_{y=0} = \frac{1}{2\lambda}K^{(2)}(x-x', t) = [4\lambda(2\pi Dt)^{\frac{1}{2}}]^{-1}\exp\left[-(x-x')^2/8Dt\right], \tag{17}$$

$$\langle\psi(x, t)^{2n}\rangle = \left(-i\frac{\delta}{\delta y(x, t)}\right)^{2n}\Phi\bigg|_{y=0} = \frac{(2n)!}{n!}\left(\frac{K^{(2)}(0, t)}{4\lambda}\right)^n = \frac{(2n)!}{n!}\left[8\lambda(2\pi Dt)^{\frac{1}{2}}\right]^{-n}, \tag{18}$$

$$\langle\psi(x, t)^{2n}\psi(x', t)^{2n'}\rangle = \left(-i\frac{\delta}{\delta y(x, t)}\right)^{2n}\left(-i\frac{\delta}{\delta y(x', t)}\right)^{2n'}\Phi\bigg|_{y=0} = (2n)!\,(2n')!\,[8\lambda(2\pi Dt)^{\frac{1}{2}}]^{-n-n'} \times \sum_{k=0}^{\min\{n,n'\}}\frac{4^k\exp\left[-k(x-x')^2/4Dt\right]}{(2k)!\,(n-k)!\,(n'-k)!}, \tag{19}$$

in which n and n' are nonnegative integers.

PROBABILITY AVERAGES IN ϕ

Now by evoking the natural analytic continuation[9] of (18) for all real continuous values of $n \geq 0$,

$$\langle|\psi(x, t)|^{2n}\rangle = [\Gamma(2n+1)/\Gamma(n+1)][8\lambda(2\pi Dt)^{\frac{1}{2}}]^{-n}, \tag{20}$$

we obtain

$$\left\langle\phi(x, t) + \epsilon^{-1}x\int_0^t J(t')\,dt'\right\rangle = \frac{D}{\mu}\frac{\partial}{\partial n}\left\langle\exp\left[n\frac{\mu}{D}\left(\phi(x, t) + \epsilon^{-1}x\int_0^t J(t')\,dt'\right)\right]\right\rangle\bigg|_{n=0} = \frac{D}{\mu}\frac{\partial}{\partial n}\langle|\psi(x, t)|^{2n}\rangle\big|_{n=0} = -\frac{D}{\mu}\{C + \ln\left[8\lambda(2\pi Dt)^{\frac{1}{2}}\right]\}, \tag{21}$$

where $C \equiv -\Gamma'(1) = 0.577\cdots$ is the Euler–Mascheroni constant. It follows from (21) that the mean value of the potential field is

$$\langle\phi(x, t)\rangle = -\epsilon^{-1}x\int_0^t J(t')\,dt' - \frac{D}{\mu}\{C + \ln\left[8\lambda(2\pi Dt)^{\frac{1}{2}}\right]\}. \tag{22}$$

Similarly, by evoking the natural analytic continuation[9] of (19) for all real continuous values of $n, n' \geq 0$,

$$\langle |\psi(x,t)|^{2n} |\psi(x',t)|^{2n'} \rangle = \Gamma(2n+1)\Gamma(2n'+1)[8\lambda(2\pi Dt)^{\frac{1}{2}}]^{-n-n'} \times \sum_{k=0}^{\infty} \frac{4^k \exp[-k(x-x')^2/4Dt]}{(2k)!\,\Gamma(n-k+1)\Gamma(n'-k+1)}, \quad (23)$$

we obtain

$$\left\langle \left(\phi(x,t) + \epsilon^{-1}x\int_0^t J(t')\,dt'\right) \times \left(\phi(x',t) + \epsilon^{-1}x'\int_0^t J(t')\,dt'\right)\right\rangle$$
$$= \left(\frac{D}{\mu}\right)^2 \frac{\partial^2}{\partial n \partial n'} \left\langle \exp\left[n\frac{\mu}{D}\left(\phi(x,t) + \epsilon^{-1}x\int_0^t J(t')\,dt'\right) + n'\frac{\mu}{D}\left(\phi(x',t) + \epsilon^{-1}x'\int_0^t J(t')\,dt'\right)\right]\right\rangle\Bigg|_{n=n'=0}$$
$$= \left(\frac{D}{\mu}\right)^2 \frac{\partial^2}{\partial n \partial n'} \langle |\psi(x,t)|^{2n} |\psi(x',t)|^{2n'}\rangle\Big|_{n=n'=0}$$
$$= \left(\frac{D}{\mu}\right)^2 (\{C + \ln[8\lambda(2\pi Dt)^{\frac{1}{2}}]\}^2 + \mathcal{F}), \quad (24)$$

in which there appears

$$\mathcal{F} \equiv \sum_{k=1}^{\infty} \frac{[(k-1)!]^2 4^k \exp[-k(x-x')^2/4Dt]}{(2k)!} = 2\sum_{k=0}^{\infty} \frac{(k!)^2 4^k \exp[-(k+1)(x-x')^2/4Dt]}{(2k+1)!\,(k+1)} = 2(\sin^{-1}\{\exp[-(x-x')^2/8Dt]\})^2, \quad (25)$$

with the second member being a tabulated series.[10] It follows from (24) that the equal-time 2-point correlation of the potential field is

$$\langle \phi(x,t)\phi(x',t)\rangle = -\epsilon^{-1}(x\langle\phi(x',t)\rangle + x'\langle\phi(x,t)\rangle)\int_0^t J(t')\,dt' - \epsilon^{-2}xx'\left(\int_0^t J(t')\,dt'\right)^2 + \left(\frac{D}{\mu}\right)^2(\{C + \ln[8\lambda(2\pi Dt)^{\frac{1}{2}}]\}^2 + \mathcal{F})$$
$$= \epsilon^{-2}xx'\left(\int_0^t J(t')\,dt'\right)^2 + \frac{D}{\epsilon\mu}(x+x')\{C + \ln[8\lambda(2\pi Dt)^{\frac{1}{2}}]\}\int_0^t J(t')\,dt' + \left(\frac{D}{\mu}\right)^2(\{C + \ln[8\lambda(2\pi Dt)^{\frac{1}{2}}]\}^2 + \mathcal{F}), \quad (26)$$

where use has been made of (22). It is easy to verify that (22) and (26) satisfy the ensemble average of the dynamical equation (3) with

$$\left\langle\left(\frac{\partial\phi}{\partial x}\right)^2\right\rangle \equiv \lim_{x'\to x}\left(\frac{\partial^2}{\partial x\partial x'}\right)\langle\phi(x,t)\phi(x',t)\rangle.$$

By employing (22) once again, the fluctuation part of (26) is obtained as

$$\langle\phi(x,t)\phi(x',t)\rangle - \langle\phi(x,t)\rangle\langle\phi(x',t)\rangle = (D/\mu)^2\mathcal{F} = 2(D/\mu)^2(\sin^{-1}\{\exp[-(x-x')^2/8Dt]\})^2. \quad (27)$$

Hence, subject to the initial probability distribution (10), the fluctuation part of the equal-time 2-point correlation of the potential field (27) is independent of the parameter λ and universal in character; the autocorrelation of the potential field

$$\langle\phi(x,t)^2\rangle - \langle\phi(x,t)\rangle^2 = \tfrac{1}{2}(\pi D/\mu)^2$$

is a constant for all x and t. We obtain the fluctuation part of the equal-time 2-point correlation of the carrier concentration from (27) be recalling (2):

$$\langle n(x,t)n(x',t)\rangle - \langle n(x,t)\rangle\langle n(x',t)\rangle = \left(\frac{\epsilon D}{q\mu}\right)^2\left(\frac{\partial^2}{\partial x^2}\right)\left(\frac{\partial^2}{\partial x'^2}\right)\mathcal{F} = 2\left(\frac{\epsilon D}{q\mu}\right)^2\left(\frac{\partial^4}{\partial x^4}\right)\left\{\sin^{-1}\left[\exp\left(\frac{-(x-x')^2}{8Dt}\right)\right]\right\}^2. \quad (28)$$

It should be noted that the only technical difficulty associated with solving the theory for a non-Gaussian initial probability measure in place of (10) is the evaluation of the functional integral for the characteristic functional (14). For such a non-Gaussian initial probability measure, functional integration approximation methods[7] appear to be necessary.

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[8] The numerical factors in Eqs. (18) and (19) are obtainable by applying combinatorial analysis to the auxiliary formula

$$\langle\psi(x_1,t)\psi(x_2,t)\cdots\psi(x_{2N-1},t)\psi(x_{2N},t)\rangle = \sum_{\substack{\text{perm.}\\ \text{distinct}\\ \text{pairings}}} \langle\psi(x_{i_1},t)\psi(x_{i_2},t)\rangle\cdots\langle\psi(x_{i_{2N-1}},t)\psi(x_{i_{2N}},t)\rangle,$$

which follows immediately from the general Gaussian character of the probability measure (11). Details of the derivation of the numerical factors in Eqs. (18) and (19) are given by G. Eckstut, thesis, Drexel Institute of Technology, Philadelphia, Pa., 1970.

[9] The analytic continuation of a function defined on nonnegative integers is, of course, not unique. In the present context, however, the natural analytic continuation is corroborated by examination of the functional integral.

[10] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1965), p. 52. To sum the infinite series directly, we put the representation

$$\frac{[(k-1)!]^2 4^k}{(2k)!} = \frac{2}{k}\int_0^1 \frac{\theta^{2k-1}}{(1-\theta^2)^{\frac{1}{2}}}\,d\theta$$

into (25), and we find

$$\begin{aligned}\mathcal{F} &= 2\int_0^1 \sum_{k=1}^{\infty} \frac{\theta^{2k-1}}{k} \exp\left[-k(x-x')^2/4Dt\right] \frac{d\theta}{(1-\theta^2)^{\frac{1}{2}}}\\ &= -2\int_0^1 (\ln\{1-\theta^2\exp\left[-(x-x')^2/4Dt\right]\}) \frac{d\theta}{\theta(1-\theta^2)^{\frac{1}{2}}}\\ &= 2(\sin^{-1}\{\exp\left[-(x-x')^2/8Dt\right]\})^2.\end{aligned}$$

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Relativistic Theory of Microelectromagnetism*

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A theory of relativistic (special theory) microelectromagnetism is proposed for the treatment of the class of physical phenomena arising from a high degree of polarization, magnetization, and rapid local field fluctuation in material bodies. The master electromagnetic balance laws are given for the resultant generalized EM fields. The local field equations and jump conditions are obtained for the moments of the electromagnetic fields up to any order p. The equations of the zeroth-order moments turn out to be Maxwell's equations and associated jump conditions. The Euclidean form of the first-order theory is presented in full.

1. INTRODUCTION

Extension of the electromagnetic theory of Maxwell to moving media has occupied a large number of research workers since the turn of the century. The problem for free space and "rigid bodies" was fairly well resolved with the introduction of the special theory of relativity. Nevertheless, certain serious questions remained unanswered for bodies undergoing deformations. For a discussion of various theories together with a definitive formulation of elastic solids and viscous fluids within the domain of special relativity, we mention the work of Grot and Eringen.[1] While these theories can explain a large class of physical phenomena of electromagnetic origin, there exists a wide variety of electromagnetic effects which fall beyond the scope of such theories. For example, the well-known magnetic domain structure in ferromagnetic materials, stable configurations, and motions of domain walls have neither been fully understood nor incorporated into a unified theory. The literature is replete with works of micromagnetism; cf. Brown.[2]

Among other important phenomena observed, we cite the behavior of electrets. They possess no net local charge within the volume; however, they may support a uniform volume polarization and/or surface charge and electric double layer; cf. Perlman and Meunier,[3] Gross and DeMoraes,[4] Thiessen *et al.*[5] For a survey of this field, see Gutman.[6]

The theory of the propagation of microwaves in solids constitutes another class of as yet unsolved problems.

We believe that the basic reason for our inability to understand the theoretical basis of these important classes of phenomena lies in the fact that the classical field theories do not contain the necessary mechanism to take into account the local degrees of freedom. When a length scale associated with the exciting agents becomes comparable to the average grains (microelements) in bodies and/or the average distance between grains, the classical continuum hypothesis is violated. Individual motions, polarizations, and magnetizations of the microelements of the body can affect the average motions and fields. Our approach to remedy this situation is to regard the microscopic

[8] The numerical factors in Eqs. (18) and (19) are obtainable by applying combinatorial analysis to the auxiliary formula

$$\langle\psi(x_1,t)\psi(x_2,t)\cdots\psi(x_{2N-1},t)\psi(x_{2N},t)\rangle = \sum_{\substack{\text{perm.}\\ \text{distinct}\\ \text{pairings}}} \langle\psi(x_{i_1},t)\psi(x_{i_2},t)\rangle\cdots\langle\psi(x_{i_{2N-1}},t)\psi(x_{i_{2N}},t)\rangle,$$

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$$\begin{aligned}\mathcal{F} &= 2\int_0^1 \sum_{k=1}^{\infty} \frac{\theta^{2k-1}}{k} \exp\left[-k(x-x')^2/4Dt\right] \frac{d\theta}{(1-\theta^2)^{\frac{1}{2}}}\\ &= -2\int_0^1 (\ln\{1-\theta^2\exp\left[-(x-x')^2/4Dt\right]\}) \frac{d\theta}{\theta(1-\theta^2)^{\frac{1}{2}}}\\ &= 2(\sin^{-1}\{\exp\left[-(x-x')^2/8Dt\right]\})^2.\end{aligned}$$

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Among other important phenomena observed, we cite the behavior of electrets. They possess no net local charge within the volume; however, they may support a uniform volume polarization and/or surface charge and electric double layer; cf. Perlman and Meunier,[3] Gross and DeMoraes,[4] Thiessen *et al.*[5] For a survey of this field, see Gutman.[6]

The theory of the propagation of microwaves in solids constitutes another class of as yet unsolved problems.

We believe that the basic reason for our inability to understand the theoretical basis of these important classes of phenomena lies in the fact that the classical field theories do not contain the necessary mechanism to take into account the local degrees of freedom. When a length scale associated with the exciting agents becomes comparable to the average grains (microelements) in bodies and/or the average distance between grains, the classical continuum hypothesis is violated. Individual motions, polarizations, and magnetizations of the microelements of the body can affect the average motions and fields. Our approach to remedy this situation is to regard the microscopic

electromagnetic fields appearing in Maxwell's equations as distributions. The macroscopic observable fields are posited to be linear functionals of these microscopic fields over the space of infinitely differentiable test functions with bounded support. Since the test functions admit power-series expansions, the resulting "moments" may, equivalently, be used as observable fields. Precise definitions of these concepts are given in Sec. 3. A hierarchy of field equations and jump conditions is obtained for all moments; the equations for the zeroth-order moments turn out to be Maxwell's equations. The main contribution of the present paper is to present the basic laws of relativistic microelectromagnetism constructed on a rational basis. In future papers, we hope to deal with the constitutive theory and solutions of some of the problems in the previously mentioned areas by use of the present theory.

2. RELATIVISTIC LAWS OF ELECTROMAGNETISM

In the special theory of relativity, space-time is regarded as a flat 4-dimensional Riemannian manifold called Minkowski space M^4. Minkowski space is endowed with a fundamental metric tensor $g_{\alpha\beta}(\mathbf{x})$ referred to a curvilinear coordinate system x^α, $\alpha, \beta = 1, 2, 3, 4$. In a rectangular frame of reference, we write $x^\alpha \equiv z^\alpha \equiv (x, y, z, ict)$, where x, y, z are the 3-dimensional rectangular coordinates, $i \equiv (-1)^{\frac{1}{2}}$, c is the speed of light in a vacuum, and t is time. In this case,

$$g_{\alpha\beta} \overset{*}{=} \delta_{\alpha\beta} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{2.1}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta and the symbol $\overset{*}{=}$ is used throughout this paper to denote equality generally valid only in a rectangular frame of reference.

The electromagnetic field[7] is described by two skew-symmetric 4-tensors $F_{\alpha\beta}$ and $G^{\alpha\beta}$ and two 4-vectors J^α and K^α called the *magnetic flux* and *electric displacement* tensors and the *current* and *surface current* vectors, respectively. These quantities are related to the classical 3-dimensional electromagnetic fields by

$$F_{\alpha\beta} = -F_{\beta\alpha} \overset{*}{=} (\text{dual } \mathbf{B}, -i\mathbf{E}), \tag{2.2a}$$

$$G^{\alpha\beta} = -G^{\beta\alpha} \overset{*}{=} (\text{dual } \mathbf{H}, -i\mathbf{D}), \tag{2.2b}$$

$$J^\alpha \overset{*}{=} (\mathbf{J}, icq), \tag{2.2c}$$

$$K^\alpha \overset{*}{=} (1 - v_{(\mathbf{n})}^2/c^2)^{-\frac{1}{2}}(\mathbf{K}, ic\sigma), \tag{2.2d}$$

where $\mathbf{E}$, $\mathbf{B}$, $\mathbf{H}$, $\mathbf{D}$, $\mathbf{J}$, $\mathbf{K}$, q, and σ are, respectively, the electric field vector, magnetic induction vector, magnetic field vector, electric displacement vector, current vector, surface current vector, volume charge density, and surface charge density of classical electromagnetism. By (2.2a) and (2.2b), we mean

$$F^{kl} = \epsilon^{klm}B_m, \quad F^{k4} = -iE^k,$$

$$G^{kl} = \epsilon^{klm}H_m, \quad G^{k4} = -iD^k,$$

where ϵ^{klm} is the 3-dimensional permutation tensor.

Both current vectors are the sum of a conduction current and a convection current, the latter being due to the motion of charges, i.e.,

$$\mathbf{J} = \mathbf{j} + q\mathbf{v}, \quad \mathbf{K} = \mathbf{k} + \sigma\mathbf{v}, \tag{2.3}$$

where $\mathbf{v}$ is the velocity vector of a point in the body and $\mathbf{v}$ is the velocity of the surface of discontinuity Γ, which bears the nonmechanical surface current $\mathbf{k}$ and surface charge σ. If the unit positive normal of Γ is denoted by $\mathbf{n}$, then $\mathbf{k}$ is perpendicular to $\mathbf{n}$, and $v_{(\mathbf{n})} \equiv \mathbf{v} \cdot \mathbf{n}$.

In an N-dimensional Riemannian space, to each covariant M-vector $\mathbf{X}$, $M \leq N$, and to each contravariant M-vector $\mathbf{Y}$ there corresponds one and only one dual vector defined by

$$\begin{aligned} \hat{X}^{a_1 \cdots a_{N-M}} &\equiv (\text{dual } \mathbf{X})^{a_1 \cdots a_{N-M}} \\ &\equiv (M!)^{-1}\epsilon^{a_1 \cdots a_{N-M}b_1 \cdots b_M}X_{b_1 \cdots b_M}, \\ \hat{Y}_{a_1 \cdots a_{N-M}} &\equiv (\text{dual } \mathbf{Y})_{a_1 \cdots a_{N-M}} \\ &\equiv (M!)^{-1}Y^{b_1 \cdots b_M}\epsilon_{b_1 \cdots b_M a_1 \cdots a_{N-M}}, \end{aligned}$$

where $\epsilon^{a_1 \cdots a_N}$ and $\epsilon_{a_1 \cdots a_N}$ are the permutation tensors. From these, it follows that

$$\text{dual dual } \mathbf{X} = \mathbf{X}.$$

Thus, for example, an area element on an M-dimensional manifold S^M, described by its Gaussian equation $x^\alpha = x^\alpha(u^1, \cdots, u^M)$ in this N-dimensional space, may be expressed in either of the two forms

$$dA_{(M)}^{a_1 \cdots a_M} = M!\,\frac{\partial x^{[a_1}}{\partial u^1} \cdots \frac{\partial x^{a_M]}}{\partial u^M}\,du^1 \cdots du^M,$$

$$d\hat{A}^{(M)}_{a_1 \cdots a_{N-M}} = (\text{dual } d\mathbf{A}_{(N)})_{a_1 \cdots a_{N-M}},$$

where brackets enclosing a set of indices indicate alternation on this set. Similarly, the electromagnetic field tensors possess dual forms, e.g.,

$$\hat{F}^{\alpha\beta} = (\text{dual } \mathbf{F})^{\alpha\beta} \overset{*}{=} (-i \text{ dual } \mathbf{E}, \mathbf{B}).$$

It is only a matter of taste or convenience to express the basic laws of electromagnetism in terms of $\mathbf{F}$ and $\mathbf{G}$ or their duals. For the sake of brevity and uniformity in the following derivations, we elect to employ the fields $\hat{F}^{\alpha\beta}$, $G^{\alpha\beta}$, J^α, and K^α.

