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Description of the Extended Tube*

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Necessary and sufficient conditions are given for the belonging of an n tuple of complex four-vectors to the extended tube.

I

THE analyticity properties of vacuum expectation values of field operators[1–6] are related to the geometric properties of the so-called extended tube R_n', which is defined as follows. An n tuple $z_1, \cdots, z_n$ of complex four-vectors belongs to R_n' if and only if there exists a proper complex Lorentz transformation Λ such that, for $p=1, \cdots, n$, the imaginary parts of Λz lie in the interior of the forward light cone. Jost[7] has given a simple characterization of the real points of R_n'. It is the purpose of this paper to give a characterization which applied to all points of R_n', brings out the role of convexity properties, and exploits the symmetry between complex four-vectors and complex 2×2 matrices.

Every complex four-vector determines, in a natural way, an element of an eight-dimensional real euclidean space $E^{(8)}$. Thus the complex four-vectors $z_\mu = x_\mu + iy_\mu$ and $c_\mu = a_\mu + ib_\mu$ correspond to the vectors

$$Z = (x_0, x_1, x_2, x_3; y_0, y_1, y_2, y_3) \tag{1}$$

and

$$C = (a_0, a_1, a_2, a_3; b_0, b_1, b_2, b_3), \tag{2}$$

respectively.

Together with an arbitrary $C \epsilon E^{(8)}$ given by (2), we can consider the vectors

$$\begin{aligned} H^{(0)} &= (b_0, b_1, b_2, b_3; a_0, a_1, a_2, a_3) \\ H^{(1)} &= (b_1, b_0, -a_3, a_2; a_1, a_0, b_3, -b_2) \\ H^{(2)} &= (b_2, a_3, b_0, -a_1; a_2, -b_3, a_0, b_1) \\ H^{(3)} &= (b_3, -a_2, a_1, b_0; a_3, b_2, -b_1, a_0). \end{aligned} \tag{3}$$

It is easy to verify that

$$\begin{aligned} H^{(i)} \cdot H^{(k)} &= |C|^2 \delta_{ik} \quad (i, k = 1, 2, 3) \\ H^{(0)} \cdot H^{(i)} &= 2[a_0 \mathbf{a} + b_0 \mathbf{b} + (\mathbf{a} \times \mathbf{b})]_i. \end{aligned} \tag{4}$$

Here the scalar product and the norms are taken in the euclidean space $E^{(8)}$.

We define now the *cone associated to* C as the set of all vectors $Z \epsilon E^{(8)}$ such that

$$Z \cdot H^{(0)} - \{ \sum_{i=1}^{3} (Z \cdot H^{(i)})^2 \}^{\frac{1}{2}} > 0. \tag{5}$$

A cone associated to a vector (2) which satisfies

$$\begin{aligned} a_\mu a^\mu - b_\mu b^\mu &> 0 \\ a_\mu b^\mu &= 0 \end{aligned} \tag{6}$$

(that is, $c_\mu c^\mu \equiv c_0^2 - \mathbf{c} \cdot \mathbf{c} > 0$), will be called a *distinguished cone*. We shall prove the following result:

An n tuple $\{z_1, \cdots, z_n\}$ belongs to the extended tube if and

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[1] A. S. Wightman, Phys. Rev. **101**, 860 (1956).
[2] D. Hall and A. S. Wightman, Mat. fys. medd. dan. vid. selsk. **31**, 5 (1957).
[3] G. Källen and A. S. Wightman, Mat. fys. skr. dan. vid. selsk. **1**, 6 (1958).
[4] G. Källen and H. Wilhelmsson, Mat. fys. skr. dan. vid. selsk. **1**, 9 (1959).
[5] D. Ruelle, Helv. Phys. Acta **32**, 135 (1959).
[6] D. Kleitman, Nuclear Phys. **11**, 459 (1959).
[7] R. Jost, Helv. Phys. Acta **30**, 409 (1957).

only if the convex body spanned by the real eight-dimensional vectors $Z_1, \cdots, Z_n$ *lies in the interior of some distinguished cone.*

The proof is given in Sec. II.