The integral balance laws of electromagnetism are the conservation of magnetic flux,

$$\oint_{S^2-\Gamma^2} \hat{F}^{\alpha\beta}\,d\hat{A}^{(2)}_{\alpha\beta} = 0, \tag{2.4}$$

and the Ampere–Gauss law,

$$-\tfrac{1}{2}\oint_{S^2-\Gamma^2} G^{\alpha\beta}\, d\hat{A}^{(2)}_{\alpha\beta} = \frac{4\pi}{c}\int_{S^3-\Gamma^2} J^\alpha\, d\hat{A}^{(3)}_\alpha - \frac{2\pi}{c}\int_{\Gamma^2} \mathcal{K}^{\alpha\beta}\, d\hat{A}^{(2)}_{\alpha\beta}, \quad (2.5)$$

where

$$\mathcal{K}^{\alpha\beta} = K^\alpha n^\beta - K^\beta n^\alpha, \quad K^\alpha n_\alpha = 0 \quad (2.6)$$

and where S^2 is a 2-dimensional closed circuit bounding S^3 and

$$n^\alpha = (1 - v^2_{(\mathbf{n})}/c^2)^{-\frac{1}{2}}(n^k, iv_{(\mathbf{n})}/c)$$

is the unit outward normal of Γ (which contains the discontinuity manifold Γ^2). The orientation of S^2 is selected so that the direction from an interior point of S^3 to S^2 followed by the orientation of S^2 constitutes a screw sense identical to that of S^3 (cf. Schouten,[8] p. 95).

The law of conservation of charge is obtained from (2.5) by closing the surface S^3. Thus,

$$\oint_{S^3-\Gamma^2} J^\alpha\, d\hat{A}^{(3)}_\alpha - \tfrac{1}{2}\int_{\Gamma^2} \mathcal{K}^{\alpha\beta}\, d\hat{A}^{(2)}_{\alpha\beta} = 0. \quad (2.7)$$

For arbitrary circuits, by use of the generalized Stokes' theorem[9] in (2.4), (2.5), and (2.7), we obtain the field equations

$$\hat{F}^{\alpha\beta}{}_{:\beta} = 0, \quad (2.8a)$$

$$G^{\alpha\beta}{}_{:\beta} = (4\pi/c)J^\alpha, \quad (2.8b)$$

$$J^\alpha{}_{:\alpha} = 0, \quad \text{in } S^4 - \Gamma, \quad (2.8c)$$

and the jump conditions

$$[\hat{F}^{\alpha\beta}]n_\beta = 0, \quad (2.9a)$$

$$[G^{\alpha\beta}]n_\beta = (4\pi/c)\mathcal{K}^{\alpha\beta}n_\beta = (4\pi/c)K^\alpha, \quad (2.9b)$$

$$[J^\alpha]n_\alpha + K^\Delta{}_{:\Delta} = 0, \quad \text{on } \Gamma, \quad (2.9c)$$

where a boldface bracket denotes the jump of the quantity enclosed across Γ, a subscript semicolon (colon) denotes partial (total) covariant differentiation, and $K_\Delta \equiv x^\alpha{}_{,\Delta}K_\alpha$ are the surface components of K_α on Γ. If the Gaussian equations of Γ are $x^\alpha = x^\alpha(u^\Delta)$, $\Delta = 1, 2, 3$, then

$$K^\Delta{}_{:\Delta} = x^\alpha{}_{,\Delta}K_\alpha{}^{:\Delta}.$$

If Γ contains a moving discontinuity line Γ'^2, then Eqs. (2.9) hold on $\Gamma - \Gamma'^2$, and (2.8) and (2.9) are supplemented by

$$[K^\alpha]n'_\alpha = 0, \quad \text{on } \Gamma'^2, \quad (2.10)$$

where

$$n'_\alpha \overset{*}{=} (1 - \mu^2_{(\mathbf{n}')}/c^2)^{-\frac{1}{2}}(n'_k, (i/c)\mu_{(\mathbf{n}')}).$$

Here, n'_k is normal to Γ'^2 subject to $n'_k n^k = 0$, and $\boldsymbol{\mu}$ is the velocity of Γ'^2. Thus, $\mu_{(\mathbf{n}')} \equiv \mu^k n'_k$ is the velocity of Γ'^2 in the $\mathbf{n}'$ direction.

In a Euclidean frame [employing (2.2)], the electromagnetic field equations (2.8) and jump conditions (2.9) take the well-known 3-dimensional forms

$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = \mathbf{0}, \qquad \nabla \cdot \mathbf{B} = 0,$$

$$\nabla \times \mathbf{H} - \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} = \frac{4\pi}{c}\mathbf{J}, \quad \nabla \cdot \mathbf{D} = 4\pi q, \quad (2.11)$$

$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{J} = 0,$$

$$\mathbf{n} \times [\mathbf{E}] - (v_{(\mathbf{n})}/c)[\mathbf{B}] = \mathbf{0}, \qquad [\mathbf{B}] \cdot \mathbf{n} = 0,$$

$$\mathbf{n} \times [\mathbf{H}] + (v_{(\mathbf{n})}/c)[\mathbf{D}] = (4\pi/c)\mathbf{K}, \quad [\mathbf{D}] \cdot \mathbf{n} = 4\pi\sigma,$$

$$\mathbf{n} \cdot [\mathbf{J} - q\mathbf{v}] + \frac{\partial \sigma}{\partial t} + K^a{}_{:a} - \sigma v_{(\mathbf{n})} b^a{}_a = 0 \quad (2.12)$$

(we have been unable to locate this last equation in the literature), where $x^k = x^k(u^a, t)$, $a = 1, 2$, is the Gaussian equation of Γ, $b^a{}_a$ is the trace of the second fundamental form of Γ, and

$$\frac{\partial \sigma}{\partial t} = \frac{\partial \sigma(u^a, t)}{\partial t}, \quad K_a = \frac{\partial x^k}{\partial u^a}K_k.$$

From (2.10), we have

$$[K^k - \sigma\mu^k]n'_k = 0, \quad \text{on } \Gamma'^2. \quad (2.13)$$

3. BALANCE LAWS OF MICROELECTROMAGNETISM

All theories of electrodynamics in the presence of matter are physically based on the assumption that on a "microscopic" scale Maxwell's equations in free space are valid. This assumption is not requisite, and one could just as easily postulate a description based on (2.4) and (2.5). The resultant equations in both cases, phenomenologically, are identical for this theory. Those favoring a minimal beginning may consider that we have made the former assumption, while for others, desiring to look into material mixtures, the latter assumption may appear to be more natural.

The derivation of the fundamental laws of microelectromagnetic theory (or, equivalently, *polar electromagnetism* or *micromorphic EM theory*) will be made through a smoothing process introduced by Eringen.[10] We imagine that the 4-dimensional manifold S^4, occupied by *body–time*, is made up of a collection of nonintersecting 4-dimensional submanifolds S^4_M, $M = 1, 2, \cdots, N$, called *micro–elements*. The EM fields associated with the points x^α of S^4_M are assumed to satisfy the fundamental laws (2.8)–(2.10) of relativistic EM theory.[11] However, these fields may be unbounded and may be discontinuous across the boundary of any two adjacent microelements S^4_M and $S^4_{M'}$, $M \neq M'$. To account for such possible discontinuities, we consider the microelectromagnetic fields as *distributions*. Let $\phi(x^\alpha)$ (called the *test*

function) be an infinitely differentiable function in S^4 that vanishes outside of a bounded 4-dimensional region (has bounded *support*) containing the body–time. The test function will be used to smooth out the discontinuities of the microelectromagnetic fields.

The following is an identity that follows from the generalized form of Stokes' theorem:

$$-\tfrac{1}{2}\oint_{S^2-\Gamma^2}\phi G'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta} = \int_{S^3-\Gamma^2}(\phi_{;\beta}G'^{\alpha\beta}+\phi G'^{\alpha\beta}{}_{;\beta})\,d\hat{A}'^{(3)}_{\alpha} - \tfrac{1}{2}\int_{\Gamma^2-\Gamma'^2}\phi[G'^{\alpha\beta}]\,d\hat{A}'^{(2)}_{\alpha\beta},$$

where all quantities carrying a prime denote microscopic fields. In the sense of distributions, the integrals on the right-hand side of this identity are meaningful.

From (2.8b) and (2.9b), this identity may also be written as

$$-\tfrac{1}{2}\oint_{S^2-\Gamma^2}\phi G'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta} = \int_{S^3-\Gamma^2}\left(\phi_{;\beta}G'^{\alpha\beta}+\frac{4\pi}{c}\phi J'^{\alpha}\right)d\hat{A}'^{(3)}_{\alpha} - \frac{2\pi}{c}\int_{\Gamma^2-\Gamma'^2}\phi\mathcal{K}'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta}. \quad (3.1)$$

We now imagine that the manifolds S^3, S^2, and Γ^2 are subdivided into a large number of nonoverlapping submanifolds S^3_J, S^2_K, Γ^2_L, $J, K, L \gg 1$. Then, clearly,

$$-\tfrac{1}{2}\sum_K\int_{S_K{}^2\subset S^2-\Gamma^2}\phi G'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta} = \sum_J\int_{S_J{}^3\subset S^3-\Gamma^2}\left(\phi_{;\beta}G'^{\alpha\beta}+\frac{4\pi}{c}\phi J'^{\alpha}\right)d\hat{A}'^{(3)}_{\alpha} - \frac{2\pi}{c}\sum_L\int_{\Gamma_L{}^2\subset\Gamma^2-\Gamma'^2}\phi\mathcal{K}'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta}. \quad (3.2)$$

The integrals taken over the open submanifolds define the following surface averages:

$$\begin{aligned}
\langle\phi G^{\alpha\beta}\rangle_{(2)}\,d\hat{A}^{(2)}_{\alpha\beta} &\equiv \lim_{S_K{}^2\to 0}\int_{S_K{}^2-\Gamma^2}\phi G'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta},\\
\langle\phi_{,\beta}G^{\alpha\beta}\rangle_{(3)}\,d\hat{A}^{(3)}_{\alpha} &\equiv \lim_{S_J{}^3\to 0}\int_{S_J{}^3-\Gamma^2}\phi_{;\beta}G'^{\alpha\beta}\,d\hat{A}'^{(3)}_{\alpha},\\
\langle\phi J^{\alpha}\rangle_{(3)}\,d\hat{A}^{(3)}_{\alpha} &\equiv \lim_{S_J{}^3\to 0}\int_{S_J{}^3-\Gamma^2}\phi J'^{\alpha}\,d\hat{A}'^{(3)}_{\alpha},\\
\langle\phi\mathcal{K}^{\alpha\beta}\rangle_{(2)}\,d\hat{A}^{(2)}_{\alpha\beta} &= \lim_{\Gamma_L{}^2\to 0}\int_{\Gamma_L{}^2-\Gamma'^2}\phi\mathcal{K}'^{\alpha\beta}\,d\hat{A}'^{(2)}_{\alpha\beta},
\end{aligned} \quad (3.3)$$

where the new area measures on the submanifolds S^2_K, S^3_J, and Γ^2_L are indicated respectively by $d\hat{A}^{(2)}_{\alpha\beta}$, $d\hat{A}^{(3)}_{\alpha}$, and $d\hat{A}^{(2)}_{\alpha\beta}$, and the subscript (2) or (3) is attached to the angular brackets as a reminder of the dimension of the submanifold over which the mean is taken.

A physical motivation for the introduction of the definitions (3.3) may be made as follows: While the local microfields $G'^{\alpha\beta}$, J'^{α}, and $\mathcal{K}'^{\alpha\beta}$ are not well behaved, nonetheless, there exists small open submanifolds S^2_K, S^3_J, and Γ^2_L over which these fields may be smoothed out by multiplying them by the test function ϕ and integrating these products over the above submanifolds. The resultant integrals can then be considered as densities associated with S^2_K, S^3_J, and Γ^2_L. The limits S^2_K, S^3_J, $\Gamma^2_L \to 0$ are to be understood only in the sense that these manifolds are so small that the summations in (3.2) may be replaced by integrations. The mathematical justification of (3.3) can also be made by providing a microsubstructure to these manifolds. This simply means that the integrations are performed over a set of new variables ξ^{α}, $\alpha = 1, 2, 3, 4$, that cover each submanifold.

From (3.2), in the limit as $J, K, L \to \infty$ and the areas of S^3_J, S^2_K, $\Gamma^2_L \to 0$, we obtain

$$-\tfrac{1}{2}\oint_{S^2-\Gamma^2}\langle\phi G^{\alpha\beta}\rangle_{(2)}\,d\hat{A}^{(2)}_{\alpha\beta} = \int_{S^3-\Gamma^2}\left(\langle\phi_{;\alpha}G^{\beta\alpha}\rangle_{(3)}+\frac{4\pi}{c}\langle\phi J^{\beta}\rangle_{(3)}\right)d\hat{A}^{(3)}_{\beta} - \frac{2\pi}{c}\int_{\Gamma^2-\Gamma'^2}\langle\phi\mathcal{K}^{\alpha\beta}\rangle\,d\hat{A}^{(2)}_{\alpha\beta}. \quad (3.4)$$

Similarly, for the $\hat{F}'^{\alpha\beta}$ field, we have

$$-\tfrac{1}{2}\oint_{S^2-\Gamma^2}\langle\phi\hat{F}^{\alpha\beta}\rangle_{(2)}\,d\hat{A}^{(2)}_{\alpha\beta} = \int_{S^3-\Gamma^2}\langle\phi_{;\alpha}\hat{F}^{\beta\alpha}\rangle_{(3)}\,d\hat{A}^{(3)}_{\beta}, \quad (3.5)$$

where the averages indicated by angular brackets are defined similarly to (3.3). If in (3.4) and (3.5) we close the surface S^3, we find

$$\oint_{S^3-\Gamma^2}\left(\langle\phi_{;\alpha}G^{\beta\alpha}\rangle_{(3)}+\frac{4\pi}{c}\langle\phi J^{\beta}\rangle_{(3)}\right)d\hat{A}^{(3)}_{\beta} - \frac{2\pi}{c}\int_{\Gamma^2-\Gamma'^2}\langle\phi\mathcal{K}^{\alpha\beta}\rangle_{(2)}\,d\hat{A}^{(2)}_{\alpha\beta} = 0, \quad (3.6)$$

$$\oint_{S^3-\Gamma^2}\langle\phi_{;\alpha}\hat{F}^{\beta\alpha}\rangle_{(3)}\,d\hat{A}^{(3)}_{\beta} = 0. \quad (3.7)$$

If Γ is a locally smooth surface (as we assume henceforth), then, using (2.6), we may express $\langle\phi\mathcal{K}^{\alpha\beta}\rangle_{(2)}$ as

$$\langle\phi\mathcal{K}^{\alpha\beta}\rangle_{(2)} = \langle\phi K^{\alpha}\rangle_{(2)}n^{\beta} - \langle\phi K^{\beta}\rangle_{(2)}n^{\alpha}; \qquad \langle\phi K^{\alpha}\rangle_{(2)}n_{\alpha} = 0.$$

Equations (3.4)–(3.7) *are postulated to be the master balance laws of microelectromagnetic theory.*

4. FIELD EQUATIONS

By applying Stokes' theorem to the integrals in (3.4)–(3.7) and postulating that the integrals are valid for all submanifolds $S^3 - \Gamma^2$, $S^2 - \Gamma^2$, and $\Gamma^2 - \Gamma'^2$ in space–time, we obtain

$$\langle \phi G^{\beta\alpha}\rangle_{(2);\alpha} - \langle \phi_{;\alpha} G^{\beta\alpha}\rangle_{(3)} = (4\pi/c)\langle \phi J^{\beta}\rangle_{(3)}, \quad (4.1)$$

$$\langle \phi_{;\alpha} G^{\beta\alpha}\rangle_{(3);\beta} + (4\pi/c)\langle \phi J^{\beta}\rangle_{(3);\beta} = 0, \quad (4.2)$$

$$\langle \phi \hat{F}^{\beta\alpha}\rangle_{(2);\alpha} - \langle \phi_{;\alpha} \hat{F}^{\beta\alpha}\rangle_{(3)} = 0, \quad (4.3)$$

$$\langle \phi_{;\alpha} \hat{F}^{\beta\alpha}\rangle_{(3);\beta} = 0, \quad \text{in } S^4 - \Gamma, \quad (4.4)$$

and the jump conditions

$$[\langle \phi G^{\alpha\beta}\rangle_{(2)}]n_\beta = (4\pi/c)\langle \phi \mathcal{K}^{\alpha\beta}\rangle_{(2)} n_\beta = (4\pi/c)\langle \phi K^{\alpha}\rangle_{(2)}, \quad (4.5)$$

$$[(c/4\pi)\langle \phi_{;\beta} G^{\alpha\beta}\rangle_{(3)} + \langle \phi J^{\alpha}\rangle_{(3)}]n_\alpha + \langle \phi K^{\Delta}\rangle_{(2);\Delta} = 0, \quad (4.6)$$

$$[\langle \phi \hat{F}^{\alpha\beta}\rangle_{(2)}]n_\beta = 0, \quad (4.7)$$

$$[\langle \phi_{;\beta} \hat{F}^{\alpha\beta}\rangle_{(3)}]n_\alpha = 0, \quad \text{on } \Gamma, \quad (4.8)$$

$$[\langle \phi K^{\alpha}\rangle_{(2)}]n'_\alpha = 0, \quad \text{on } \Gamma'^2. \quad (4.9)$$

Equations (4.1)–(4.4) are the *master differential field equations* and (4.5)–(4.9) are the *master jump conditions of relativistic microelectromagnetic theory.*

By use of these equations, we can derive theories involving various order moments of the electromagnetic fields. To this end, we recall that the test function $\phi(x'^\alpha)$ is expandable in each S^3_J, S^2_K, and Γ^2_L about a point x^α, i.e.,

$$\phi(x'^\alpha) = \phi(x^\alpha) + \phi_{;\lambda}(x^\alpha)\xi^\lambda + (1/2!)\phi_{;\lambda\mu}(x^\alpha)\xi^\lambda\xi^\mu + \cdots, \quad x^\alpha, x'^\alpha \in S^3_J \text{ or } S^2_K \text{ or } \Gamma^2_L, \quad (4.10)$$

where

$$\xi^\lambda \equiv \mathbf{g}^\lambda(x^\alpha)\cdot[\mathbf{p}(x'^\alpha) - \mathbf{p}(x^\alpha)].$$

Here the $\mathbf{g}^\lambda$ are the reciprocal base vectors to $\mathbf{g}_\lambda$, and $\mathbf{p}$ is the position vector.