II

Given two complex four-vectors c_μ and z_μ, consider the real number $f(c,z)$ defined by

$$f(c,z)=v_0-|\mathbf{v}| \tag{7}$$

and

$$v_0=Im(c_0z_0+\mathbf{c}\cdot\mathbf{z}) \tag{8}$$

$$v=Im(c_0\mathbf{z}+z_0\mathbf{c}+i(\mathbf{c}\times\mathbf{z})). \tag{9}$$

It is easy to see that the function $f(c,z)$ has the following convexity properties; if $0\leqslant\lambda\leqslant 1$, then

$$f(\lambda c'+(1-\lambda)c'',z)\geqslant\lambda f(c',z)+(1-\lambda)f(c'',z) \tag{10}$$

$$f(c,\lambda z'+(1-\lambda)z'')\geqslant\lambda f(c,z')+(1-\lambda)f(c,z''). \tag{11}$$

Furthermore, for any real positive number γ

$$f(\gamma c,z)=f(c,\gamma z)=\gamma f(c,z). \tag{12}$$

We shall now prove the following lemma:

An n tuple $\{z_1, \cdots, z_n\}$ belongs to the extended tube if and only if there exists a complex four-vector c_μ such that

$$c_\mu c^\mu=1 \tag{13}$$

$$f(c,z)_p>0 \quad (p=1, \cdots, n). \tag{14}$$

Proof: Instead of the four vectors c_μ and z_μ, we may consider the matrices

$$c=\begin{pmatrix} c_0+c_3 & c_1-ic_2 \\ c_1+ic_2 & c_0-c_3 \end{pmatrix} \tag{15}$$

$$z=\begin{pmatrix} z_0+z_3 & z_1-iz_2 \\ z_1+iz_2 & z_0-z_3 \end{pmatrix}. \tag{16}$$

It is known (see e.g., Jost[7]) that $\{z_1, \cdots, z_n\}$ belongs to the extended tube if and only if there exists a matrix c such that

$$\det c=1, \tag{17}$$

and that the complex four-vectors $w_{p\mu}$, corresponding to the matrices

$$w_p=cz_p \quad (p=1, \cdots, n) \tag{18}$$

have their imaginary parts in the interior of the forward light-cone. Because of (15) and (16), Eqs. (18) can be written as

$$w_0=c_0z_0+\mathbf{c}\cdot\mathbf{z} \tag{19}$$

$$\mathbf{w}=c_0\mathbf{z}+z_0\mathbf{c}+i(\mathbf{c}\times\mathbf{z}) \tag{20}$$

and (17) as

$$c_\mu c^\mu=1. \tag{21}$$

The assertion of the lemma now follows from the definition of the function $f(c,z)$, with $v_0=\mathrm{Im}w_0$, and $\mathbf{v}=\mathrm{Im}\mathbf{w}$.

If the inequalities (14) are satisfied, then by (11), $f(c,z)>0$ in the closed convex body spanned by $z_1, \cdots, z_n$. Conversely, if $f(c,z)>0$ in that body, then obviously $f(c,z)_p>0$ $(p=1, \cdots n)$.

If we introduce now (instead of the complex four-vectors c_μ and z_μ) the real eight-vectors (1) and (2), then Eqs. (8) and (9) become

$$v_0=Z\cdot H^{(0)} \tag{22}$$

$$v_i=Z\cdot H^{(i)} \quad (i=1, 2, 3), \tag{23}$$

where $H^{(0)}$ and $H^{(i)}$ are given by (3). Consequently,

$$f(c,z)=Z\cdot H^{(0)}-\{\sum_{i=1}^{3}(Z\cdot H^{(i)})^2\}^{\frac{1}{2}} \tag{24}$$

and the statement of the theorem follows from the lemma, the definition of distinguished cones, and the Eq. (12). The inequality (11), together with Eq. (12), also shows that the sets which we called cones are indeed convex cones.

III

We shall now illustrate the thorem just proved by a few simple examples.