By use of (4.10), we may write

$$\begin{aligned}
\langle \phi G^{\alpha\beta}\rangle_{(2)} &\equiv \phi G^{\alpha\beta} + \sum_{p=1} \phi_{;\lambda_1\cdots\lambda_p} G^{\alpha\beta\lambda_1\cdots\lambda_p},\\
\langle \phi_{;\beta} G^{\alpha\beta}\rangle_{(3)} &\equiv \sum_{p=1} \phi_{;\lambda_1\cdots\lambda_p} \mathcal{G}^{\alpha\lambda_1\cdots\lambda_p},\\
\langle \phi J^{\alpha}\rangle_{(3)} &\equiv \phi J^{\alpha} + \sum_{p=1} \phi_{;\lambda_1\cdots\lambda_p} J^{\alpha\lambda_1\cdots\lambda_p},\\
\langle \phi \mathcal{K}^{\alpha\beta}\rangle_{(2)} &\equiv \phi \mathcal{K}^{\alpha\beta} + \sum_{p=1} \phi_{;\lambda_1\cdots\lambda_p} \mathcal{K}^{\alpha\beta\lambda_1\cdots\lambda_p},\\
\langle \phi \hat{F}^{\alpha\beta}\rangle_{(2)} &\equiv \phi \hat{F}^{\alpha\beta} + \sum_{p=1} \phi_{;\lambda_1\cdots\lambda_p} \hat{F}^{\alpha\beta\lambda_1\cdots\lambda_p},\\
\langle \phi_{;\beta} \hat{F}^{\alpha\beta}\rangle_{(3)} &\equiv \sum_{p=1} \phi_{;\lambda_1\cdots\lambda_p} \hat{\mathcal{F}}^{\alpha\lambda_1\cdots\lambda_p},
\end{aligned} \quad (4.11)$$

where we have defined

$$G^{\alpha\beta\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle G^{\alpha\beta}\xi^{(\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(2)}, \quad (4.12a)$$

$$\mathcal{G}^{\alpha\beta\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle G^{\alpha(\beta}\xi^{\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(3)}, \quad (4.12b)$$

$$J^{\alpha\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle J^{\alpha}\xi^{(\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(3)}, \quad (4.12c)$$

$$\mathcal{K}^{\alpha\beta\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle \mathcal{K}^{\alpha\beta}\xi^{(\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(2)} = K^{\alpha\lambda_1\cdots\lambda_p}n^\beta - K^{\beta\lambda_1\cdots\lambda_p}n^\alpha, \quad (4.12d)$$

$$K^{\alpha\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle K^{\alpha}\xi^{(\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(2)}, \quad (4.12e)$$

$$\hat{F}^{\alpha\beta\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle \hat{F}^{\alpha\beta}\xi^{(\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(2)}, \quad (4.12f)$$

$$\hat{\mathcal{F}}^{\alpha\beta\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle \hat{F}^{\alpha(\beta}\xi^{\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(3)}, \quad (4.12g)$$

and a parenthesis enclosing a set of indices denotes symmetrization. Upon substituting (4.11) into the master equations (4.1)–(4.9) and noting that they are to hold identically for all admissible values of $\phi_{;\lambda_1\cdots\lambda_p}$, we obtain the field equations

$$G^{\alpha\beta}{}_{;\beta} = (4\pi/c)J^\alpha, \quad (4.13a)$$

$$G^{\alpha\beta\lambda_1\cdots\lambda_p}{}_{;\beta} + G^{\alpha(\lambda_1\cdots\lambda_p)} - \mathcal{G}^{\alpha\lambda_1\cdots\lambda_p} = (4\pi/c)J^{\alpha\lambda_1\cdots\lambda_p}, \; p \geq 1, \quad \text{in } S^4 - \Gamma, \quad (4.13b)$$

$$\hat{F}^{\alpha\beta}{}_{;\beta} = 0, \quad (4.13c)$$

$$\hat{F}^{\alpha\beta\lambda_1\cdots\lambda_p}{}_{;\beta} + \hat{F}^{\alpha(\lambda_1\cdots\lambda_p)} - \hat{\mathcal{F}}^{\alpha\lambda_1\cdots\lambda_p} = 0, \quad p \geq 1, \quad \text{in } S^4 - \Gamma, \quad (4.13d)$$

$$J^\alpha{}_{;\alpha} = 0, \quad (4.13e)$$

$$J^{\alpha\lambda_1}{}_{;\alpha} + J^{\lambda_1} = -(c/4\pi)\mathcal{G}^{\alpha\lambda_1}{}_{;\alpha} \equiv \mathcal{J}^{\lambda_1}, \quad (4.13f)$$

$$J^{\alpha\lambda_1\cdots\lambda_p}{}_{;\alpha} + J^{(\lambda_1\cdots\lambda_p)} = -(c/4\pi)\times(\mathcal{G}^{\alpha\lambda_1\cdots\lambda_p}{}_{;\alpha} + \mathcal{G}^{(\lambda_1\cdots\lambda_p)}) \equiv \mathcal{J}^{\lambda_1\cdots\lambda_p}, \quad p \geq 2, \quad \text{in } S^4 - \Gamma, \quad (4.13g)$$

$$\hat{\mathcal{F}}^{\alpha\beta}{}_{;\beta} = 0, \quad (4.13h)$$

$$\hat{\mathcal{F}}^{\beta\lambda_1\cdots\lambda_p}{}_{;\beta} + \hat{\mathcal{F}}^{(\lambda_1\cdots\lambda_p)} = 0, \quad p \geq 1, \quad \text{in } S^4 - \Gamma, \quad (4.13i)$$

and jump conditions

$$[G^{\alpha\beta}]n_\beta = (4\pi/c)\mathcal{K}^{\alpha\beta}n_\beta = (4\pi/c)K^\alpha, \quad (4.14a)$$

$$[G^{\alpha\beta\lambda_1\cdots\lambda_p}]n_\beta = (4\pi/c)\mathcal{K}^{\alpha\beta\lambda_1\cdots\lambda_p}n_\beta = (4\pi/c)K^{\alpha\lambda_1\cdots\lambda_p}, \quad p \geq 1, \quad \text{on } \Gamma - \Gamma'^2, \quad (4.14b)$$

$$[\hat{F}^{\alpha\beta}]n_\beta = 0, \quad (4.14c)$$

$$[\hat{F}^{\alpha\beta\lambda_1\cdots\lambda_p}]n_\beta = 0, \quad p \geq 1, \quad \text{on } \Gamma - \Gamma'^2, \quad (4.14d)$$

$$[J^\alpha]n_\alpha + K^\Delta{}_{;\Delta} = 0, \quad (4.14e)$$

$$[J^{\alpha\lambda_1\cdots\lambda_p} + (c/4\pi)\mathcal{G}^{\alpha\lambda_1\cdots\lambda_p}]n_\alpha + K^{\Delta\lambda_1\cdots\lambda_p}{}_{;\Delta} + K^{(\lambda_1\cdots\lambda_p)} = 0, \quad p \geq 1, \quad \text{on } \Gamma - \Gamma'^2, \quad (4.14f)$$

$$[\hat{\mathcal{F}}^{\alpha\lambda_1\cdots\lambda_p}]n_\alpha = 0, \quad p \geq 1, \quad \text{on } \Gamma - \Gamma'^2, \quad (4.14g)$$

$$[K^{\alpha\lambda_1\cdots\lambda_p}]n'_\alpha = 0, \quad \text{on } \Gamma'^2. \quad (4.14h)$$

Symmetry properties of these tensors are noted by the following identities:

$$\begin{aligned}
G^{\alpha\beta} &= -G^{\beta\alpha},\\
G^{\alpha\beta\lambda_1\cdots\lambda_p} &= -G^{\beta\alpha\lambda_1\cdots\lambda_p} = G^{\alpha\beta(\lambda_1\cdots\lambda_p)},\\
\mathfrak{G}^{\alpha\lambda_1\cdots\lambda_p} &= \mathfrak{G}^{\alpha(\lambda_1\cdots\lambda_p)},\\
\hat{F}^{\alpha\beta} &= -\hat{F}^{\beta\alpha},\\
\hat{F}^{\alpha\beta\lambda_1\cdots\lambda_p} &= -\hat{F}^{\beta\alpha\lambda_1\cdots\lambda_p} = \hat{F}^{\alpha\beta(\lambda_1\cdots\lambda_p)},\\
\hat{\mathfrak{F}}^{\alpha\lambda_1\cdots\lambda_p} &= \hat{\mathfrak{F}}^{\alpha(\lambda_1\cdots\lambda_p)},\\
J^{\alpha\lambda_1\cdots\lambda_p} &= J^{\alpha(\lambda_1\cdots\lambda_p)},\\
\mathfrak{J}^{\lambda_1\cdots\lambda_p} &= \mathfrak{J}^{(\lambda_1\cdots\lambda_p)}, \text{ (see Ref. 12)},\\
\mathfrak{K}^{\alpha\beta\lambda_1\cdots\lambda_p} &= K^{\alpha\lambda_1\cdots\lambda_p}n^{\beta} - K^{\beta\lambda_1\cdots\lambda_p}n^{\alpha},\\
K^{\alpha\lambda_1\cdots\lambda_p} &= K^{\alpha(\lambda_1\cdots\lambda_p)},\\
K^{\alpha\lambda_1\cdots\lambda_p}n_{\alpha} &= 0.
\end{aligned} \tag{4.15}$$

The first two sets of (4.13) and (4.14) (equations for $\mathbf{G}$'s) constitute a generalization of the Ampere–Gauss law, the second two (equations for $\hat{\mathbf{F}}$'s) are a generalization of the conservation of magnetic flux, and the last three sets (equations satisfied by $\mathbf{J}$'s) are the generalization of the law of conservation of charge. A *microelectromagnetic theory of grade p* will be defined as that theory for which the $(p+1)$th averages of all the aforementioned averages [$(p+1)$th moment of fields] vanish. For example, Maxwell's equations constitute a theory of grade zero. The theory of grade 1 is presented in Sec. 5. Theories higher than grade 1 are clearly quite complicated.

5. MICROELECTROMAGNETIC THEORY OF GRADE 1

Polar electromagnetic theory of grade 1 (alternatively, *micromorphic* EM *theory*) is embodied in the field equations

$$G^{\alpha\beta}{}_{;\beta} = (4\pi/c)\,J^{\alpha}, \tag{5.1a}$$

$$G^{\alpha\beta\lambda}{}_{;\beta} + G^{\alpha\lambda} - \mathfrak{G}^{\alpha\lambda} = (4\pi/c)\,J^{\alpha\lambda}, \tag{5.1b}$$

$$\hat{F}^{\alpha\beta}{}_{;\beta} = 0, \tag{5.1c}$$

$$\hat{F}^{\alpha\beta\lambda}{}_{;\beta} + \hat{F}^{\alpha\lambda} - \hat{\mathfrak{F}}^{\alpha\lambda} = 0, \quad \text{in} \quad S^4 - \Gamma, \tag{5.1d}$$

and in the jump conditions

$$\begin{aligned}
[G^{\alpha\beta}]n_{\beta} &= (4\pi/c)K^{\alpha},\\
[G^{\alpha\beta\lambda}]n_{\beta} &= (4\pi/c)K^{\alpha\lambda},\\
[\hat{F}^{\alpha\beta}]n_{\beta} &= 0,\\
[\hat{F}^{\alpha\beta\lambda}]n_{\beta} &= 0, \quad \text{on } \Gamma.
\end{aligned} \tag{5.2}$$

According to (4.15), the tensors appearing in these equations possess the following properties:

$$G^{\alpha\beta} = -G^{\beta\alpha}, \quad \hat{F}^{\alpha\beta} = -\hat{F}^{\beta\alpha},$$
$$G^{\alpha\beta\lambda} = -G^{\beta\alpha\lambda}, \quad \hat{F}^{\alpha\beta\lambda} = -\hat{F}^{\beta\alpha\lambda}.$$

Equations (4.13e)–(4.13i) and the jumps (4.14e)–(4.14h) become, for grade 1,

$$\mathfrak{G}^{(\mu\lambda)} = -(4\pi/c)J^{(\mu\lambda)} = -(4\pi/c)\mathfrak{J}^{(\mu\lambda)}, \tag{5.3a}$$

$$\hat{\mathfrak{F}}^{(\mu\lambda)} = 0, \tag{5.3b}$$

$$\mathfrak{G}^{\mu\lambda}{}_{;\mu} = -(4\pi/c)\mathfrak{J}^{\lambda}, \tag{5.3c}$$

$$\hat{\mathfrak{F}}^{\mu\lambda}{}_{;\mu} = 0, \tag{5.3d}$$

$$J^{\mu}{}_{;\mu} = 0, \tag{5.3e}$$

$$J^{\mu\lambda}{}_{;\mu} + J^{\lambda} - \mathfrak{J}^{\lambda} = 0, \quad \text{in} \quad S^4 - \Gamma, \tag{5.3f}$$

$$[\mathfrak{G}^{\lambda\mu} + (4\pi/c)J^{\lambda\mu}]n_{\lambda} = -(4\pi/c)(K^{\mu} + K^{\Delta\mu}{}_{;\Delta}), \tag{5.4a}$$

$$[\hat{\mathfrak{F}}^{\lambda\mu}]n_{\lambda} = 0, \tag{5.4b}$$

$$[J^{\mu}]n_{\mu} + K^{\Delta}{}_{;\Delta} = 0, \tag{5.4c}$$

$$K^{(\mu\lambda)} = 0, \quad \text{on} \quad \Gamma - \Gamma'^{2}, \tag{5.4d}$$

$$[K^{\mu}]n'_{\mu} = 0, \tag{5.4e}$$

$$[K^{\mu\lambda}]n'_{\mu} = 0, \quad \text{on} \quad \Gamma'^{2}. \tag{5.4f}$$

We recall that $K^{\mu}n_{\mu} = K^{\mu\lambda}n_{\mu} = 0$.

From (5.3a) and (5.3b), we see that $\hat{\mathfrak{F}}^{\mu\lambda}$ is skew, and the symmetric part of $\mathfrak{G}^{\mu\lambda}$ is determined when $J^{(\mu\lambda)}$ is known. Equations (5.1b), (5.1d), (5.3c), (5.3d), (5.4a), and (5.4b) may thus be written as

$$G^{\alpha\beta\lambda}{}_{;\beta} + G^{\alpha\lambda} - \mathfrak{G}^{[\alpha\lambda]} = (4\pi/c)J^{[\alpha\lambda]}, \tag{5.5a}$$

$$\hat{F}^{\alpha\beta\lambda}{}_{;\beta} + \hat{F}^{\alpha\lambda} - \hat{\mathfrak{F}}^{[\alpha\lambda]} = 0, \tag{5.5b}$$

$$\mathfrak{G}^{[\mu\lambda]}{}_{;\lambda} = (4\pi/c)(J^{\mu} - J^{[\mu\lambda]}{}_{;\lambda}), \tag{5.5c}$$

$$\hat{\mathfrak{F}}^{[\mu\lambda]}{}_{;\lambda} = 0, \tag{5.5d}$$

$$[\mathfrak{G}^{[\lambda\mu]} + (4\pi/c)J^{[\lambda\mu]}]n_{\mu} = (4\pi/c)(K^{\lambda} + K^{\Delta\lambda}{}_{;\Delta}), \tag{5.6a}$$

$$[\hat{\mathfrak{F}}^{[\lambda\mu]}]n_{\mu} = 0. \tag{5.6b}$$

Thus, for the theory of grade 1, we need only concern ourselves with the skew parts of $\mathfrak{G}$, $\hat{\mathbf{F}}$, and $\mathbf{J}$. Hence, we adopt the following convention: By writing $\mathfrak{G}^{\alpha\beta}$, $\hat{\mathfrak{F}}^{\alpha\beta}$, and $J^{\alpha\beta}$ we mean $\mathfrak{G}^{[\alpha\beta]}$, $\hat{\mathfrak{F}}^{[\alpha\beta]}$, and $J^{[\alpha\beta]}$.

We now proceed to give the forms of the above field equations in a Euclidean frame of reference. To this end, we employ (2.2) and the additional fields $\mathfrak{E}$, $\mathfrak{B}$, $\mathfrak{K}$, and $\mathfrak{D}$ defined by

$$\begin{aligned}
\mathfrak{F} &\overset{*}{=} (\text{dual } \mathfrak{B}, -i\mathfrak{E}),\\
\mathfrak{G} &\overset{*}{=} (\text{dual } \mathfrak{K}, -i\mathfrak{D}).
\end{aligned} \tag{5.7}$$

Further, $\hat{F}^{\alpha\beta\lambda}$ and $G^{\alpha\beta\lambda}$ may be given uniquely by

$$\begin{aligned}
F_{kl}{}^{r} &\overset{*}{=} \epsilon_{klm}B^{mr}, & F_{k4}{}^{r} &\overset{*}{=} -iE_{k}{}^{r},\\
F_{kl}{}^{4} &\overset{*}{=} i\epsilon_{klm}B^{m4}, & F_{k4}{}^{4} &\overset{*}{=} E_{k}{}^{4},\\
G^{klr} &\overset{*}{=} \epsilon^{klm}H_{m}{}^{r}, & G^{k4r} &\overset{*}{=} -iD^{kr},\\
G^{kl4} &\overset{*}{=} i\epsilon^{klm}H_{m}{}^{4}, & G^{k44} &\overset{*}{=} D^{k4}.
\end{aligned} \tag{5.8}$$

If we recall the definitions (4.12c) for $J^{\alpha\beta}$, we see that $J^{[\alpha\beta]} = \langle J^{[\alpha}\xi^{\beta]}\rangle_{(3)}$ is none other than the polarization tensor of classical electromagnetism (cf. Grot and

Eringen, Ref. 1, p. 643). Hence, we set

$$\mathbf{J} \overset{*}{=} [\text{dual}\,(-c\mathbf{M} - \mathbf{P} \times \mathbf{v}), -ic\mathbf{P})], \tag{5.9}$$

where $\mathbf{M}$ is the magnetization, $\mathbf{P}$ is the polarization, and $\mathbf{v}$ is the velocity vector. Using the properties of $K^{\alpha\beta}$ given in (5.4d) and its definition $K^{\alpha\beta} = \langle K^{[\alpha}\xi^{\beta]}\rangle_{(2)}$, we can express it in a unique form

$$\mathbf{K} \overset{*}{=} (1 - v_{(\mathfrak{n})}^2/c^2)^{-\frac{1}{2}}[\text{dual}\,(-c\mu\mathfrak{n} - \boldsymbol{\pi} \times v_{(\mathfrak{n})}\mathfrak{n}), -ic\boldsymbol{\pi}], \tag{5.10}$$

where

$$\boldsymbol{\pi} \cdot \mathfrak{n} = 0.$$

Therefore, the discontinuity surface can only support a surface polarization $\boldsymbol{\pi}$, perpendicular to the normal, and a surface magnetization $\mu\mathfrak{n}$, parallel to the normal.

Employing the above definitions (5.7)–(5.10) and (2.2) in (5.1) and (5.2), we obtain the field equations

$$\begin{gathered}
D^k{}_{;k} = 4\pi q, \quad D^{lk}{}_{;l} + D^k - \mathfrak{D}^k = 4\pi P^k, \quad D^{k4}{}_{;k} = 0, \\
\epsilon^{klm}H_{m;l} - \frac{1}{c}\frac{\partial D^k}{\partial t} = \frac{4\pi}{c}J^k, \\
\epsilon^{kmn}H_n{}^l{}_{;m} - \frac{1}{c}\frac{\partial D^{kl}}{\partial t} + \epsilon^{klm}(H_m - \mathcal{H}_m) \\
= -4\pi\epsilon^{klm}\left(M_m + \epsilon_{mrs}P^r\frac{v^s}{c}\right), \\
\epsilon^{klm}H_m{}^4{}_{;l} - \frac{1}{c}\frac{\partial D^{k4}}{\partial t} - (D^k - \mathfrak{D}^k) = -4\pi P^k, \\
B^k{}_{;k} = 0, \quad B^{lk}{}_{;l} + B^k - \mathfrak{B}^k = 0, \quad B^{k4}{}_{;k} = 0, \\
\epsilon^{klm}E_{m;l} + \frac{1}{c}\frac{\partial B^k}{\partial t} = 0, \\
\epsilon^{kmn}E_n{}^l{}_{;m} + \frac{1}{c}\frac{\partial B^{kl}}{\partial t} + \epsilon^{klm}(E_m - \mathfrak{E}_m) = 0, \\
\epsilon^{klm}E_m{}^4{}_{;l} + \frac{1}{c}\frac{\partial B^{k4}}{\partial t} + B^k - \mathfrak{B}^k = 0, \quad \text{in} \quad \mathcal{U} - \Gamma,
\end{gathered} \tag{5.11}$$

and the jump conditions

$$\begin{gathered}
[D^k]n_k = 4\pi\sigma, \quad [D^{kl}]n_k = 4\pi\pi^l, \quad [D^{k4}]n_k = 0, \\
\epsilon^{klm}n_l[H_m] + v_{(\mathfrak{n})}c^{-1}[D^k] = (4\pi/c)K^k, \\
\epsilon^{kmn}n_m[H_n{}^l] + v_{(\mathfrak{n})}c^{-1}[D^{kl}] \\
= -4\pi\epsilon^{klm}(\mu n_m + v_{(\mathfrak{n})}c^{-1}\epsilon_{mrs}\pi^r n^s), \\
\epsilon^{klm}n_l[H_m{}^4] + v_{(\mathfrak{n})}c^{-1}[D^{k4}] = -4\pi\pi^k, \\
[B^k]n_k = 0, \quad [B^{kl}]n_k = 0, \quad [B^{k4}]n_k = 0, \\
\epsilon^{klm}n_l[E_m] - v_{(\mathfrak{n})}c^{-1}[B^k] = 0, \\
\epsilon^{kmn}n_m[E_n{}^l] - v_{(\mathfrak{n})}c^{-1}[B^{kl}] = 0, \\
\epsilon^{klm}n_l[E_m{}^4] - v_{(\mathfrak{n})}c^{-1}[B^{k4}] = 0, \quad \text{on } \Gamma,
\end{gathered} \tag{5.12}$$

where $\mathcal{U}$ is the region of 3-dimensional space where the EM fields are continuous and Γ is the discontinuity surface. The field equations and jump conditions (5.5c), (5.5d), and (5.6) for the script capital fields become

$$\mathfrak{D}^k{}_{;k} = 4\pi(q - P^k{}_{;k}), \tag{5.13a}$$

$$\epsilon^{klm}\mathcal{H}_{m;l} - \frac{1}{c}\frac{\partial \mathfrak{D}^k}{\partial t} = \frac{4\pi}{c}\left(J^k + \frac{\partial P^k}{\partial t} + \epsilon^{klm}(cM_m + \epsilon_{mrs}P^r v^s)_{;l}\right), \tag{5.13b}$$

$$\mathfrak{B}^k{}_{;k} = 0, \tag{5.13c}$$

$$\epsilon^{klm}\mathfrak{E}_{m;l} + \frac{1}{c}\frac{\partial \mathfrak{B}^k}{\partial t} = 0, \quad \text{in} \quad \mathcal{U} - \Gamma, \tag{5.13d}$$

$$[\mathfrak{D}^l]n_l = 4\pi(\sigma - \pi^a{}_{;a}) - 4\pi[P^k]n_k, \tag{5.14a}$$

$$\begin{gathered}
\epsilon^{klm}n_l[\mathcal{H}_m] + v_{(\mathfrak{n})}c^{-1}[\mathfrak{D}^k] = \frac{4\pi}{c}\Big[K^k + x^k{}_{,a} \\
\times \left(\frac{\partial \pi^a}{\partial t} - \pi^a v_{(\mathfrak{n})}b^c{}_c + c\epsilon^{ab}\mu_{;b}\right) - v_{(\mathfrak{n})}n^k\pi^a{}_{;a}\Big] \\
+ \frac{4\pi}{c}\{\epsilon^{klm}n_l[cM_m + \epsilon_{mrs}P^r v^s] - v_{(\mathfrak{n})}[P^k]\},
\end{gathered} \tag{5.14b}$$

$$[\mathfrak{B}^k]n_k = 0, \tag{5.14c}$$

$$\epsilon^{klm}n_l[\mathfrak{E}_m] - v_{(\mathfrak{n})}c^{-1}[\mathfrak{B}^k] = 0, \quad \text{on } \Gamma. \tag{5.14d}$$

From (5.3e), (5.4c), and (5.4e) the zeroth moment of the conservation of charge equation is

$$\begin{gathered}
\frac{\partial q}{\partial t} + J^k{}_{;k} = 0, \quad \text{in} \quad \mathcal{U} - \Gamma, \\
[J^k - qv^k]n_k + \frac{\partial \sigma}{\partial t} + K^a{}_{;a} - \sigma v_{(\mathfrak{n})}b^a{}_a = 0, \\
\text{on} \quad \Gamma - \Gamma'^2, \\
[K^k - \sigma\mu^k]n'_k = 0, \quad \text{on} \quad \Gamma'^2.
\end{gathered} \tag{5.15}$$

The first moment [excluding (5.4f)] is identical to Eqs. (5.13a), (5.13b), (5.14a), and (5.14b). Finally, (5.4f) is

$$[\pi^k]n'_k = 0, \tag{5.16a}$$

$$\epsilon^{klm}n'_l[c\mu n_m + v_{(\mathfrak{n})}\epsilon_{mrs}\pi^r n^s] - \mu_{(\mathfrak{n}')}[\pi^k] = 0, \quad \text{on } \Gamma'^2. \tag{5.16b}$$

It is to be noted that, in the microelectromagnetic theory of grade 1, Maxwell's equations are supplemented with additional field equations and jump conditions for the new vector fields $\mathfrak{E}_k$, $\mathfrak{B}^k$, $\mathcal{H}^k$, $\mathfrak{D}^k$, $H_k{}^4$, $E_k{}^4$, $D_k{}^4$, and $B_k{}^4$ and the new tensor fields $H_k{}^l$, $E_k{}^l$, D^{kl}, and B^{kl}.

A comparison of Maxwell's equations for ponderable matter with Eqs. (5.1)–(5.4) is in order. If we

assume that, for the grade 1 theory,

(1) microscopically, $F'_{\alpha\beta} = G'_{\alpha\beta}$,

(2) the moments of the electromagnetic field $F'_{\alpha\beta}$, and the surface current $\mathcal{K}'^{\alpha\beta}$, vanish while the moments of the current J'^{μ} do not,

then Maxwell's equations in the presence of matter are equivalent to (5.1)–(5.4). For, under these assumptions,

$$G^{\mu\lambda\alpha} = F^{\mu\lambda\alpha} = 0,$$

which imply [cf. (5.1b), (5.1d)]

$$F^{\mu\lambda} = \mathcal{F}^{\mu\lambda},$$

$$G^{\mu\lambda} = \mathcal{G}^{\mu\lambda} + (4\pi/c)J^{\mu\lambda},$$

and since $F^{\mu\lambda}$, $\mathcal{F}^{\mu\lambda}$, and now $\mathcal{G}^{\mu\lambda}$ [cf. (5.5c), (5.6a) and recall $K^{\mu\lambda} = 0$] satisfy the identical relations as (dual **B**, $-i$**E**) of Maxwell's equations in matter, then

$$F^{\mu\lambda} = \mathcal{F}^{\mu\lambda} = \mathcal{G}^{\mu\lambda},$$

and thus (5.1)–(5.4) are identical to (2.8) and (2.9). Hence, Maxwell's equations for ponderable matter are a special case of the laws for an electromagnetic polar medium of grade 1.

For a complete theory, the aforementioned balance laws must be supplemented with the mechanical laws of motion and constitutive equations. The straightforward case of a rigid linear medium can be dispensed with by taking $F_{\mu\lambda}$, $\mathcal{F}_{\mu\lambda}$, and $F_{\mu\lambda}{}^{\alpha}$ as linear functions of $G_{\mu\lambda}$, $\mathcal{G}_{\mu\lambda}$, and $G_{\mu\lambda}{}^{\alpha}$. However, constitutive equations for a deformable medium require the general thermodynamic considerations appropriate to the *complete* polar electromagnetic theory with mechanical interaction and will be considered in a later paper.

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[10] A. C. Eringen, in *Mechanics of Generalized Continua*, E. Kröner, Ed. (Springer, New York, 1968).

[11] If one desires to employ Maxwell's equations in free space, then one must take $F^{\alpha\beta} = G^{\alpha\beta}$ microscopically.

[12] Instead of abstractly defining the quantities $\mathcal{J}^{\lambda_1\cdots\lambda_p}$, we may introduce them in a natural manner: If the averaging procedure is extended to (2.7) alone, then the resultant field equations are

$$J^{\alpha\lambda_1\cdots\lambda_p}{}_{;\alpha} + J^{(\lambda_1\cdots\lambda_p)} - \mathcal{J}^{\lambda_1\cdots\lambda_p} = 0, \quad p \geq 1,$$

where $J^{\alpha\lambda_1\cdots\lambda_p}$ is defined as above [see (4.12c)], and, in addition, the quantities $\mathcal{J}^{\lambda_1\cdots\lambda_p}$ are defined by

$$\mathcal{J}^{\alpha\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle J^{(\alpha}\xi^{\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(4)}.$$

This definition thus gives further insight into $\mathcal{J}^{\lambda_1\cdots\lambda_p}$.

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Nonuniqueness of the Energy Correction in Application of the WKB Approximation to Radial Problems

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An infinite set of transformations is given that convert a radial energy-eigenvalue problem into a 1-dimensional problem. Langer's transformations are included in this set. The transformations introduce no spurious, real-axis singularities into the effective potential, and yield wavefunctions that meet 1-dimensional boundary conditions and are asymptotically satisfactory for virtually all power law potentials. The first-order radial WKB quantization condition is transformation dependent through two parameters. It may be distinct from the Langer–Kemble condition obtained by substituting $(l + \frac{1}{2})^2$ for $l(l + 1)$ in the effective potential. Here, l is the rotational quantum number. For the vibrating rotator, a rough test of the usefulness of the $(l + \frac{1}{2})^2$ substitution is described; flexibility advantages provided by the new transformations are pointed out.

I. INTRODUCTION

The first-order WKB quantization condition[1–3] provides a method for determining approximate energy eigenvalues in 1-dimensional quantum mechanical problems. This approximation is also applied to radial problems through use of an effective potential energy. Langer[4] developed a transformation method for turning a radial problem into a 1-dimensional problem, whereby the radial quantization condition is a particular modification of the 1-dimensional WKB condition. However, the Langer transformations are not unique, as indicated by Krieger[5]; also

assume that, for the grade 1 theory,

(1) microscopically, $F'_{\alpha\beta} = G'_{\alpha\beta}$,

(2) the moments of the electromagnetic field $F'_{\alpha\beta}$, and the surface current $\mathcal{K}'^{\alpha\beta}$, vanish while the moments of the current J'^{μ} do not,

then Maxwell's equations in the presence of matter are equivalent to (5.1)–(5.4). For, under these assumptions,

$$G^{\mu\lambda\alpha} = F^{\mu\lambda\alpha} = 0,$$

which imply [cf. (5.1b), (5.1d)]

$$F^{\mu\lambda} = \mathcal{F}^{\mu\lambda},$$

$$G^{\mu\lambda} = \mathcal{G}^{\mu\lambda} + (4\pi/c)J^{\mu\lambda},$$

and since $F^{\mu\lambda}$, $\mathcal{F}^{\mu\lambda}$, and now $\mathcal{G}^{\mu\lambda}$ [cf. (5.5c), (5.6a) and recall $K^{\mu\lambda} = 0$] satisfy the identical relations as (dual **B**, $-i$**E**) of Maxwell's equations in matter, then

$$F^{\mu\lambda} = \mathcal{F}^{\mu\lambda} = \mathcal{G}^{\mu\lambda},$$

and thus (5.1)–(5.4) are identical to (2.8) and (2.9). Hence, Maxwell's equations for ponderable matter are a special case of the laws for an electromagnetic polar medium of grade 1.

For a complete theory, the aforementioned balance laws must be supplemented with the mechanical laws of motion and constitutive equations. The straightforward case of a rigid linear medium can be dispensed with by taking $F_{\mu\lambda}$, $\mathcal{F}_{\mu\lambda}$, and $F_{\mu\lambda}{}^{\alpha}$ as linear functions of $G_{\mu\lambda}$, $\mathcal{G}_{\mu\lambda}$, and $G_{\mu\lambda}{}^{\alpha}$. However, constitutive equations for a deformable medium require the general thermodynamic considerations appropriate to the *complete* polar electromagnetic theory with mechanical interaction and will be considered in a later paper.

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[11] If one desires to employ Maxwell's equations in free space, then one must take $F^{\alpha\beta} = G^{\alpha\beta}$ microscopically.

[12] Instead of abstractly defining the quantities $\mathcal{J}^{\lambda_1\cdots\lambda_p}$, we may introduce them in a natural manner: If the averaging procedure is extended to (2.7) alone, then the resultant field equations are

$$J^{\alpha\lambda_1\cdots\lambda_p}{}_{;\alpha} + J^{(\lambda_1\cdots\lambda_p)} - \mathcal{J}^{\lambda_1\cdots\lambda_p} = 0, \quad p \geq 1,$$

where $J^{\alpha\lambda_1\cdots\lambda_p}$ is defined as above [see (4.12c)], and, in addition, the quantities $\mathcal{J}^{\lambda_1\cdots\lambda_p}$ are defined by

$$\mathcal{J}^{\alpha\lambda_1\cdots\lambda_p} \equiv (1/p!)\langle J^{(\alpha}\xi^{\lambda_1}\cdots\xi^{\lambda_p)}\rangle_{(4)}.$$

This definition thus gives further insight into $\mathcal{J}^{\lambda_1\cdots\lambda_p}$.

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Nonuniqueness of the Energy Correction in Application of the WKB Approximation to Radial Problems

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An infinite set of transformations is given that convert a radial energy-eigenvalue problem into a 1-dimensional problem. Langer's transformations are included in this set. The transformations introduce no spurious, real-axis singularities into the effective potential, and yield wavefunctions that meet 1-dimensional boundary conditions and are asymptotically satisfactory for virtually all power law potentials. The first-order radial WKB quantization condition is transformation dependent through two parameters. It may be distinct from the Langer–Kemble condition obtained by substituting $(l + \frac{1}{2})^2$ for $l(l + 1)$ in the effective potential. Here, l is the rotational quantum number. For the vibrating rotator, a rough test of the usefulness of the $(l + \frac{1}{2})^2$ substitution is described; flexibility advantages provided by the new transformations are pointed out.

I. INTRODUCTION

The first-order WKB quantization condition[1–3] provides a method for determining approximate energy eigenvalues in 1-dimensional quantum mechanical problems. This approximation is also applied to radial problems through use of an effective potential energy. Langer[4] developed a transformation method for turning a radial problem into a 1-dimensional problem, whereby the radial quantization condition is a particular modification of the 1-dimensional WKB condition. However, the Langer transformations are not unique, as indicated by Krieger[5]; also

they may lead to poorer eigenvalues than those obtained from an uncorrected first-order 1-dimensional WKB condition.[6] It is the primary purpose of this paper to point out a more general class of transformations that accomplish the same end as Langer's but that may lead to different eigenenergies. The new transformations, like Langer's, introduce no spurious, real-axis singularities in the effective potential, and yield wavefunctions that meet 1-dimensional boundary conditions and are asymptotically satisfactory for power law potentials. Finally, we indicate a rough test for utility of Langer's transformations and illustrate the flexibility of the new transformations in application to the vibrating rotator.

II. THE WKB QUANTIZATION CONDITION

The first-order, 1-dimensional WKB quantization condition is

$$n + \tfrac{1}{2} = \frac{2(2m)^{\frac{1}{2}}}{h}\int_{x_1}^{x_2}[E_n - V(x)]^{\frac{1}{2}}\,dx. \qquad (1)$$

In Eq. (1), n is a nonnegative integer, m is the particle mass, h is Planck's constant, E_n is the nth approximate energy eigenvalue, $V(x)$ is the potential energy of m, and x_1 and x_2 are the classical turning points determined from the equation $E_n - V(x) = 0$. In this paper, we assume that for each E_n there are two and only two turning points. Equation (1) is applicable to the eigenvalue problem defined by the equation

$$\psi''(x) + q^2(x)\psi(x) = 0$$

and the boundary conditions $\psi(\pm\infty) = 0$, where

$$q^2(x) = (8\pi^2m/h^2)[E_n - V(x)].$$

Equation (1) should not be applied directly to a radial eigenvalue problem defined by the equation

$$R''(r) + Q^2(r)R(r) = 0$$

and the boundary conditions $R(0) = R(\infty) = 0$. Here,

$$Q^2(r) = \frac{8\pi^2m}{h^2}[E_n - V_{\text{eff}}(r)]$$
$$= \frac{8\pi^2m}{h^2}\left(E_n - V(r) - \frac{h^2}{8\pi^2m}\frac{l(l+1)}{r^2}\right), \qquad (2)$$

with l the rotational quantum number. This is because of the distinction between the boundary condition $\psi(-\infty) = 0$ and the origin condition $R(0) = 0$. Recently, there has been considerable interest in the application of altered forms of Eq. (1) to radial problems.[5–9] Discussions can be found in the works of Fröman and Fröman[8] and of Heading.[10]

III. LANGER'S TRANSFORMATIONS

Langer's link between the 1-dimensional problem and the radial problem was made through use of two transformations. These are a transformation of the independent variable r and of the dependent variable $R(r)$ through

$$r(x) = e^x, \qquad (3a)$$
$$R(r(x)) = e^{\frac{1}{2}x}\chi(x). \qquad (3b)$$

Application of these transformations to the radial Schrödinger equation results in

$$\chi''(x) + e^{2x}\{(8\pi^2m/h^2)[E_n - V(x)] - (l+\tfrac{1}{2})^2e^{-2x}\}\chi(x) = 0. \qquad (4)$$

This equation is of the same form as the original equation for $R(r)$. However, in Eq. (4), the independent variable x can take values from $-\infty$ to $+\infty$, and $\chi(x)$ satisfies 1-dimensional boundary conditions. Therefore, the new dependent variable $\chi(x)$ is the solution to a 1-dimensional problem. Applying Eq. (1) to Eq. (4) and transforming back to the independent variable r yields the quantization condition

$$(n + \tfrac{1}{2}) = \frac{2(2m)^{\frac{1}{2}}}{h}\int_{r_1}^{r_2}\left(E_n - V(r) - \frac{h^2}{8\pi^2m}\frac{(l+\frac{1}{2})^2}{r^2}\right)^{\frac{1}{2}}dr. \qquad (5)$$

Here, r_1 and r_2 are determined from the condition

$$E_n - V(r) - \frac{h^2}{8\pi^2m}\frac{(l+\frac{1}{2})^2}{r^2} = 0.$$

The origin difficulty is taken into account in Eq. (5) by replacing $l(l+1)$ by $(l+\frac{1}{2})^2$ in the centrifugal term of the effective potential. That is, $h^2/32\pi^2mr^2$ has been added to the effective potential. This replacement is sometimes known as the Langer–Kemble[11] (LK) correction and is so denoted here. Significantly, the LK correction introduces no new singularities in the effective potential [except in the case $l = 0$ for $V(r)$ analytic at $r = 0$]. Further, Langer showed that his transformations were applicable as $x \to -\infty$ and as $x \to +\infty$. As has been pointed out (Ref. 8, pp. 113–14), Langer used this treatment only for the Coulomb potential $V(r) = k/r$, without implying its universal applicability to all radial problems.

IV. OTHER TRANSFORMATION PAIRS

A set of transformations, which moves the origin to $-\infty$ as Langer's does, but which is more general, is

$$r(y) = r_0\exp[\tfrac{1}{2}(y^p + py)], \qquad (6a)$$
$$R(r(y)) = (y^{p-1} + 1)^{\frac{1}{2}}\exp[\tfrac{1}{4}(y^p + py)]\chi(y). \qquad (6b)$$

Here, p is a positive odd integer and r_0 is a scaling factor with the dimensions of r. The result of using these transformations on the radial Schrödinger equation is again an equation of the form

$$\chi''(y) + \tilde{Q}^2(y)\chi(y) = 0, \tag{7}$$

where

$$\tilde{Q}^2(y) = \left(\frac{8\pi^2 m}{h^2}(E - V)\frac{p^2}{4}(y^{p-1} + 1)^2 r_0^2 \times \exp(y^p + py) - [(l + \tfrac{1}{2})^2]\frac{p^2}{4}(y^{p-1} + 1)^2 + \frac{(p-1)(p-2)y^{p-3}}{2(y^{p-1} + 1)} - \frac{3(p-1)^2 y^{2p-4}}{4(y^{p-1} + 1)^2}\right). \tag{8}$$

Using Eq. (1) to determine the energy eigenvalues of Eq. (7), one obtains

$$n + \tfrac{1}{2} = \frac{1}{\pi}\int_{y_1}^{y_2} \tilde{Q}(y)\, dy, \tag{9}$$

where y_1 and y_2 are the values of y for which $\tilde{Q}^2(y) = 0$. When Eq. (9) is re-expressed in terms of r, it becomes

$$(n + \tfrac{1}{2}) = \frac{2(2m)^{\frac{1}{2}}}{h}\int_{r_1}^{r_2}\left[E_n - V - \frac{h^2}{8\pi^2 m r^2} \times \left((l + \tfrac{1}{2})^2 - \frac{2(p-1)(p-2)y^{p-3}}{p^2(y^{p-1} + 1)^3} + \frac{3(p-1)^2 y^{2p-4}}{p^2(y^{p-1} + 1)^4}\right)\right]^{\frac{1}{2}} dr. \tag{10}$$

In Eq. (10), r_1 and r_2 are the transformed values of y_1 and y_2 and $y(r)$ is the function of r defined by

$$y^p + py - 2\ln(r/r_0) = 0. \tag{11}$$

To obtain an explicit expression for $y(r)$, Eq. (11) must be inverted; Hille[12] describes a method of inversion for general p. For the special case of $p = 3$, y is expressible in terms of radicals and it is

$$y(r) = \{\ln(r/r_0) + [1 + \ln^2(r/r_0)]^{\frac{1}{2}}\}^{\frac{1}{3}} + \{\ln(r/r_0) - [1 + \ln^2(r/r_0)]^{\frac{1}{2}}\}^{\frac{1}{3}}. \tag{12}$$

One should note that Eqs. (6)–(11) reduce to the corresponding Langer expressions when $p = 1$.

The noteworthy aspect of Eqs. (6) is that they lead to a new radial quantization condition (10), which is transformation dependent through parameters p and r_0. The sum of the two new terms in Eq. (10) may be positive or negative, depending on p and y. For $p = 3$ at $y = 0$ ($r = r_0$), the sum is of opposite sign and $\frac{16}{9}$ as large as the LK term $-h^2/(32\pi^2 m r^2)$. As $y \to \pm\infty$, the new terms are of order $[1/\ln^2(r/r_0)]$ times the LK term and so are dominated by it.

The derivation of Eq. (10) is based on the implicit assumptions that the transformed differential equation (7) has solutions that meet the conditions $\chi(\pm\infty) = 0$ and are asymptotically satisfactory. It is not difficult to show that $\chi(y)$ must satisfy the boundary conditions for a 1-dimensional problem. Remembering that $R(r)$ must decrease at least as fast as r in the limit as $r \to 0$, one sees that $\chi(y)$ goes to 0 as least as fast as $(y^{p-1} + 1)^{-\frac{1}{2}} \exp[\frac{1}{4}(y^p + py)]$, as $y \to -\infty$. Further, if the boundary condition $R(r) \to 0$ as $r \to \infty$ is to be met, then $\chi(y)$ must go to zero faster than $(y^{p-1} + 1)^{-\frac{1}{2}} \exp[-\frac{1}{4}(y^p + py)]$, as $y \to +\infty$. A criterion for asymptotically satisfactory solutions at the boundaries has been given by Langer and it is that the integral

$$I \equiv \int^{y} |\theta(y)/\tilde{Q}(y)|\, dy$$

be convergent when y is allowed to recede to the boundaries. Here, $\theta(y) = S''(y)/S(y)$, where

$$S(y) = \tilde{Q}^{-\frac{1}{2}}(y)\xi^{\frac{1}{2}-\mu}, \quad \xi = \int^{y} \tilde{Q}(y)\, dy,$$

and $\mu = 1/(\nu + 2)$, where ν is the order of the zero of $\tilde{Q}^2(y)$ at the nearest turning point. We have examined the convergence of I for all potentials asymptotically of the form $V(r) = kr^\delta$ with k and δ real constants. We found that I is convergent as $y \to \pm\infty$ for all p, k, and δ, with one exception. For constants $p = 1$, $\delta = -2$, $k = -h^2(l + \frac{1}{2})^2/8\pi^2 m$, then $I(-\infty)$ is divergent. This one failure occurs for a reason analogous to the failure of the ordinary WKB method at turning points, i.e., $\tilde{Q}(-\infty) = 0$, while $\theta(-\infty) \neq 0$.