Consider first the distinguished cone associated to a vector (2) with $a_0=1$, $a_i=b_i=b_0=0$. If the convex body spanned by $Z_1, \cdots, Z_n$ lies within this particular distinguished cone, then the n tuple $\{z_1, \cdots, z_n\}$ belongs to the so-called forward tube. Indeed, for any Z given by (1), $Z\cdot H^{(0)}=y_0$ $Z\cdot H^{(i)}=y_i$; so (5) becomes just the condition that the imaginary parts of all the $z-s$ lie in the forward light-cone.

Next, it is easy to verify that if $z_\mu z^\mu\geqslant 0$, then the corresponding Z cannot belong to any distinguished cone.

Finally, if x_μ is real and space-like, then $Z=(x_\mu;0)$ lies in the distinguished cone associated with $C=(0;x_\mu)$.

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Pair Distribution Function of a Hard Sphere Bose System Calculated by the Pseudo-Potential Method*†

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The pair distribution function for a hard sphere Bose system has been calculated by using a method in which the hard sphere potential is replaced by the so-called pseudo-potential. The problem is carried through using the quasi-particle formalism of Bogoliubov. In this calculation one considers a system of bosons interacting via the pseudo-potential which can be regarded as a weak interaction when the system is very dilute. The Hamiltonian of the system is diagonalized by means of a canonical transformation which has the effect of separating the energy into two parts, one of which is the ground state energy and the other corresponds to an ideal Bose gas composed of "elementary excitations" or "quasi-particles." This formalism is applied to the calculation of the pair distribution function. This quantity is calculated by averaging over a grand canonical ensemble constructed with the total number of elementary excitations. A result which is seen to be valid both for the condensed and gaseous phases of the system and also for any distance r between the particles is obtained.

A discussion of the difference between these results and the ones obtained in a previous calculation and a comparison between both results and the experimental ones is also given.

INTRODUCTION

IN a previous calculation,[1,2] we have obtained the pair distribution function (pdf) for a hard sphere Bose system to first order in a/λ by using the Binary Collision Expansion (BCE) method of Yang and Lee. The parameter a is the radius of the spheres and λ is the thermal wavelength, $h(2\pi mkT)^{-\frac{1}{2}}$. As we have mentioned in I, the result has the disadvantage of being applicable only for the "gaseous phase" and for large interparticle distances. The first limitation is a result of the appearance of functions $g_\sigma(z,s)$ and $g_\sigma(z)$ which for any value of σ converge only if $|z|<1$. The second arises from the fact that one of the terms in the expansion for the pdf is inversely proportional to r, the distance between any two particles.

In this paper we wish to calculate the pdf for the hard sphere Bose system to the same order in a/λ, so that the result is sufficiently general to be valid for the condensed and gaseous phases and at any value of the interparticle separation. We shall use for this purpose the formalism of Bogoliubov[3] in his theory of the superfluidity of He II. We shall apply it to the case of a dilute hard sphere Bose system interacting through the pseudo-potential which we regard as a weak interaction.

The first section of this paper will be devoted to a discussion of Bogoliubov's method. In the following section we shall evaluate the pair correlation function for any weakly interacting system. The calculation will be performed by averaging the matrix elements of the corresponding operator over the grand canonical ensemble constructed by the total number of "quasi-particles" or elementary excitations. In Sec. 3, the resulting formula will be applied to the ideal gas and the hard sphere gas, to order a/λ, in the gaseous phase. In Sec. 4, we shall compare the two results (i.e., the one obtained in I and the one obtained in the present paper), with the experimental results for liquid helium at 4.2°K. Finally, in Sec. 5 some comments will be made concerning the connection between the two methods and their validity.