The new transformations given by Eqs. (6) introduce no spurious singularities on the real positive r axis and are applicable as $r \to 0$ and as $r \to +\infty$. However, that caution must be exercised in dealing with generalized Langer transformations is illustrated by the following examples. Consider first

$$r(y) = r_0 \exp(y^p), \tag{13a}$$

$$R[r(y)] = (y^{p-1})^{\frac{1}{2}} \exp(\tfrac{1}{2}y^p)\chi(y), \tag{13b}$$

with r_0 and p defined as for Eqs. (6). The $\chi(y)$, defined in Eq. (13b), $\to 0$ and also meets Langer's asymptotic condition as $y \to \pm\infty$ for the same potentials as $\chi(y)$ defined in Eq. (6b). However, because $dr/dy = 0$ at $y = 0$, a spurious logarithmic singularity is introduced into the effective potential at $r = r_0$. Furthermore, $I = \int^{y(r_0)} |\theta/\tilde{Q}|\, dy$ is divergent. Consider next the transformations

$$r(y) = r_0 \exp[\exp(py)], \tag{14a}$$

$$R[r(y)] = \exp(\tfrac{1}{2}py) \exp[\tfrac{1}{2}\exp(py)]\chi(y), \tag{14b}$$

with r_0 and p defined as above. Through Eq. (14a) the domain (r_0, ∞) is transformed to $(-\infty, \infty)$. Again, a spurious singularity is introduced into the effective potential at r_0. Also, the usual 1-dimensional boundary condition $\chi(-\infty) = 0$ cannot, in general, be met, since $\exp(\frac{1}{2}py) \to 0$ and $R(r_0) \neq 0$.

V. THE VIBRATING-ROTATOR CORRECTION

For certain special cases, the LK correction is very effective. In the cases of the radial, isotropic, harmonic oscillator and the Coulomb binding problem, the first-order LK corrected energy eigenvalues are exact.[7,8,13]

For a vibrating rotator one can use the following "rough" test for applicability of the LK correction near the vicinity of a true potential minimum r_e. It has been pointed out[7] that, for effective potentials with a second-order pole at $r = 0$ and $l \neq 0$, origin corrections in the second-order WKB differential equation are made by substituting $l(l+1) - 1/[64l(l+1)]$ for $l(l+1)$. This indicates that radial corrections to second-order WKB calculations are of fourth order in $h/\sqrt{m}$. To be accurate to second order, one may use Dunham's[14] second-order 1-dimensional results even in an origin-uncorrected radial problem. Thus, one may test the size of the Dunham second-order 1-dimensional corrections against the LK radial correction in the vicinity of the minimum of $V(r)$. It was shown[15] that the LK correction to the zero-point energy is equal to $\frac{1}{4}B_e$ plus negligible higher-order terms. Here, B_e is a spectroscopic constant proportional to the inverse moment of inertia. On the other hand, the dominant Dunham second-order correction to the zero-point energy is $\frac{1}{4}B_e\gamma$, with $\gamma = [\frac{3}{2}a_2 - \frac{7}{8}a_1^2]$. Here, a_1 is the cubic coefficient and a_2 the quartic coefficient in a potential expansion of $V(r)$ about r_e. Thus, if γ is close to unity, one obtains second-order accuracy by applying the LK correction in a first-order WKB calculation. If, on the other hand, γ is close to zero, it appears justifiable to neglect entirely a radial WKB correction in the vicinity of the potential minimum.

If one wishes to obtain a zero-point energy with second-order accuracy from a first-order WKB calculation, one can use the transformations of Eqs. (6). The adjustable parameters r_0 and p can be chosen to satisfy the zero-point energy and at least one other condition. The zero-point condition is met if

$$\frac{1}{4} - \frac{2(p-1)(p-2)y_e^{p-3}}{p^2(y_e^{p-1}+1)^3} + \frac{3(p-1)^2y_e^{2p-4}}{p^2(y_e^{p-1}+1)^4} = \tfrac{1}{4}\gamma, \tag{15}$$

where y_e corresponds to r_e. For the ground state of H_2,[16] for example, $\gamma = 0.60$. This is about midway between the case of no radial correction and the LK value of unity. However, Eq. (15) can be satisfied if $p = 3$ and $r_0 = 2.20r_e$ or $r_0 = 0.455r_e$, as well as with other $p - r_0$ combinations.

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Internal Symmetry Cannot Be Concealed*

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We consider the problem of determining whether a given "particle" is elementary or is some member of a degenerate multiplet corresponding to an exact symmetry. We discuss a double-scattering experiment which can make this determination *unless* the members of the multiplet are unable to distinguish one another. Finally, such an inability is shown to be incompatible with the usual relation between spin and statistics and known analyticity properties of scattering amplitudes for strongly interacting particles.

1. INTRODUCTION

In discussions of internal symmetry the question arises, "How could we know if something which we regard as an elementary particle actually has an additional internal quantum number?" Of course if the symmetry is broken, as the proton charge breaks the isotopic spin symmetry of the proton–neutron doublet, there is no problem. Suppose, however, that the internal symmetry is *not* broken by any interactions, so that the generators of it commute with the time development operator H. How can we tell that a "hidden degeneracy" exists? Two partial answers to this question seem to be widely known. First, if the particles in question are fermions one can *imagine* confining them to a box and measuring the Fermi energy as a function of particle number. The hidden degeneracy will of course lower the Fermi energy. Second, there is always the possibility that the members of the multiplet can distinguish *each other* and the degeneracy is then revealed by a suitable double-scattering experiment. We show that the analyticity of scattering amplitudes as a function of center-of-mass scattering angle requires that this possibility is the *only* one, provided that the particles have definite statistics.

The remainder of this paper is divided into three sections. In Sec. 2 we analyze the relevant double-scattering experiment. In Sec. 3 we apply the constraints imposed by analyticity and definite statistics. A brief discussion is given in Sec. 4.

2. HYPOTHETICAL DOUBLE-SCATTERING EXPERIMENT

If something which we regard as an elementary particle has a hidden internal quantum number then every such particle in a beam or target must be described by a density matrix[1] as far as the internal quantum number is concerned. Similarly a 2-particle system will be described by a density matrix. It is convenient to represent this matrix in terms of the representations of the internal symmetry group. We assume that the multiplet to be discovered transforms according to some representation D of the internal symmetry group. We expand the density matrix in terms of the projection operators for states transforming according to all the representations $D^{(I)}$ which appear in the Clebsch–Gordan series which reduces $D \otimes D$. Let $\mathfrak{P}_{I,i}$ be the projector corresponding to the ith partner of the I representation. Thus we write

$$\rho_{\text{initial}} = \sum_{I,i} \omega(I, i)\mathfrak{P}_{I,i}. \tag{1}$$

We normalize to unit flux, setting

$$\sum_{I,i} \omega(I, i) = 1. \tag{2}$$

Now let $T(I, i, E, z)$ be the scattering amplitude in the state (I, i) corresponding to center-of-mass total energy E and scattering angle θ, $z = \cos\theta$. After a single scattering the density matrix is

$$\rho_{\text{once}} = \sum_{I,i} \omega(I, i)\mathfrak{P}_{I,i}|T(I, i, E, z)|^2$$

and the corresponding flux is

$$\mathfrak{F}_{\text{once}} = \sum_{I,i} \omega(I, i)\,|T(1, i, E, z)|^2. \tag{3}$$

We now imagine that the scattered and recoiling particles are transported in such a way that they collide again. If no particles are lost from the beam this will not change the density matrix (because the symmetry is exact and all "external" fields are invariant under it). Now let the particles undergo a second scattering at the *same* center-of-mass energy and scattering angle. The resulting density matrix is

$$\rho_{\text{twice}} = \sum_{I,i} \omega(I, i)\mathfrak{P}_{I,i}|T(I, i, E, z)|^4 \tag{4}$$

and

$$\mathfrak{F}_{\text{twice}} = \sum_{I,i} \omega(I, i)\,|T(I, i, E, z)|^4. \tag{5}$$

For compactness we will set

$$\lambda(I, i) \equiv |T(I, i, E, z)|^2 \geq 0. \tag{6}$$

Now consider the case where D is 1 dimensional (that is, no hidden degeneracy). Then each sum reduces to one term and we have

$$\mathcal{F}_{\text{twice}} = (\mathcal{F}_{\text{once}})^2. \tag{7}$$

Suppose that the degenerate case manages to simulate this result. The necessary condition is

$$\sum \omega(I, i)\lambda(I, i)^2 = [\sum \omega(I, i)\lambda(I, i)]^2. \tag{8}$$

Making use of Eq. (2) we can rewrite this as

$$\sum_{\substack{I,i \\ I,j}} \omega(I, i)\omega(J, j)[\lambda(I, i)^2 - \lambda(I, i)\lambda(J, j)] = 0. \tag{9}$$

Interchanging indices and adding the resulting equations we find that

$$\sum \omega(I, i)\omega(J, j)[\lambda(I, i) - \lambda(J, j)]^2 = 0. \tag{10}$$

Thus the necessary condition (8) requires that $|T(I, i)|^2$ be independent of i (which is guaranteed by the symmetry) and also independent of I. We now show that in the degenerate case this last constraint is in fact impossible.

3. STATISTICS AND ANALYTICITY

To show that the functions $T(I, E, z)$ cannot all have the same magnitude we need two facts. First, at each value of E, every $T(I, E, z)$ is an analytic function[2] of z in some neighborhood of the point $z = 0$. Hence the ratio

$$\phi_{IJ}(z) \equiv T(I, E, z)/T(J, E, z) \tag{11}$$

is analytic in some neighborhood, except possibly for poles. The condition of indistinguishability requires that ϕ have unit modulus on the real axis between $z = -1$ and $z = +1$. This means that ϕ cannot be an *odd* function. The fact that $|\phi| = 1$ would require $z = 0$ to be a singular point, but in the neighborhood of a pole an analytic function must grow without bound.

Now we show that, if there is more than one amplitude $T(I, E, z)$, at least one of the functions ϕ_{IJ} must be odd and hence cannot have unit modulus. To do this we note first that, using the usual relation between spin and statistics[3] we can require the amplitude to have definite transformation properties under exchange of the space, spin, *and* internal coordinates of the final state particles. For the spin singlet-to-singlet transition amplitude this requires that the amplitude be even under simultaneous interchange of space coordinates ($z \to -z$) and internal symmetry coordinates.

Since the generators of internal symmetry for two independent particles commute we can take each of the internal symmetry wavefunctions labeled by I to be either even or odd under interchange of internal symmetry coordinates. To see that both types must occur simply consider the (unreduced) tensor product $D \otimes D$ resolved into odd and even parts,

$$\mathfrak{D}^{(\pm)}_{ik;jl}(g) = D_{ik}(g)D_{jl}(g) \pm D_{jk}(g)D_{il}(g). \tag{12}$$

If either part vanishes we may multiply the resulting equation by $[D^{-1}(g)]_{mi}$ and sum on i to obtain

$$\delta_{mk}D_{jl}(g) \pm \delta_{ml}D_{jk}(g) = 0. \tag{13}$$

If the representation D is more than 1 dimensional we may choose $l \neq m = k$ and prove that $D_{jl}(g) = 0$, for all j and l.

Thus, there must be at least one even and one odd T_I and their ratio ϕ is subject to the analysis given above, showing that the T_I cannot all have the same modulus and proving that the internal degeneracy cannot be concealed.

4. DISCUSSION

The analysis presented here is, I think, of no practical significance. The only particles for which we can readily imagine performing the experiment of Sec. 2 are protons, and the success of the nuclear shell model makes it already clear that there is no degeneracy. It however, is of some philosophical interest to see that the degeneracy can never fully conceal itself and it is intriguing that such powerful tools enter into the proof.

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Massive Vector Field: Covariant Definition of Independent Components and Quantization

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A new approach to the theory of the vector field is presented in which inelegant features like negative terms in the energy do not make an appearance at any stage. All components of the field are handled in a completely symmetric fashion and the explicitly covariant appearance of the theory is preserved in the process of quantization as well as in earlier stages. Though the special features which arise when the mass vanishes are pointed out, a detailed treatment of that case is not included here and will be given separately.

I. INTRODUCTION

The basic field equations for free relativistic particles of spin 1 were formulated over thirty years ago in several equivalent forms. One of the most familiar, the spin-1 specialization of the general Fierz–Pauli form[1] employs a 4-vector field A^μ obeying the Klein–Gordon equation and a supplementary condition analogous to the Lorentz condition of electrodynamics[2]

$$(\partial^\mu\partial_\mu + m^2)A^\nu = 0, \tag{1a}$$

$$\partial_\nu A^\nu = 0. \tag{1b}$$

These equations follow directly from the Proca equations[3]

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu, \tag{2a}$$

$$\partial_\nu F^{\mu\nu} = m^2 A^\mu, \tag{2b}$$

which in turn are nothing but a special representation of the Kemmer equation[4] for spin 1. The familiar approach to the quantization of the vector field, as presented for example by Bogoliubov and Shirkov[5] treats (1a) as the basic field equation and (1b) merely as a supplementary condition, useful, to be sure, in getting rid of unwelcome terms with negative sign in the expression for the energy of the field, but a nuisance where quantization is concerned: It necessitates the elimination of one of the four components A^μ in a manner which destroys *manifest* covariance in order to arrive at three independent quantities on which quantum conditions can be imposed. The final result is of course again manifestly covariant. This procedure does not lead one into any conceptual difficulties but it is quite inelegant—unnecessarily so, as we shall see. Part of the reason for presenting a new approach to this old problem is thus aesthetic. But the main interest lies in the guidelines it provides towards a more satisfactory handling of a problem which does pose conceptual difficulties, namely the theory of the massless vector field. The application to the latter will be dealt with in a separate paper in view of important differences in matters of detail between the massive and massless cases.

Our starting point will be the field equations in Proca form or, rather, the equation

$$(\partial^\mu\partial_\mu + m^2)A^\nu - \partial^\nu\partial_\mu A^\mu = 0 \tag{3}$$

resulting from the substitution of Eq. (2a) in (2b). Equation (3) is obtainable from the Lagrangian density

$$\mathfrak{L} = -\tfrac{1}{4}(\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu) + m^2 A_\mu A^\mu, \tag{4}$$

by applying the usual variational procedure with respect to the field variables A^μ. It is important to note that this equation is equivalent to both of Eqs. (1), when $m \neq 0$. For $m = 0$, it does not imply the two separate equations (1a) and (1b), nor do the Maxwell equations. In fact, Eq. (3) with $m = 0$ is precisely what one obtains from the Maxwell field equations on expressing the electric and magnetic fields in terms of the potentials A^μ.

What we will now show is that by taking advantage of the content of Eq. (3) as it stands, avoiding an artificial separation into two equations of unequal status (one "field equation" and one "supplementary condition"), it becomes possible to lay down a quantization procedure which is manifestly covariant all the way and is elegant in that no unsymmetric elimination of components, for example, will be involved.

II. THE PLANE-WAVE SOLUTIONS

The essential step consists in expressing the A^μ in terms of the appropriate plane-wave solutions of (3). For a plane wave characterized by the propagation 4-vector $k \equiv (k^0, \mathbf{k})$, one has

$$[(k^2 - m^2)\delta^\nu_\mu - k^\nu k_\mu]A^\mu(k) = 0. \tag{5}$$

Here $k^2 = k_\rho k^\rho$. We have used the same symbol A^μ for the field in the configuration space as well as for its momentum-space counterpart which appears in (5). The argument k will be always explicitly indicated in the latter case to avoid confusion.

Viewing (5) as a matrix equation,

$$M^\nu_\mu A^\mu(k) = 0 \tag{6a}$$

with

$$M^{\nu}_{\mu} = (k^2 - m^2)\delta^{\nu}_{\mu} - k^{\nu}k_{\mu}, \tag{6b}$$

we observe that admissible 4-vectors $A^{\mu}(k)$ *must be eigenvectors belonging to zero eigenvalues of* M. Now, it is a simple matter to verify that the eigenvalues of M are

$$(k^2 - m^2), \quad \text{3-fold and } -m^2 \text{ once.} \tag{7}$$

At this point it is necessary to distinguish between massive and massless vector fields.

A. Case (i): $m = 0$

It is clear that in this case M can have zero eigenvalues and hence can lead to nontrivial solutions for (5) or (6a) only if the 4-vector k^{μ} is such that

$$k^2 = m^2. \tag{8}$$

We will therefore take this to be true of the k^{μ} in terms of which M is defined. The eigenvectors, say $u_{(1)}$, $u_{(2)}$, and $u_{(3)}$, belonging to the three equal eigenvalues $k^2 - m^2 = 0$ can now be verified to be determined by

$$k_{\mu}u^{\mu}_{(i)} = 0, \quad i = 1, 2, 3. \tag{9}$$

The remaining eigenvector, say $u^{\mu}_{(0)}$, belonging to the nonzero eigenvalue $-m^2$ cannot be a solution of (5), but it is nevertheless useful to note its explicit form

$$u^{\mu}_{(0)} = k^{\mu}/m, \tag{10}$$

including a convenient normalization factor $1/m$. The general solution of (5) is[6]

$$A^{\mu}(\mathbf{k}) = \sum_{i=1}^{3} a_i u^{\mu}_{(i)}. \tag{11}$$

It should be observed that Eqs. (8) and (9) as applied to (11) are nothing but the two equations (1).

For the further development of the theory we need the following properties of the vectors $u^{\mu}_{(\alpha)}$, $\alpha = 0, 1, 2, 3$. First, since the $u^{\mu}_{(i)}$, according to (9), are orthogonal to the timelike vector k^{μ}, they can be chosen to be real, mutually orthogonal, and spacelike, and hence normalized according to

$$u_{(i)\mu}u^{\mu}_{(j)} = -\delta_{ij}. \tag{12a}$$

Further, from (8) and (10),

$$u_{(0)\mu}u^{\mu}_{(0)} = 1 \tag{12b}$$

and, from (9) and (10),

$$u_{(0)\mu}u^{\mu}_{(i)} = 0. \tag{12c}$$

Thus we have, associated with any vector k^{μ} obeying (9), an orthonormal tetrad of vectors $u^{\mu}_{(\alpha)}$:

$$u_{(\alpha)\mu}u^{\mu}_{(\beta)} = \eta_{\alpha\beta},$$
$$\eta \text{ diag}, \ -\eta_{00} = \eta_{11} = \eta_{22} = \eta_{33} = -1, \tag{13}$$

which spans the 4-dimensional vector space. Their completeness can be expressed through the identity[7]

$$\delta^{\mu}_{\nu} = u^{\mu}_{(\alpha)}u^{(\alpha)}_{\nu} \equiv u^{\mu}_{(0)}u_{(0)\nu} - u^{\mu}_{(1)}u_{(1)\nu} - u^{\mu}_{(2)}u_{(2)\nu} - u^{\mu}_{(3)}u_{(3)\nu}. \tag{14}$$

We will have occasion to make good use of this identity in the sequel.

B. Case (ii): $m = 0$

In this case M has one zero eigenvalue $-m^2 = 0$, irrespective of what k^2 is, and so Eq. (5) has solutions violating the Klein–Gordon condition $k^2 = m^2 \equiv 0$. This solution, for $k^2 \neq 0$, is of the form $u^{\mu}_{(0)} \propto k^{\mu}$ and, clearly, it does not satisfy the Lorentz condition either.

For vectors k^{μ} with $k^2 = 0$, however, a new situation arises. All the four eigenvalues are now zero and since the matrix itself is nonzero, it is clearly nondiagonalizable. This is the special feature which leads to the complications (and, curiously enough, also shows the way out of them) in the case of the massless field. We reserve a detailed discussion of this case to a separate paper.[8,9]

III. QUANTIZATION

We are now in a position to exploit the fact established in the last section that all the four $A^{\mu}(k)$ can be expressed in a fully covariant way in terms of just three amplitudes a_i. Let us consider first the expressions for the total energy and momentum of the field in terms of these. The energy–momentum density tensor

$$T^{\mu}_{\nu} = \frac{\partial \mathfrak{L}}{\partial(\partial_{\mu}A_{\rho})}\partial_{\nu}A_{\rho} - \mathfrak{L}\delta^{\mu}_{\nu} \tag{15}$$

obtained from $\mathfrak{L}$, as given in Eq. (4), is

$$T^{\mu}_{\nu} = -(\partial^{\mu}A^{\rho} - \partial^{\rho}A^{\mu})\partial_{\nu}A_{\rho} - \mathfrak{L}\delta^{\mu}_{\nu} \tag{16}$$

and it can be symmetrized by making use of the equations of motion (3) and dropping a divergence term. The result (which we will continue to denote by T^{μ}_{ν}) is

$$T^{\mu}_{\nu} = (\partial^{\mu}A^{\rho} - \partial^{\rho}A^{\mu})(\partial_{\rho}A_{\nu} - \partial_{\nu}A_{\rho}) + m^2A^{\mu}A_{\nu} - \mathfrak{L}\delta^{\mu}_{\nu}. \tag{17}$$

Now, decomposing the A^{μ} into plane waves

$$A^{\mu}(x) = (2\pi)^{-\frac{3}{2}}\int \frac{d^3k}{(2k^0)^{\frac{1}{2}}}\left[A^{\mu}(\mathbf{k})e^{-ik\cdot x} + A^{\mu *}(\mathbf{k})e^{ik\cdot x}\right] \tag{18}$$

and, introducing them into (17), we obtain, on integration of $T^{0\mu}$ over all space, the total energy–momentum vector

$$P^{\mu} = -\tfrac{1}{2}\int d^3k k^{\mu}[A^{\rho}(\mathbf{k})A^{*}_{\rho}(\mathbf{k}) + A^{*}_{\rho}(\mathbf{k})A^{\rho}(\mathbf{k})]. \tag{19}$$

Now, from the representation (11) for $A^\mu(k)$ and the orthonormality properties (12), we find that

$$A^\rho(\mathbf{k})A^*_\rho(\mathbf{k}) = \sum_{ij} a_i a_j^* u^\rho_{(i)} u_{(j)\rho} = -\sum_i a_i a_i^*, \quad (20)$$

so that we have for the total energy, for instance,

$$P^0 \equiv H = \tfrac{1}{2}\int d^3k k^0 \sum (a_i a_i^* + a_i^* a_i). \quad (21)$$

It is no surprise that this is positive definite as it stands.

It is now obvious that the quantization is to be carried out by requiring the independent amplitudes to obey the commutation relations

$$[a_i(\mathbf{k}), a_j^*(\mathbf{k}')] = \delta_{ij}\delta(\mathbf{k} - \mathbf{k}'), \quad (22)$$

with all other commutators vanishing. The commutator of $A^\mu(\mathbf{k})$ and $A^{\nu *}(\mathbf{k}')$ is then

$$[A^\mu(\mathbf{k}), A^{\nu *}(\mathbf{k}')] = \sum_{ij} u^\mu_{(i)} u^\nu_{(j)} [a_i(\mathbf{k}), a_j^*(\mathbf{k}')]$$
$$= \sum_i u^\mu_{(i)} u^\nu_{(i)} \cdot \delta(\mathbf{k} - \mathbf{k}'). \quad (23)$$

On raising the index ν in (14), we find that the sum occurring in the last expression is just

$$\sum_i u^\mu_{(i)} u^\nu_{(i)} = -g^{\mu\nu} + u^\mu_{(0)} u^\nu_{(0)} \equiv -\left(g^{\mu\nu} - \frac{k^\mu k^\nu}{m^2}\right). \quad (24)$$

It will be noticed that we have not had to make any particular choice (e.g., longitudinal and transverse in the 3-dimensional sense) of the vectors $u^\mu_{(i)}$. The result should be and is independent of any such choice.

From (24) we now recover the familiar commutator

$$[A^\mu(\mathbf{k}), A^{\nu *}(\mathbf{k}')] = -(g^{\mu\nu} - k^\mu k^\nu/m^2) \cdot \delta(k - k'), \quad (25)$$

which in turn leads to the well-known result[5]

$$[A_\mu(x), A_\nu(y)] = \left(g_{\mu\nu} + \frac{1}{m^2}\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\nu}\right) iD(x - y). \quad (26)$$

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Boundary-Value Problems for the Integro–Differential Equations of Nonlocal Wave Interaction. I*

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It is shown that the linear 2-point boundary-value problems for the integro–differential equations of nonlocal wave interaction may be reduced to Cauchy systems. This provides new equations for the study of solid state plasmas, electron–electron interactions, the anomalous skin effect, and helicon propagation near doppler-shifted cyclotron resonance. The Cauchy system is of analytic interest and computational utility.

1. INTRODUCTION

In the study of electromagnetic fields in metallic slabs and semiconductors of finite thickness we are led to certain integro–differential equations for the electric field. These equations have the form

$$\frac{d^2e(t)}{dt^2} + Ae(t) = \int_0^L k(|t - t'|)e(t')\,dt', \quad 0 \le t \le L,$$

where A is a constant. In addition, boundary conditions are specified at $t = 0$ and $t = L$. See the paper on the anomalous skin effect by Reuter and Sondheimer.[1] Three decisive papers[2–4] by Baraff provide additional references and an approach to the analysis through a Wiener–Hopf technique. Our approach is along different lines and grew out of studies in radiative transfer and control theory.

Now, from the representation (11) for $A^\mu(k)$ and the orthonormality properties (12), we find that

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It is shown that the linear 2-point boundary-value problems for the integro–differential equations of nonlocal wave interaction may be reduced to Cauchy systems. This provides new equations for the study of solid state plasmas, electron–electron interactions, the anomalous skin effect, and helicon propagation near doppler-shifted cyclotron resonance. The Cauchy system is of analytic interest and computational utility.

1. INTRODUCTION

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where A is a constant. In addition, boundary conditions are specified at $t = 0$ and $t = L$. See the paper on the anomalous skin effect by Reuter and Sondheimer.[1] Three decisive papers[2–4] by Baraff provide additional references and an approach to the analysis through a Wiener–Hopf technique. Our approach is along different lines and grew out of studies in radiative transfer and control theory.

At present, it is known that various 2-point boundary-value problems,[5,6] integral equations,[7,8] and variational problems[9,10] can be transformed into Cauchy systems, i.e., initial-value problems. Such transformations are of analytical interest. They are also of computational utility,[11,12] in view of the ability of modern computers to integrate large systems of ordinary differential equations subject to known initial conditions.[13]

The purpose of this paper is to show that another large class of functional equations—integro–differential equations—subject to boundary conditions can be transformed into Cauchy systems. Such integro–differential equations arise in modern physics in situations where nonlocal interactions must be considered.[1,2]

To expose the chain of reasoning involved, consider determining the function $u = u(t)$, $0 \leq t \leq c$, where u is a solution of the integro–differential equation

$$\ddot{u}(t) + Au(t) = \int_0^c k(|t - y|)u(y)\,dy, \quad 0 < t < c,$$

with, for simplicity, the boundary conditions

$$\dot{u}(0) = 0, \quad u(c) = 1.$$

The basic technique is to imbed the original problem in a class of problems and interconnect the solutions of neighboring members of the class.[14] In this instance, the interval length c is viewed not as a constant, but as an essential variable of the problem. The solution u is studied primarily as a function of the interval length. Our principal analytical tools are the principle of superposition for linear systems and the assumed uniqueness of solution of certain linear variational equations.

First the Cauchy problem is stated. This is followed by a derivation of the Cauchy problem from the boundary-value problem for the integro–differential equation. Next some numerical aspects are discussed. The concluding section is devoted to various extensions.

2. STATEMENT OF CAUCHY PROBLEM

Let the functions u and v be solutions of the linear 2-point boundary-value problem

$$\dot{u}(t, x) = v(t, x), \tag{1}$$

$$\dot{v}(t, x) + Au(t, x) = \int_0^x k(|t - y|)u(y, x)\,dy, \quad 0 \leq t \leq x \leq c, \tag{2}$$

$$v(0, x) = 0, \tag{3}$$

$$u(x, x) = 1, \tag{4}$$

where c is sufficiently small, the dot refers to differentiation with respect to t, and

$$k(p) = \int_a^b e^{-p/z'}w(z')\,dz', \quad p > 0. \tag{5}$$

Physical applications[4] suggest the form given in Eq. (5). The functions J and M are solutions of the system

$$\dot{J}(t, x, z) = M(t, x, z), \tag{6}$$

$$\dot{M}(t, x, z) + AJ(t, x, z) = e^{-(x-t)/z} + \int_0^x k(|t - y|)J(y, x, z)\,dy, \quad 0 \leq t \leq x, \quad a \leq z \leq b, \tag{7}$$

$$M(0, x, z) = 0, \tag{8}$$

$$J(x, x, z) = 0. \tag{9}$$

The functions e, r, α, and R are defined by means of the relations

$$e(x, v) = \int_0^x e^{-(x-y)/v}u(y, x)\,dy, \tag{10}$$

$$r(v, z, x) = \int_0^x e^{-(x-y)/v}J(y, x, z)\,dy, \tag{11}$$

$$\alpha(x, z) = M(x, x, z), \tag{12}$$

$$R(x) = v(x, x),^{15} \tag{13}$$

where

$$0 \leq x \leq c, \quad a \leq v, z \leq b.$$

Then the functions e, r, α, and R satisfy the Cauchy system

$$e_x(x, v) = 1 - v^{-1}e(x, v) - R(x)e(x, v) + \int_a^b r(v, z', x)w(z')\,dz', \tag{14}$$

$$e(0, v) = 0, \tag{15}$$

$$r_x(v, z, x) = -(v^{-1} + z^{-1})r(v, z, x) - \alpha(x, z)e(x, v), \tag{16}$$

$$r(v, z, 0) = 0, \tag{17}$$

$$\alpha_x(x, z) = 1 + \int_a^b r(z', z, x)w(z')\,dz' - \alpha(x, z)[z^{-1} + R(x)], \tag{18}$$

$$\alpha(0, z) = 0, \tag{19}$$

$$R_x(x) = -A + \int_a^b [e(x, z') + \alpha(x, z')] \times w(z')\,dz' - R^2(x), \tag{20}$$

$$R(0) = 0, \tag{21}$$

where

$$0 \leq x \leq c, \quad a \leq v, z \leq b.$$

Let t be a real number for which

$$0 \leq t \leq c. \tag{22}$$

At $x = t$, the initial conditions on the functions u, v, J, and M are

$$u(t, t) = 1, \tag{23}$$

$$v(t, t) = R(t), \tag{24}$$

$$J(t, t, z) = 0, \tag{25}$$

$$M(t, t, z) = \alpha(t, z). \tag{26}$$

For

$$x \geq t, \quad \text{and} \quad a \leq z \leq b,$$

the functions u, v, J, and M satisfy the differential equations

$$u_x(t, x) = -R(x)u(t, x) + \int_a^b J(t, x, z')w(z')\,dz', \tag{27}$$

$$v_x(t, x) = -R(x)v(t, x) + \int_a^b M(t, x, z')w(z')\,dz', \tag{28}$$

$$J_x(t, x, z) = -z^{-1}J(t, x, z) - \alpha(x, z)u(t, x), \tag{29}$$

$$M_x(t, x, z) = -z^{-1}M(t, x, z) - \alpha(x, z)v(t, x). \tag{30}$$

3. DERIVATION OF THE CAUCHY SYSTEM

Consider the differential–integral equations

$$\dot{u}(t, x) = v(t, x), \tag{31}$$

$$\dot{v}(t, x) + Au(t, x) = \int_0^x k(|t - y|)u(y, x)\,dy, \quad 0 \leq t \leq x, \tag{32}$$

where the dependent variables are subject to the inhomogeneous boundary conditions

$$v(0, x) = 0, \tag{33}$$

$$u(x, x) = 1. \tag{34}$$

It is assumed that the kernel k may be represented in the form

$$k(r) = \int_a^b e^{-r/z'}w(z')\,dz', \quad r > 0. \tag{35}$$

Differentiation with respect to x in Eqs. (31)–(34) yields the relations

$$\dot{u}_x(t, x) = v_x(t, x), \tag{36}$$

$$\dot{v}_x(t, x) + Au_x(t, x) = k(x - t)u(x, x) + \int_0^x k(|t - y|)u_x(y, x)\,dy, \quad 0 \leq t \leq x, \tag{37}$$

$$v_x(0, x) = 0, \tag{38}$$

$$\dot{u}(x, x) + u_2(x, x) = 0. \tag{39}$$

In Eq. (39), we have used the dot to represent partial differentiation of u with respect to the first argument and the subscript "2" to represent differentiation with respect to the second argument.

Introduce the functions Φ and Ψ as the solutions of the inhomogeneous differential–integral equations

$$\dot{\Phi}(t, x) = \Psi(t, x), \tag{40}$$

$$\dot{\Psi}(t, x) + A\Phi(t, x) = k(x - t) + \int_0^x k(|t - y|)\Phi(y, x)\,dy, \quad 0 \leq t \leq x, \tag{41}$$

and the homogeneous boundary conditions

$$\Psi(0, x) = 0, \tag{42}$$

$$\Phi(x, x) = 0. \tag{43}$$

Regard Eqs. (36)–(39) as an inhomogeneous system of differential-integral equations for the functions u_x and v_x subject to inhomogeneous boundary conditions. Use of the superposition principle for linear systems then provides the solution

$$u_x(t, x) = -\dot{u}(x, x)u(t, x) + u(x, x)\Phi(t, x), \tag{44}$$

$$v_x(t, x) = -\dot{u}(x, x)v(t, x) + u(x, x)\Psi(t, x), \quad x \geq t. \tag{45}$$

Equations (44) and (45) are viewed as ordinary differential equations for the functions u and v, where t is a fixed parameter and the independent variable is x, with $x \geq t$. The boundary condition in Eq. (34) disposes of $u(x, x)$. The functions Φ and Ψ, $-\dot{u}(x, x)$, and the initial conditions on the functions u and v at $x = t$ will now be considered.

Introduce the two new functions

$$J = J(t, x, z), \tag{46}$$

$$M = M(t, x, z), \quad 0 \leq t \leq x, \quad a \leq z \leq b, \tag{47}$$

as the solutions of the system

$$\dot{J}(t, x, z) = M(t, x, z), \tag{48}$$

$$\dot{M}(t, x, z) + AJ(t, x, z) = e^{-(x-t)/z} + \int_0^x k(|t - y|)J(y, x, z)\,dy, \quad 0 \leq t \leq x, \quad a \leq z \leq b, \tag{49}$$

$$M(0, x, z) = 0, \tag{50}$$

$$J(x, x, z) = 0. \tag{51}$$

In view of the representation for the kernel k in Eq. (35) and the Eqs. (40)–(43) for the functions Φ and Ψ, it is clear that the functions Φ and Ψ may be represented in terms of the functions J and M in the

form

$$\Phi(t, x) = \int_a^b J(t, x, z')w(z')\,dz', \tag{52}$$

$$\Psi(t, x) = \int_a^b M(t, x, z')w(z')\,dz', \quad 0 \le t \le x. \tag{53}$$

We now shift our attention to the determination of the functions J and M.

Through differentiation with respect to x, Eqs. (48)–(51) become

$$\dot{J}_x(t, x, z) = M_x(t, x, z), \tag{54}$$

$$\dot{M}_x(t, x, z) + AJ_x(t, x, z) = -z^{-1}e^{-(x-t)/z} + k(x - t)J(x, x, z) + \int_0^x k(|t - y|)J_x(y, x, z)\,dy, \tag{55}$$

$$M_x(0, x, z) = 0, \tag{56}$$

$$\dot{J}(x, x, z) + J_2(x, x, z) = 0. \tag{57}$$

Since

$$J(x, x, z) = 0$$

and

$$-\dot{J}(x, x, z) = -M(x, x, z),$$

it is seen that

$$J_x(t, x, z) = -z^{-1}J(t, x, z) - M(x, x, z)u(t, x), \tag{58}$$

$$M_x(t, x, z) = -z^{-1}M(t, x, z) - M(x, x, z)v(t, x), \tag{59}$$

where

$$x \ge t, \quad a \le z \le b.$$

Introduce the function α to be

$$\alpha(x, z) = M(x, x, z), \quad x \ge 0, \quad a \le z \le b. \tag{60}$$

It follows, from Eqs. (49) and (59), that

$$\alpha_x(x, z) = \dot{M}(x, x, z) + M_2(x, x, z) = -AJ(x, x, z) + 1 + \int_0^x k(x - y)J(y, x, z)\,dy - z^{-1}M(x, x, z) - M(x, x, z)v(x, x) \tag{61}$$

or

$$\alpha_x(x, z) = 1 + \int_0^x k(x - y)J(y, x, z)\,dy - \alpha(x, z)[z^{-1} + v(x, x)]. \tag{62}$$

It is now convenient to introduce the additional terminology that

$$r(v, z, x) = \int_0^x e^{-(x-y)/v}J(y, x, z)\,dy, \quad a \le v, z \le b, \quad x \ge 0, \tag{63}$$

and

$$R(x) = v(x, x), \quad x \ge 0.[16] \tag{64}$$

Again recalling the representation for the kernel k in Eq. (35), we write

$$\alpha_x(x, z) = 1 + \int_0^x \int_a^b e^{-(x-y)/z'}w(z')\,dz'J(y, x, z)\,dy - \alpha(x, z)[z^{-1} + R(x)]. \tag{65}$$

This becomes, finally,

$$\alpha_x(x, z) = 1 + \int_a^b r(z', z, x)w(z')\,dz' - \alpha(x, z)[z^{-1} + R(x)]. \tag{66}$$

Now we turn to the function r. Through differentiation of both sides of Eq. (63) with respect to x, we find that

$$r_x(v, z, x) = J(x, x, z) - v^{-1}r(v, z, x) + \int_0^x e^{-(x-y)/v}[-z^{-1}J(y, x, z) - \alpha(x, z)u(y, x)]\,dy. \tag{67}$$

Upon simplification, this last equation becomes

$$r_x(v, z, x) = -(z^{-1} + v^{-1})r(v, z, x) - \alpha(x, z)e(x, v), \tag{68}$$

where

$$e(x, v) = \int_0^x e^{-(x-y)/v}u(y, x)\,dy, \quad x \ge 0, \quad a \le v \le b. \tag{69}$$

We now obtain the differential equation for the function e. From Eq. (69), we see that

$$e_x(x, v) = u(x, x) - v^{-1}e(x, v) + \int_0^x e^{-(x-y)/v}[-\dot{u}(x, x)u(y, x) + u(x, x)\Phi(y, x)]\,dy. \tag{70}$$

In obtaining the above equation, use has been made of the differential equation for the function u in Eq. (44). From this it is seen that

$$e_x(x, v) = 1 - v^{-1}e(x, v) - R(x)e(x, v) + \int_0^x e^{-(x-y)/v}\Phi(y, x)\,dy. \tag{71}$$

Note that

$$\dot{u}(x, x) = v(x, x) = R(x). \tag{72}$$

The integral in Eq. (71) is transformed by employing Eq. (52). It becomes

$$\int_0^x e^{-(x-y)/v} \int_a^b J(y, x, z')w(z')\,dz'\,dy = \int_a^b w(z')\,dz' \int_0^x e^{-(x-y)/v}J(y, x, z')\,dy, \tag{73}$$

$$\int_0^x e^{-(x-y)/v}\Phi(y, x)\,dy = \int_a^b r(v, z', x)w(z')\,dz'. \tag{74}$$

The result is that the differential equation for the function e is

$$e_x(x, v) = 1 - v^{-1}e(x, v) - R(x)e(x, v) + \int_a^b r(v, z', x)w(z')\,dz', \quad a \le v \le b. \tag{75}$$

We now turn our attention to the function R, defined earlier to be

$$R(x) = v(x, x). \tag{76}$$

Differentiation shows that

$$\begin{aligned} R_x(x) &= \dot{v}(x, x) + v_2(x, x) \\ &= -Au(x, x) + \int_0^x k(x - y)u(y, x)\,dy \\ &\quad - \dot{u}(x, x)v(x, x) + \Psi(x, x)u(x, x) \\ &= -A + \int_0^x \int_a^b e^{-(x-y)/z'}w(z')\,dz'u(y, x)\,dy \\ &\quad - R^2(x) + \int_a^b M(x, x, z')w(z')\,dz' \\ &= -A + \int_a^b e(x, z')w(z')\,dz' \\ &\quad - R^2(x) + \int_a^b \alpha(x, z')w(z')\,dz'. \end{aligned} \tag{77}$$

The differential equations for the functions R, e, α, and r have now been obtained. They are contained in Eqs. (77), (75), (66), and (68). They hold for $x \ge 0$. Furthermore, from the definitions, it is seen that the initial conditions on these functions at $x = 0$ are

$$R(0) = 0, \tag{78}$$

$$e(0) = 0, \tag{79}$$

$$\alpha(0, z) = 0, \quad a \le z \le 1, \tag{80}$$

$$r(v, z, 0) = 0, \quad a \le v, z \le b. \tag{81}$$

In this way it is seen that the four auxiliary functions R, e, α, and r satisfy a Cauchy system.