1. METHOD OF BOGOLIUBOV

We consider a system of N weakly interacting bosons whose Hamiltonian, in the language of second quantization, is given by

$$H=\sum_p |p|^2 a_p^* a_p + \frac{1}{2\Omega}\sum_{(p_1+p_2=p_1'+p_2')} v(p_1-p_1')a_{p_1}^* a_{p_2}^* a_{p_2'} a_{p_1'}, \quad (1)$$

where $\mathbf{p}$ is the particle momentum, $v(p)$ is the Fourier transform of the interaction potential for a pair of particles (this quantity is assumed to be proportional to some small parameter), Ω is the volume of the system and a_p^* and a_p are the boson creation and annihilation operators. We shall, for the time being, choose our system of units such that $\hbar=2m=1$.

Bogoliubov[3] has shown that in the presence of a weak interaction, one can assume that the overwhelming majority of the particles will be in the particle ground state, i.e., that there exists a condensate in the system. If this condensate contains N_0 particles, where

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[1] L. S. Garcia-Colín and J. Peretti, J. Math. Phys 1, 97 (1960).

[2] Hereafter we shall refer to this paper as I.

[3] N. N. Bogoliubov, J. Phys. (U.S.S.R.) 11, 23 (1947); N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau, New York, 1959), Chap. I.

$N_0 \gg 1$, the expression

$$a_0 a_0^* - a_0^* a_0 = 1$$

is small compared with a_0 and a_0^* themselves since $N_0 = a_0^* a_0$. We, therefore, may treat these operators as c numbers, neglecting their noncommutativity. Then, on introducing the operators,

$$b_p = a_0^* N_0^{-\frac{1}{2}} a_p \quad b_p^* = a_0 N_0^{-\frac{1}{2}} a_p^*, \tag{2}$$

we may rewrite Eq. (1) as follows:

$$\begin{aligned} H &= H_0 + H_{\text{int}} \\ H_0 &= \sum_p |p|^2 b_p^* b_p \\ H_{\text{int}} &= \frac{N_0^2}{\Omega} \nu(0) + \frac{N_0}{2\Omega} \sum_{p \neq 0} \nu(p) \\ &\quad \times (b_p^* b_{-p}^* + b_p b_{-p} + 2 b_p^* b_p), \end{aligned} \tag{3}$$

where we have neglected terms of an order larger than second in b_p^* and b_p because they are of order $N_0^{\frac{1}{2}}$ and 1. This corresponds to the solution of the equation of motion of the system by using a field operator of the type

$$\Psi = \Omega^{-\frac{1}{2}} a_0 + \theta,$$

where θ is a small quantity, and where all those terms involving second and higher orders of θ have been neglected.

We now introduce two operators ξ_p and ξ_p^* by means of the transformation

$$\begin{aligned} b_p &= u_p \xi_p + v_p \xi_{-p}^* \\ b_{-p} &= u_p \xi_{-p} + v_p \xi_p^*, \end{aligned} \tag{4}$$

where u_p and v_p are real c numbers, functions of p, such that they satisfy the relations

$$u_p^2 - v_p^2 = 1; \quad u_{-p} = u_p; \quad v_{-p} = v_p.$$

It is then easy to show that the ξ's satisfy the same commutation relations as the a's, and thus they are Bose amplitudes. Under the transformation defined by Eq. (4), Eq. (3) reduces to[4]

$$\begin{aligned} H &= H_1 + \sum_{p \neq 0} \omega(p) \xi_p^* \xi_p \\ H_1 &= \frac{N_0^2}{\Omega} \nu(0) + \tfrac{1}{2} \sum_{p \neq 0} [\omega(p) - E(p) - J(p)], \end{aligned} \tag{5}$$

where

$$\begin{aligned} E(p) &= p^2 \qquad J(p) = \frac{N_0 \nu(p)}{\Omega} \\ \omega(p) &= [E(p)^2 + 2E(p)J(p)]^{\frac{1}{2}} \end{aligned} \tag{6}$$

provided that u_p and v_p satisfy the relation

$$2u_p v_p [E(p) + J(p)] + (u_p^2 + v_p^2) J(p) = 0. \tag{7}$$

Thus the total energy of the system is equal to the ground state energy H_1 and the energy of the "elementary excitations" or "quasi-particles," described by the operators ξ and ξ^*. As it is shown in Eq. (5), these elementary excitations, represented by the term $\sum_{p \neq 0} \omega(p) \xi_p^* \xi_p$ form a perfect Bose gas.