Let t be a fixed nonnegative number. Then, for $x \ge t$, the differential equations for the functions J, M, u, and v are given in Eqs. (58), (59), (44), and (45). They may be written more conveniently in the form

$$J_x(t, x, z) = z^{-1}J(t, x, z) - \alpha(x, z)u(t, x), \tag{82}$$

$$M_x(t, x, z) = -z^{-1}M(t, x, z) - \alpha(x, z)v(t, x), \tag{83}$$

$$u_x(t, x) = -R(x)u(t, x) + \int_a^b J(t, x, z')w(z')\,dz', \tag{84}$$

$$v_x(t, x) = -R(x)v(t, x) + \int_a^b M\ t, x, z')w(z')\,dz', \quad x \ge t. \tag{85}$$

The initial conditions at $x = t$ are

$$J(t, t, z) = 0, \tag{86}$$

$$M(t, t, z) = \alpha(t, z), \quad a \le z \le b, \tag{87}$$

$$u(t, t) = 1, \tag{88}$$

$$v(t, t) = R(t). \tag{89}$$

This completes the derivation of the Cauchy system.

4. NUMERICAL ASPECTS

Previous experience with similar Cauchy systems[6,11,12] indicates that the method of lines[17] provides an effective means of solving such Cauchy systems numerically. Let us merely indicate its employment in the numerical solution of the Cauchy system for the functions R, e, α, and r in Eqs. (77), (75), (66), (68), and Eqs. (78)–(81). A suitable quadrature formula is used to approximate the integrals on the interval (a, b) that occur:

$$\int_a^b f(z')w(z')dz' \cong \sum_{i=1}^N f(z_i)c_i. \tag{90}$$

A low-order Gaussian quadrature formula has proved to be efficacious in similar circumstances.[11] In this instance the nodes $z_1, z_2, \cdots, z_N$ are the roots of the Nth-order polynomial in the system of orthogonal polynomials in the interval (a, b), and the numbers $c_1, c_2, \cdots, c_N$ are the corresponding Christoffel weights. For the interval $(0, 1)$, these numbers are tabulated[18] for $N = 3, 4, \cdots, 15$. We introduce the functions $e_i(x)$, $r_{ij}(x)$, and $\alpha_i(x)$ for $i, j, \cdots, N, x \ge 0$, by means of the equations

$$e_i(x) = e(x, z_i), \tag{91}$$

$$r_{ij}(x) = r(z_i, z_j, x), \tag{92}$$

$$\alpha_i(x) = \alpha(x, z_i). \tag{93}$$

The exact equations (77), (75), (66), and (68) are replaced by the approximate system

$$e_i'(x) = 1 - z_i^{-1}e_i(x) - R(x)e_i(x) + \sum_{m=1}^N r_{im}c_m, \tag{94}$$

$$r_{ij}'(x) = -(z_i^{-1} + z_j^{-1})r_{ij}(x) - \alpha_j(x)e_i(x), \tag{95}$$

$$\alpha_i'(x) = 1 + \sum_{m=1}^N r_{mi}c_m - \alpha_i(x)[z_i^{-1} + R(x)], \tag{96}$$

$$R'(x) = -A + \sum_{m=1}^N [e_m(x) + \alpha_m(x)]c_m - R^2(x), \quad i, j = 1, 2, \cdots, N, \quad x \ge 0. \tag{97}$$

The initial conditions, of course, are

$$e_i(0) = 0, \tag{98}$$

$$r_{ij}(0) = 0, \tag{99}$$

$$\alpha_i(0) = 0, \tag{100}$$

$$R(0) = 0, \tag{101}$$

for $i, j = 1, 2, \cdots, N$. Such systems of $N^2 + 2N + 1 = (N + 1)^2$ ordinary differential equations subject to known initial conditions are readily solved numerically on modern computing machines for $N \leq 50$.

The functions R, e, α, and r could be produced numerically and stored. Then the Cauchy system in Eqs. (82)–(89) for the functions J, M, u, and v could be handled similarly. Actually, it is simpler to adjoin the differential equations and initial conditions for the functions J, M, u, and v to the differential equations for the functions R, e, α, and r at $x = t$ and integrate the entire system to $x = c$.[10] In the event that values of the functions u and v are required for $t = t_1, t_2, \cdots, t_M$ each time $x = t_i$, $i = 1, 2, \cdots, M$, an appropriate system of ordinary differential equations corresponding to Eqs. (82)–(85) is adjoined, together with the initial conditions.

5. DISCUSSION

In subsequent papers in this series, we shall extend and apply the theory presented here in several ways. First, we must show that the solution of the Cauchy system actually provides the solution of the boundary value problem for the integro-differential equation. This amounts to establishing the converse of the theorem in Sec. 2 and will be given for more general boundary conditions than those considered here or in the papers by Baraff. Secondly, results of numerical experiments will be presented. Thirdly, certain nonlinear integro-differential equations will be treated.[19] Next the invariant imbedding approach to the eigenvalue problem will be given.[20] Lastly, physical interpretations of the new equations of the Cauchy system must be provided.

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Differential Forms and Maxwell's Field: An Application of Harmonic Integrals

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Maxwell's equations are derived under the assumption of 4-dimensionality of Euclidean space from a somewhat different definition of time from that considered by Einstein, using differential forms and de Rham's theorem in the theory of harmonic integrals. It is shown that the continuity equation of the current density is an elementary consequence of the Jordan–Brouwer theorem of topology under the requirement of integrability of the field. Matter appears as a singular point of the field, and introduces various kinds of "currents," in the sense of de Rham and Kodaira, according to the topological character of the domain of integration of the field. These "currents" describe characters of the material, and are represented not by ordinary functions, but by generalized functions in the Schwartz sense. Examples of these "currents," such as electric and magnetic polarizations and the supercurrent, are given, and the origin of the fundamental difficulties with dimensions in the usual theory of electromagnetism is attributed to this fact.

I. INTRODUCTION

Flanders[1] has suggested that differential forms are more powerful than the usual tensor analysis. In the introduction of his book he indicates the various weak points of the latter. For example, he says, "in classical tensor analysis, one never knows what is the range of applicability simply because one is never told what the space is. Everything seems to work in a coordinate patch, but we know this is inadequate for most applications." Another important point is the fact that, while tensor analysis is founded on the transformation of the coordinate frames, the theory of differential forms needs no such transformation in its foundation. In physical language, tensor analysis needs two observers, but the differential forms need only one observer. Therefore, the latter has the possibility of eliminating coordinate transformations between different observers.

In this paper, we show that this idea can, in fact, be realized for the problem of light. Furthermore, we show that this elimination enables us to derive Maxwell's equations from the invariance of the speed of light, using de Rham's theorem of harmonic integrals (Sec. V). The present derivation also gives some useful information on the way one can take into account the topological character of the domain of integration of the field (Secs. V and VI).

In Sec. II, we begin with a criticism of Einstein's theory of relativity. We introduce the differential forms in Sec. III. In Sec. IV, we write Maxwell's equations using differential forms according to Flanders. In Sec. VI we briefly discuss electric and magnetic polarizations in connection with the problem of dimensions in electromagnetism and the persistent current in a superconducting ring.

II. THE PHYSICAL MOTIVE

A. Criticism of Einstein's Concept of Time

Though it is true that Einstein's theory of relativity[2] (TR) is one of the most fascinating parts of physics, it still has some difficult points which we discuss in the following.

(A) In TR, two clocks at different points are set by using the concept of the velocity of light. However, this concept cannot logically be defined without setting the clocks. In other words, the definition of time in TR is circular. In order to define the concept of time, we must not use the concept of velocity.

(B) In TR, it is assumed that in every Lorentz frame (LF) we can use the "same" measure; this assumption means that we can take the unit of spatial distance which is common to all LF's. However, this assumption can never be justified because, to examine whether the two measures are the same or not, we must place them on a single LF, as Einstein says.[2] The two measures of different LF's can never be placed on the single LF because of their definition. In other words, there exists no way to investigate whether the two units of different LF's are the same or not.

(C) In TR, it is assumed that the quantity

$$(\Delta s)^2 \equiv (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2 - (c\Delta t)^2$$

is invariant for all LF's. However, this assumption is meaningless because, as we have shown in argument (B), we have no guarantee that we are able to take units of distance and time[3] common to all LF's. The concepts of absolute units of distance and time must be given up.

These three defects can be eliminated only if we remember that the distance traveled by light in a

vacuum defines the concept of time T to the observer and that the fundamental relation for light is not the invariance of the quantity $(\Delta s)^2$, but, accordingly, the invariance of the equation

$$(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2 - (\Delta T)^2 = 0. \qquad (1)$$

Here it is to be noted that nothing is mentioned about the state of the light emitter, whether it is moving or not, because these concepts can be rigorously defined only after the concept of time has been resolved. According to this definition, the time interval required during which light advances, in a vacuum, from one spatial point to another is measured by the spatial distance between these two points. If the unit of distance changes, then the unit of time also changes. However, the ratio c of the interval of space to that of time which is required for light to pass through the former is always constant even if the unit of distance should change; this means that, in a vacuum, the velocity of light c is independent of the motion of the light emitter.[4] Thus, one of the basic postulates in TR follows from our new definition of time. Equation (1) is the mathematical expression of the definition in an isotropic Euclidean space (x, y, z, T). In the units used in Eq. (1), we have $c = 1$, but we know experimentally the value of c in the cgs system, in which the units of length and time t are decided separately; i.e., originally, the former referred to the meridian of the earth and the latter to its revolution around the sun:

$$c = 3 \times 10^{10}\ \text{cm/sec}, \quad T = ct = 3 \times 10^{10} t.$$

In the following, we explain the basic idea of the derivation of Maxwell's equations based on Eq. (1).

B. The Basic Idea of Maxwell's Equations

In argument (C) above we showed that there exists no way to investigate whether the quantity $(\Delta s)^2$ is invariant for all LF's or not. However, according to our definition of time, relation (1), i.e., $(\Delta s)^2 = 0$, for the wavefront of light still has it own meaning for every observer, because this relation is homogeneous with respect to the quantities x, y, z, and t. Therefore, a change of units implies simply the multiplication of the entire left-hand side of this equation by some constant number. By the same reason, only the homogeneous equation with respect to the variables x, y, z, and t can be adopted as the equation representing the property of light. Therefore, it can be represented in the form of a differential equation as[5]

$$\Box\phi \equiv \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi = 0. \qquad (2)$$

Here, if we use the invariance of the quantity $(\Delta s)^2$ instead of the invariance of Eq. (1), then we can never take the right-hand side of Eq. (2) to be zero. Equation (2) is second-order homogeneous partial differential equation, and, therefore, we have two linearly independent solutions ϕ on which we do not have any kind of boundary conditions to impose at this stage. Instead of considering that we have two independent solutions for Eq. (2), we can formally regard that we have four solutions ϕ_μ, $\mu = 1, 2, 3, 4$, for this equation, which are mutually dependent by the additional two independent conditions which we seek. Let us call these solutions ϕ_μ the 4-component potential. It is to be noted that these conditions are also necessarily homogeneous because they must be form invariant to the observer, whom we can choose arbitrarily. We seek these conditions in the following. Thus far, we have implicitly omitted from our consideration the location of the light emitters; these places are formally represented as the singular points of the potential ϕ_μ with respect to the observer. Let the values of the quantities $(-c/4\pi)\Box\phi_\mu$ at these singular points be formally equal to some prescribed values J_μ with respect to the observer; we call this quantity $J_\mu(x, y, z, t)$ the 4-current density with respect to him. Of course, in the nonsingular region, the value of the density $J_\mu(x, y, z, t)$ is equal to zero. Thus we have the following equations:

$$\Box\phi_\mu = (-4\pi/c)J_\mu, \quad \mu = 1, 2, 3, 4; \qquad (3)$$

these equations with two additional independent conditions completely represent the behavior of light in the space–time continuum which formally include the singular points. It is to be noted that Eqs. (3) are just for some particular observer because these equations are not homogeneous in a different way from Eq. (2); however, this observer can be chosen arbitrarily with a corresponding change of the contents of the density J_μ. As for the additional two conditions, we can take the following two mutually independent homogeneous equations, one of which refers to the nonsingular region and the other to the singular region:

$$\frac{\partial\phi_\mu}{\partial x_\mu} = 0 \qquad (4a)$$

and

$$\frac{\partial J_\mu}{\partial x_\mu} = 0, \qquad (4b)$$

where $x_4 = ict$ and the summation convention over μ is used. In order to rewrite Eqs. (4) using real variables, we need only write the potential ϕ_μ and

the current density J_μ as $(\mathbf{A}, i\phi)$ and $(\mathbf{J}, ic\rho)$, respectively. Thus, we can find that Eqs. (4) represent the Lorentz condition and the continuity of the current density in the ordinary electromagnetic field theory. If we call the quantities

$$E_j \equiv \frac{1}{i}\left(\frac{\partial \phi_j}{\partial x_4} - \frac{\partial \phi_4}{\partial x_j}\right) \quad \text{and} \quad H_j \equiv \frac{\partial \phi_l}{\partial x_k} - \frac{\partial \phi_k}{\partial x_l}, \quad (5)$$

where $j = 1, 2, 3$ and (j, k, l) is their cyclic permutation, the electric and magnetic fields, respectively, then Eqs. (3) can be transformed by applying the conditions (4) to the usual Maxwell equations for the fields $\mathbf{E}$ and $\mathbf{H}$.[6] Actually, conditions (4) are needed only in the derivation of their inhomogeneous part; the homogeneous part follows directly from the definitions (5) alone. In Sec. V, we clarify the fundamental reason for this fact.

It is to be noted that, in the above discussions of the derivation of Maxwell's equations, we need not to introduce the concept of LF.

III. THE CALCULUS OF DIFFERENTIAL FORMS

In the preceding section, we derived Maxwell's equations for $\mathbf{E}$ and $\mathbf{H}$ from the invariance of Eq. (1) in an illuminating way. The subsequent sections are devoted to the more rigorous mathematical formulation and generalization of the idea. In this section, we explain the calculus of differential forms[1] in order to introduce Flanders' idea[1] of Maxwell's equations in the next section.

Let P be a point in an n-dimensional Euclidean space E^n. The 1-forms at P are the expressions

$$\sum_1^n a_i\, dx^i,$$

with the a_i constant. These form an n-dimensional linear space $L = L_P$. The p-forms at P are the elements of

$$\bigwedge^p L = \bigwedge^p L_P, \quad p \leq n,$$

i.e., the p-forms are the expressions

$$\sum a_H\, dx^{h_1} \cdots dx^{h_p},$$

with the a_H constant and $H = (h_1, \cdots, h_p)$. Here, the multiplication of differentials $dx^i\, dx^j$ means the exterior product $dx^i \wedge dx^j$ and obeys the following rules:

$$\begin{aligned}
(a_1\alpha_1 + a_2\alpha_2) \wedge dx^i - a_1(\alpha_1 \wedge dx^i) - a_2(\alpha_2 \wedge dx^i) &= 0,\\
dx^i \wedge (a_1\alpha_1 + a_2\alpha_2) - a_1(dx^i \wedge \alpha_1) - a_2(dx^i \wedge \alpha_2) &= 0,\\
dx^i \wedge dx^i &= 0,\\
dx^i \wedge dx^j + dx^j \wedge dx^i &= 0,
\end{aligned} \quad (6)$$

where the quantities α_j denote any one of the basis vectors dx^i, $i = 1, \cdots, n$, of L_P or any linear combination of them and the a_j are real numbers. If dx^i and $dx^j, j \neq i$, are dependent, say $dx^j = a\, dx^i$, then

$$dx^i \wedge dx^j = a(dx^i \wedge dx^i) = 0$$

according to our reductions. Otherwise, $dx^i \wedge dx^j \neq 0$. Furthermore, we have the following relations for the p-forms:

$$\begin{aligned}
(a_1\alpha_1 + a_2\alpha_2) \wedge dx^2 \wedge \cdots \wedge dx^p &\\
= a_1(\alpha_1 \wedge dx^2 \wedge \cdots \wedge dx^p) &\\
+ a_2(\alpha_2 \wedge dx^2 \wedge \cdots \wedge dx^p), &
\end{aligned} \quad (7a)$$

which is the same if any dx^i is replaced by a linear combination;

$$\alpha_1 \wedge \cdots \wedge \alpha_p = 0 \quad (7b)$$

if $\alpha_i = \alpha_j$ for some pair of indices $i \neq j$;

$$\alpha_1 \wedge \cdots \wedge \alpha_p \quad (7c)$$

changes sign if any two α_i are interchanged. We multiply a p-form λ by a q-form μ to obtain a $(p+q)$-form $\lambda \wedge \mu$ (which is zero by definition if $p + q > n$):

$$\wedge : (\bigwedge^p L) \times (\bigwedge^q L) \to \bigwedge^{p+q} L.$$

The basic properties of this exterior product are

$$\lambda \wedge \mu \text{ is distributive}, \quad (8a)$$

$$\lambda \wedge (\mu \wedge \nu) = (\lambda \wedge \mu) \wedge \nu, \text{ the associative law}, \quad (8b)$$

$$\mu \wedge \lambda = (-1)^{p \cdot q} \lambda \wedge \mu. \quad (8c)$$

Now let U denote an (open) domain in E^n. A p-form on U is obtained by choosing at each point P of U a p-form at that point, and doing this smoothly. Thus, a p-form ω has the representation

$$\omega = \sum a_H(x^1, \cdots, x^n)\, dx^H,$$

where the functions $a_H(\mathbf{x})$ are smooth functions on U, differentiable as often as we please.

The exterior algebra applies at each point of U and so may be interpreted on the differential forms on U itself. Thus, if ω is a p-form and η is a q-form in U, then $\omega \wedge \eta$ is a $(p+q)$-form on U. (Of course, $\omega \wedge \eta = 0$ if $p + q > n$.) If

$$\omega = \sum a_H\, dx^H, \quad \eta = \sum b_K\, dx^K,$$

then

$$\omega \wedge \eta = \sum a_H b_K\, dx^H\, dx^K,$$

so that the coefficients of $\omega \wedge \eta$ are again smooth functions, polynomials in the coefficients of ω and η.

We denote by $F^p(U)$ the totality of p-forms on U. In particular, $F^0(U)$ is simply the set of all smooth

functions on U. We can prove[1] the existence and uniqueness of an operator d, which takes each p-form ω to a $(p+1)$-form $d\omega$,

$$d: F^p(U) \to F^{p+1}(U),$$

such that

$$d(\omega + \eta) = d\omega + d\eta, \tag{9a}$$

$$d(\omega \wedge \eta) = d\omega \wedge \eta + (-1)^{(\deg \omega)}\omega \wedge d\eta, \tag{9b}$$

for each ω,

$$d(d\omega) = 0, \tag{9c}$$

for each function f,

$$df = \sum \frac{\partial f}{\partial x^i} dx^i. \tag{9d}$$

The operator d, called the exterior derivative, is completely independent of coordinate systems, and subsumes the ordinary gradient, rotation, and divergence. Property (9c) is nothing more than the equality of mixed second-order partial derivatives. It is the source of most "integrability conditions" of partial differential equations. It is usually referred to as the Poincaré lemma. We can prove[1] the following theorem, the converse of the Poincaré lemma.

Theorem: Let U be a domain in E^n which can be deformed to a point. Let ω be a $(p+1)$-form on U such that $d\omega = 0$, then there exists a p-form α on U such that

$$\omega = d\alpha.$$

It can also be shown that if $p \geq 1$, given one solution α, then the general solution is $\alpha + d\lambda$, where a $(p-1)$-form λ is absolutely arbitrary. (When $p = 0$, $d\lambda$ is constant.)

These results are used in the next section.

IV. MAXWELL'S EQUATIONS IN DIFFERENTIAL FORM

It is necessary to introduce inner products into differential forms, to discuss our subject. An inner product (α, β) of a space L is a real-valued function on $L \times L$ which is

(i) linear in each variable, (10a)

(ii) symmetric: $(\alpha, \beta) = (\beta, \alpha)$, (10b)

(iii) nondegenerate: if for fixed α, $(\alpha, \beta) = 0$ for all β, then $\alpha = 0$. (10c)

An orthonormal basis of L consists of a basis $\sigma^1, \cdots, \sigma^n$ such that

$$(\sigma^i, \sigma^j) = \pm\delta^{ij}.$$

If there are r plus signs and s minus signs, then $r + s = n$, and $t = r - s$ is the signature of the inner product. It does not depend on the choice of basis. It can be proved[1] that each inner product space has an orthonormal basis. We can also prove[1] the following basic property of inner-product spaces which we need below.

Theorem: Let f be a linear functional on L. Then there exists a unique vector β in L such that

$$f(\alpha) = (\alpha, \beta).$$

Next, we define an induced inner product on each of the spaces $\bigwedge^p L$. We set

$$(\lambda, \mu) = |(\alpha_i, \beta_j)|$$

for $\lambda = \alpha_1 \wedge \cdots \wedge \alpha_p$ and $\mu = \beta_1 \wedge \cdots \wedge \beta_p$, where the right-hand side denotes the determinant. It is easily seen that this definition satisfies requirements (10).