The explicit dependence on the momentum p of the c numbers u_p and v_p appearing in Eq. (4) is obtained by solving Eq. (7). This is most easily done by introducing an angle φ_p through the relations

$$u_p = \cosh \varphi_p \quad v_p = \sinh \varphi_p. \tag{8}$$

One then finds that

$$\begin{aligned} \cosh 2\varphi_p &= E(p) + J(p)/\omega(p) \\ \sinh 2\varphi_p &= -[J(p)/\omega(p)] \end{aligned} \tag{9}$$

so that φ_p is a negative number, which approaches zero as $J(p)$ goes to zero. We now define a positive number $\alpha(p)$ by means of the expression,

$$-\alpha(p) = \tanh \varphi_p = (v_p/u_p). \tag{10}$$

From Eqs. (9) and (10) it is easily found that

$$\alpha(p) = J(p)^{-1} [E(p) + J(p) - \omega(p)] \tag{11}$$

and that

$$\begin{aligned} u_p^2 &= [1 - \alpha^2(p)]^{-1} \quad v_p^2 = \alpha^2(p) [1 - \alpha^2(p)]^{-1} \\ u_p v_p &= -\alpha(p) [1 - \alpha^2(p)]^{-1}, \end{aligned} \tag{12}$$

which are the desired relations. One might mention that for a hard sphere Bose gas, where $\nu(p) = 8\pi a$, "a" being the *diameter* of the spheres, Eq. (11) reduces to the result given by Lee, Huang, and Yang.[5]

2. PAIR DISTRIBUTION FUNCTION IN BOGOLIUBOV'S FORMALISM

After using the results sketched in the previous section, we proceed to evaluate the pair distribution function for a system of weakly interacting bosons.

In the language of second quantization the pair distribution function operator is given by

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \Psi^*(\mathbf{r}_1) \Psi^*(\mathbf{r}_2) \Psi(\mathbf{r}_2) \Psi(\mathbf{r}_1), \tag{13}$$

where the field operator Ψ is given by

$$\Psi(\mathbf{r}) = \Omega^{-\frac{1}{2}} (a_0 + \sum_{p \neq 0} a_p e^{i\mathbf{p} \cdot \mathbf{r}}), \tag{14}$$

where we have explicitly written the term for zero momentum.

By introducing a new field operator $\varphi(\mathbf{r})$, given by

$$\varphi(\mathbf{r}) = \rho_0^{\frac{1}{2}} + \Omega^{-\frac{1}{2}} \sum_{p \neq 0} b_p e^{i\mathbf{p} \cdot \mathbf{r}}, \tag{15}$$

where ρ_0 is the particle density in the ground state

[4] The reasons leading to such transformations are given in footnote 3.

[5] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).

N_0/Ω, we can write Eq. (13) as follows:

$$\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=\varphi^*(\mathbf{r}_1)\varphi^*(\mathbf{r}_2)\varphi(\mathbf{r}_2)\varphi(\mathbf{r}_1). \tag{16}$$

The substitution of Eq. (4) into Eq. (15) yields

$$\varphi(\mathbf{r})=\rho_0^{\frac{1}{2}}+U(\mathbf{r})+V^*(\mathbf{r}), \tag{17}$$

where

$$U(\mathbf{r})=\Omega^{-\frac{1}{2}}\sum_{p\neq 0}u_p e^{i\mathbf{p}\cdot\mathbf{r}}\xi_p \tag{18a}$$

and

$$V(\mathbf{r})=\Omega^{-\frac{1}{2}}\sum_{p\neq 0}v_p e^{-i\mathbf{p}\cdot\mathbf{r}}\xi_p. \tag{18b}$$