We shall define an operation $*$, called the Hodge star operator. We now fix λ in $\bigwedge^p L$. The mapping

$$\mu \to \lambda \wedge \mu, \quad \mu \in \bigwedge^{n-p} L,$$

is a linear transformation on $\bigwedge^{n-p} L$ into the 1-dimensional[7] space $\bigwedge^n L$. We may write

$$\lambda \wedge \mu = f_\lambda(\mu)\sigma,$$

where f_λ is a linear functional on $\bigwedge^{n-p} L$ and σ is an orthonormal basis of $\bigwedge^n L$. By the fact stated above, there exists a unique $(n-p)$-form, which we denote $*\lambda$ to indicate its dependence on λ, such that

$$\lambda \wedge \mu = (*\lambda, \mu)\sigma.$$

This equation defines the $*$ map which is evidently linear on $\bigwedge^p L$ into $\bigwedge^{n-p} L$. Let $\sigma^1, \cdots, \sigma^n$ be an orthonormal basis of L and $\sigma^H = \sigma^1 \wedge \sigma^2 \wedge \cdots \wedge \sigma^p$, $\sigma^K = \sigma^{p+1} \wedge \cdots \wedge \sigma^n$. It is then easily shown[1] that

$$*\sigma^K = (-1)^{p(n-p)}(\sigma^H, \sigma^H)\sigma^H. \tag{11}$$

Thus, we are ready to rewrite Maxwell's equations using differential forms.[1] Maxwell's equations in ordinary vector notation are

$$\text{rot } \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} \text{ (Faraday's law of induction)}, \tag{12a}$$

$$\text{rot } \mathbf{H} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} \quad \text{(Ampère's law)}, \tag{12b}$$

$$\text{div } \mathbf{D} = 4\pi\rho \quad \text{(true charge)}, \tag{12c}$$

$$\text{div } \mathbf{B} = 0 \quad \text{(nonexistence of true magnetism)}. \tag{12d}$$

Here, c is the speed of light. We put these equations into the language of exterior forms. To this end, we set

$$\begin{aligned}\alpha &= (E_1\,dx^1 + E_2\,dx^2 + E_3\,dx^3)(c\,dt)\\ &\quad + (B_1\,dx^2\,dx^3 + B_2\,dx^3\,dx^1 + B_3\,dx^1\,dx^2),\\ \beta &= -(H_1\,dx^1 + H_2\,dx^2 + H_3\,dx^3)(c\,dt)\\ &\quad + (D_1\,dx^2\,dx^3 + D_2\,dx^3\,dx^1 + D_3\,dx^1\,dx^2),\\ \gamma &= (J_1\,dx^2\,dx^3 + J_2\,dx^3\,dx^1 + J_3\,dx^1\,dx^2)\,dt\\ &\quad - \rho\,dx^1\,dx^2\,dx^3.\end{aligned} \tag{13}$$

It can easily be seen that the homogeneous equations (12a) and (12d) become

$$d\alpha = 0 \tag{14}$$

and the inhomogeneous equations (12b) and (12c) become

$$d\beta + 4\pi\gamma = 0. \tag{15}$$

Applying d to this last equation yields

$$d\gamma = 0; \tag{16}$$

using vector notation, we obtain the equation of continuity

$$\operatorname{div}\mathbf{J} + \frac{\partial\rho}{\partial t} = 0. \tag{16'}$$

From Eq. (14) one concludes that, at least in any region of space–time which can be shrunk to a point, there exists a 1-form λ such that

$$d\lambda = \alpha. \tag{17}$$

We introduce the vector potential $\mathbf{A}$ and a scalar A_0 by writing

$$\lambda = A_1\,dx^1 + A_2\,dx^2 + A_3\,dx^3 - A_0 c\,dt. \tag{18}$$

Equation (17) in vector form is

$$\begin{aligned}\operatorname{rot}\mathbf{A} &= \mathbf{B},\\ -\operatorname{grad}A_0 - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} &= \mathbf{E}.\end{aligned} \tag{19}$$

In free space, everything simplifies according to

$$\mathbf{E} = \mathbf{D},\quad \mathbf{H} = \mathbf{B},\quad \mathbf{J} = 0,\quad \rho = 0.$$

We introduce the metric into 4-space, whereby dx^1, dx^2, dx^3, $c\,dt$ form an orthonormal basis:

$$\begin{aligned}(dx^i, dx^j) &= \delta^{ij},\quad (dx^i, c\,dt) = 0,\\ (c\,dt, c\,dt) &= -1.\end{aligned} \tag{20}$$

The signature is $3 - 1 = 2$. According to formula (11),

$$\begin{aligned}*(dx^1\,dx^2) &= -dx^3(c\,dt),\quad \text{etc.},\\ *(dx^1 c\,dt) &= dx^2\,dx^3,\quad \text{etc.}\end{aligned} \tag{21}$$

We see that

$$\begin{aligned}\alpha &= (E_1\,dx^1 + \cdots)(c\,dt) + (H_1\,dx^2\,dx^3 + \cdots),\\ \beta &= -(H_1\,dx^1 + \cdots)(c\,dt) + (E_1\,dx^2\,dx^3 + \cdots)\\ &= *\alpha.\end{aligned}$$

Consequently, Maxwell's equations in free space are simply

$$d\alpha = 0$$

and

$$d*\alpha = 0. \tag{22}$$

V. DERIVATION OF MAXWELL'S EQUATIONS: AN APPLICATION OF DE RHAM'S THEOREM

In the preceding section, we rewrote the usual Maxwell equations (12) as Eqs. (13)–(15), according to Flanders. Thus, the derivation of the Maxwell equations reduces to that of Eqs. (14) and (15). In other words, our task is to derive these equations from the invariant equation (1).

We introduce the Laplacian operator.[1] Let f be a function on E^n. Then the Laplacian Δf of a 0-form f is defined as

$$d*df = (\Delta f)\sigma, \tag{23}$$

where σ is the volume element $\sigma^1 \wedge \sigma^2 \wedge \cdots \wedge \sigma^n$.

In the following, we introduce theorems[1] without their proofs on the integration of forms over a manifold, which are needed later because we consider also the singular points of differential forms.[8]

Stokes' Theorem: Let ω be a p-form on a manifold M and $\mathbf{c}$ a $(p+1)$-"chain." Then we have

$$\int_{\partial\mathbf{c}}\omega = \int_{\mathbf{c}} d\omega, \tag{24}$$

where $\partial\mathbf{c}$ denotes the "boundary" of the chain $\mathbf{c}$.

Stokes' theorem is the generalization of Gauss', Green's, and Stokes' theorems in ordinary vector analysis.

A "closed form" is a differential form ω on M satisfying $d\omega = 0$. An "exact form" is a differential form ω on M satisfying $\omega = d\eta$ for some form η on M; in this case, ω is integrable on M.

To each p-"cycle" $\mathbf{z}$ on M, i.e., a p-chain $\mathbf{z}$ which has no boundary, $\partial\mathbf{z} = 0$, there corresponds a "period" $\int_{\mathbf{z}}\omega$ of ω.

De Rham's First Theorem: A closed form is exact if and only if all of its periods vanish.

De Rham's Second Theorem: Suppose that to each p-cycle $\mathbf{z}$ there is assigned a number per $(\mathbf{z})$ subject

to the consistency relations that whenever

$$\sum a_i \mathbf{z}_i = \text{boundary}, \tag{25a}$$

then

$$\sum a_i \,\text{per}\,(\mathbf{z}_i) = 0. \tag{25b}$$

Then there exists a closed form ω on M which has the assigned periods

$$\int_{\mathbf{z}} \omega = \text{per}\,(\mathbf{z}) \quad \text{for each } p\text{-cycle } \mathbf{z}. \tag{26}$$

Thus, we are ready to proceed to the derivation of Maxwell's equations from Eq. (1). Equation (1) shows, in the limit of $\Delta x^i \to dx^i$, $i = 1, 2, 3$, and $\Delta t \to dt$, the dependence of the differential dt on dx^i. Therefore, we have the following physical requirement of our 1-forms, as is seen from the definition of the exterior product:

$$dx \wedge dy \wedge dz \wedge dt = 0. \tag{27}$$

It is to be emphasized that requirement (27) does not follow from the invariance of the quantity $(\Delta s)^2$, which is used in the theory of Lorentz transformations.

Because of the 4-dimensionality of our space (x, y, z, t) and requirement (27), the differential forms of highest degree which we must integrate are those of 3-form. Let ω_3 be one such 3-form; then $d\omega_3 = 0$ on E^4 because of the requirement (27). De Rham's first theorem guarantees the integrability of ω_3 on our space E^4, provided all of its periods vanish. We show in the following that this condition in the presence of a singular point can be interpreted as the continuity equation of the current density, i.e., Eq. (4b). The period of ω_3 is defined as $\int_{\mathbf{z}_3} \omega_3$, where $\mathbf{z}_3$ is a 3-cycle in E^4. By the Jordan–Brouwer theorem[9] of topology, $\mathbf{z}_3$ decomposes E^4 into exactly two regions, the inside M and the outside. In other words, any 3-cycle $\mathbf{z}_3$ is a boundary in our space, i.e., $\mathbf{z}_3 = \partial M$. Thus, if there exists no singular point in E^4, then all periods of ω_3 are zero according to Stokes' theorem. Therefore, by de Rham's first theorem, ω_3 is exact, i.e., integrable on E^4 in this case. However, if there exists a singular point P_0 in E^4, we must modify the argument. The "period" of a form around a singular point can be represented[10] not by the class of ordinary functions, but by that of generalized functions in the Schwartz sense.[11] Let this "period" be called the "current" according to de Rham.[10,12] Thus, we have the following formal equation which includes the singular point:

$$\omega_3 = \omega_3', \tag{28}$$

where ω_3' is a 3-form whose components can be represented by the generalized functions J_i and ρ:

$$\omega_3' = -4\pi(J_1\, dx^2\, dx^3 + J_2\, dx^3\, dx^1 + J_3\, dx^1\, dx^2)\, dt + 4\pi\rho\, dx^1\, dx^2\, dx^3. \tag{29}$$

Thus, the vanishing of the period means

$$0 = \int_{\mathbf{z}_3} \omega_3 = \int_{\mathbf{z}_3} \omega_3' = \int_{\partial \mathbf{M}} \omega_3' = \int_{\mathbf{M}} d\omega_3', \tag{30}$$

where we have used Stokes' theorem.[13] Therefore we have, formally,

$$d\omega_3' = 0, \tag{31}$$

which is the expression in terms of differential forms of the continuity equation, i.e., Eq. (16). Thus, the 3-form ω_3 is integrable if and only if condition (31) is satisfied; then there exists a 2-form ω_2 on $M - \{P_0\}$ such that[14]

$$\omega_3 = d * \omega_2. \tag{32}$$

The singular points of ω_2 may, generally, introduce another type of "current" according to the topological character of 2-cycles. This point is discussed in the next section, and we proceed under the assumption of the integrability of ω_2. We have a 1-form ω_1 such that

$$\omega_2 = d\omega_1. \tag{33}$$

Furthermore, we assume the integrability of the 1-form

$$\omega_1 = d\omega_0, \tag{34}$$

where ω_0 is a 0-form, i.e., a function $\chi(x, y, z, t)$:

$$\omega_0 = \chi. \tag{35}$$

It is to be noted that, in Eq. (33), according to the theorem of Sec. III, ω_1 is determined up to an arbitrary additive 1-form $d\omega_0$:

$$\omega_2 = d\lambda_1 \quad \text{for} \quad \lambda_1 = \omega_1 + d\omega_0. \tag{36}$$

By requirement (27), we have the following conditions for 4-forms:

$$d * \omega_1 = 0 \tag{37}$$

and

$$d * d\omega_0 = 0. \tag{38}$$

Our task is to interpret Eqs. (32)–(38) in physical language, with the help of the discussion in Sec. IV. Equations (28), (32), and (33) yield the equations

$$d * \omega_2 = \omega_3' \tag{39}$$

and

$$d\omega_2 = 0, \tag{40}$$

which correspond to Eqs. (22) if we neglect the current ω_3'. Thus, the components of the 2-form ω_2 are interpreted as the "electric field" **E** and the

"magnetic field" **H**:

$$\omega_2 = (E_1\,dx^1 + \cdots)(c\,dt) + (H_1\,dx^2\,dx^3 + \cdots). \tag{41}$$

Equations (39) and (40) are Maxwell's equations for **E** and **H** including the current. Therefore, the 1-form ω_1 corresponds to the electromagnetic potential A_μ, i.e., Eq. (18). Equation (33) corresponds to Eq. (19). Equation (36) represents the gauge transformation. Equations (37) and (38) are the Lorentz condition for the potential and the wave equation for the gauge function χ in the usual theory of electromagnetic field, respectively. These facts can easily be seen, using the relations

$$*dx^\alpha = dx^\beta\,dx^\gamma\,dx^\delta, \quad \alpha \neq 4,$$

$$*c\,dt = -dx^1\,dx^2\,dx^3,$$

and

$$dx^\alpha\,dx^\beta\,dx^\gamma\,dx^\delta = \sigma,$$

where $dx^4 = c\,dt$ and $(\alpha, \beta, \gamma, \delta)$ are cyclic permutations of $(1, 2, 3, 4)$ and σ is the volume element of E^4.

VI. ON THE ELECTRIC AND MAGNETIC POLARIZATIONS

In the preceding section, we saw that a singular point in space–time introduces a "current" into the differential form according to its topological character, in the sense of de Rham and Kodaira.[10] "Matter" can be considered as a singular point (or an assembly of singular points) of the Maxwell field. The "current" is represented by the class of generalized functions. Therefore, the properties of matter are to be represented by generalized functions. This statement is similar to that expressed by Papoulis,[15] in which it is suggested that "physical quantities" are to be characterized by generalized functions. In this section, we point out the significance of this fact in the electromagnetism of matter, as an example.

In the usual experiment in solid state physics, using electromagnetic field, the spatial surface S^2 of a sphere surrounding the sample material is considered as a 2-cycle in E^3 which cannot be deformed to a point. Therefore, the material introduces the "currents" ω_2' and ω_2'' into the 2-forms ω_2 and $*\omega_2$, Eq. (41):

$$\omega_2 = \omega_2' \quad \text{and} \quad *\omega_2 = \omega_2''. \tag{42}$$

In the usual theory of electromagnetism, we know that the electric and the magnetic fields "in the material" are modified by the "electric polarization" **P** and the "magnetization" **M**[16]:

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P},$$

$$\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}, \tag{43}$$

where **D** and **B** are called the "electric induction" and the "magnetic induction", respectively. Therefore, ω_2' and ω_2'' are expected to represent the physical quantities **P** and **M**[17]:

$$\omega_2' = -4\pi(M_1\,dx^2\,dx^3 + M_2\,dx^3\,dx^1 + M_3\,dx^1\,dx^2)$$

and

$$\omega_2'' = -4\pi(P_1\,dx^2\,dx^3 + P_2\,dx^3\,dx^1 + P_3\,dx^1\,dx^2). \tag{44}$$

Similarly, Eqs. (39) and (40) are modified to become

$$d*\omega_2 = \omega_3' + d\omega_2''$$

and

$$d\omega_2 = d\omega_2', \tag{45}$$

which correspond to the "formal" equations (12). In other words, Eqs. (44) are the physical interpretation of the "currents" ω_2' and ω_2'', which express the "character of the material." It is to be emphasized that the components of ω_2' and ω_2'', i.e., **P** and **M**, are represented by the class of generalized functions, not by the class of ordinary functions. The usual Maxwell equations (12) neglect this fact, and mix up (ordinary) functions **E** (or **H**) and generalized functions **P** (or **M**) with result"functions" **D** (or **B**). As opposed to ordinary functions, generalized functions are linear functionals defined on a certain function space, and are usually represented by using certain integrations.[11] Therefore, generalized functions **P** (or **M**) have "global" character in spite of the fact that functions **E** (or **H**) have local character. In physical language, the dimensions of the quantities **P** (or **M**) and **E** (or **H**) are different by the dimension related to the integration by which the generalized function **P** (or **M**) is represented. The usual equations[16]

$$\mathbf{D} = \epsilon\mathbf{E} \quad \text{and} \quad \mathbf{B} = \mu\mathbf{H},$$

where ϵ and μ are called the "dielectric permeability" and the "magnetic permeability" respectively, neglect this fact. There exists no guarantee of the equivalence of the dimensions of **E** (or **H**) and **P** (or **M**). Therefore, the difficulty on the dimensions of ϵ and μ arises. This fact explains the origin of the fundamental difficulties[18] on the dimensions in the usual theory of electromagnetism.

Next we consider the "current" appearing in the 1-form ω_1, i.e., Eq. (18) or (34). In the experiment of the persistent current in a superconducting ring[19] we can form the 1-cycle in E^3 which cannot be deformed to a point without cutting across the ring. Therefore, the ring introduces the "current" ω_1' into the 1-form

$$\omega_1 = \omega_1'.$$

This equation corresponds to the London equation[20] in the theory of superconductivity, which connects the electromagnetic potential to the current density $\mathbf{J}'$ according to the relation

$$\omega_1' = -\Lambda c(J_1' dx^1 + J_2' dx^2 + J_3' dx^3),$$

where Λ is a constant depending on the material.

VII. CONCLUSIONS

We have discussed Maxwell's field in 4-dimensional Euclidean space using the technique of differential forms. In these discussions it has clarified that the Maxwell equations for electromagnetic fields are elementary consequences of the definition of time postulated in Sec. II or, roughly speaking, the invariance of the speed of light. Thus we have shown, from "first principles," the interrelationship between electromagnetic fields and light that has been suggested for some time. It has also shown that the topological character of the space has the particular importance for the integration of the field and that singular points introduce various kinds of "currents." The character of a material is described by these "currents," which are represented by generalized functions. This fact has particular significance for those various branches of physics in which integrations including singular points are used.[21] Furthermore, we have seen, in Sec. V, that the usual continuity equation of the current density is the elementary consequence of the Jordan–Brouwer theorem applied to our 4-dimensional Euclidean space under the requirement of integrability of the field.

It is to be noted that we have not used in the above discussions the concept of Lorentz transformation at all.

[1] H. Flanders, *Differential Forms with Applications to the Physical Sciences* (Academic, New York, 1963). Recently the following text book has also been published: Y. Choquet-Bruhat, *Géométrie differentielle et systémes extérieurs* (Dunod, Paris, 1968).

[2] A. Einstein, *The Meaning of Relativity* (Princeton U.P., Princeton, N.J., 1955), 5th ed.

[3] Remember that, in TR, the unit of time is defined in connection with that of spatial distance. See Ref. 2.

[4] This fact enables us to prove, without assuming the "contraction of length" and the "duration of time," the nonoccurrence of the interference pattern in Michelson and Morley's experiment because the time required to go and return between the observer and the mirror is equal to twice the time required to go, independently of the motion of the light emitter. See C. Møller, *The Theory of Relativity* (Oxford U.P., London, 1952).

[5] See I. G. Petrovskii, *Lectures on Partial Differential Equations* (Gos. Izd. Tekh.-Teor. Lit., Moscow, 1953), 2nd ed.

[6] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1955), Sec. 35.

[7] It can easily be seen that the dimension of the space $\Lambda^p L$ is given by $\binom{n}{p}$.

[8] In this introduction, we use some topological terminologies without explanation. See Ref. 1. A physical example of a "chain" is the path of integration in Ampères's law in electromagnetism.

[9] P. Alexandroff and H. Hopf, *Topologie* (Chelsea, New York, 1965).

[10] G. de Rham and K. Kodaira, *Harmonic Integrals* (Institute for Advanced Study, Princeton, N.J., 1950); Y. Akizuki, *Harmonic Integrals* (in Japanese) (Iwanami, Tokyo, 1955).

[11] L. Schwartz, *Théorie des distributions I, II* (Hermann, Paris, 1950–51).

[12] It appears that this "current" is identical to the physical 4-current density from the subsequent discussions.

[13] Concerning the detailed definition of the exterior derivative of a current, see Ref. 10.

[14] Here the metric (20) is used. Under this metric, the difference between ω_2 and $*\omega_2$ is only in the sign of its components; both are 2-forms.

[15] A. Papoulis, *The Fourier Integral and its Applications* (McGraw-Hill, New York, 1962), Appendix.

[16] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, Oxford, 1960).

[17] See Eqs. (13) and (41)–(43).

[18] T. Takano, "Study on the Systems of Units in Electromagnetism," (in Japanese), Tohoku University, Sendai, Japan, 1959 (unpublished). In this article, complete criticism of the usual systems of units has been given. The present author is indebted to Professor T. Takano for presenting a copy to him.

[19] J. M. Blatt, *Theory of Superconductivity* (Academic, New York, 1964).

[20] F. and H. London, Proc. Roy. Soc. (London) **A149**, 71 (1935). See also J. M. Blatt, Ref. 19.

[21] Concerning the difficulty on the volume integral of the radiation energy, see S. Hido, *Study of Foundations of Mathematics* (in Japanese) (Sankohdoh, Tokyo, 1967).