The operator $\varphi^*(\mathbf{r})$ is given by the hermitian conjugate of Eq. (17). Substitution of Eq. (17) and its complex conjugate into Eq. (16) would give the pair distribution operator in terms of the quasi-particle creation and annihilation operators. As it will be seen later, we are interested in calculating only the diagonal elements of this operator in the quasi-particle representation. It is then easy to see that those terms having $\rho_0^{\frac{3}{2}}$ and $\rho_0^{\frac{1}{2}}$ as coefficients give a zero contribution to such diagonal terms, and for this reason we shall ignore them. The remaining terms giving a nonzero contribution are

$$\begin{aligned}[\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2)]_{\text{diag}}&=[\rho_0^2+\rho_0\{U^*(\mathbf{r}_1)V(\mathbf{r}_2)+V(\mathbf{r}_1)U^*(\mathbf{r}_2)+U(\mathbf{r}_2)V^*(\mathbf{r}_1)\\&+V^*(\mathbf{r}_2)U(\mathbf{r}_1)+U^*(\mathbf{r}_1)U(\mathbf{r}_1)+U^*(\mathbf{r}_1)U(\mathbf{r}_2)\\&+U^*(\mathbf{r}_2)U(\mathbf{r}_1)+U^*(\mathbf{r}_2)U(\mathbf{r}_2)+V(\mathbf{r}_1)V^*(\mathbf{r}_1)\\&+V(\mathbf{r}_2)V^*(\mathbf{r}_1)+V(\mathbf{r}_1)V^*(\mathbf{r}_2)+V(\mathbf{r}_2)V^*(\mathbf{r}_2)\}\\&+U^*(\mathbf{r}_1)U^*(\mathbf{r}_2)U(\mathbf{r}_2)U(\mathbf{r}_1)+U^*(\mathbf{r}_1)V(\mathbf{r}_2)\\&\times U(\mathbf{r}_2)V^*(\mathbf{r}_1)+U^*(\mathbf{r}_1)V(\mathbf{r}_2)V^*(\mathbf{r}_2)U(\mathbf{r}_1)\\&+V(\mathbf{r}_1)U^*(\mathbf{r}_2)U(\mathbf{r}_2)V^*(\mathbf{r}_1)+V(\mathbf{r}_1)U^*(\mathbf{r}_2)\\&\times V^*(\mathbf{r}_2)U(\mathbf{r}_1)+V(\mathbf{r}_1)V(\mathbf{r}_2)V^*(\mathbf{r}_2)V^*(\mathbf{r}_1)]_{\text{diag}}.\end{aligned} \tag{19}$$

The evaluation of Eq. (19) is long but straightforward. The first term contributes ρ_0^2 since it is a constant; the term having ρ_0 as a coefficient yields after some manipulations, the following result:

$$\Delta_1=\frac{\rho_0}{\Omega}\sum_{p\neq 0}[(u_pv_p+v_p^2)(e^{i\mathbf{p}\cdot\mathbf{r}}+e^{-i\mathbf{p}\cdot\mathbf{r}})+2v_p^2]+\frac{\rho_0}{\Omega}\sum_{p\neq 0}[(2u_pv_p+u_p^2+v_p^2)(e^{i\mathbf{p}\cdot\mathbf{r}}+e^{-i\mathbf{p}\cdot\mathbf{r}})+2(u_p^2+v_p^2)]\xi_p^*\xi_p. \tag{20}$$

Finally, the independent term yields the following expression:

$$\begin{aligned}\Delta_2=\Omega^{-2}&\sum_{\substack{p,q\\p\neq q}}[u_p^2u_q^2e^{-i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}}+u_pv_pu_qv_q(e^{-i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+e^{-i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}}+e^{+i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+e^{i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}})+v_p^2v_q^2e^{i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}]\\&\times\xi_p^*\xi_p\xi_q^*\xi_q+\Omega^{-2}\sum_{p,q}[u_p^2u_q^2+2u_p^2v_q^2+v_p^2v_q^2+u_p^2v_q^2e^{-i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+v_p^2u_q^2e^{i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}}]\xi_p^*\xi_p\xi_q^*\xi_q\\&+\Omega^{-2}\sum_{\substack{p,q\\p\neq q}}[u_pv_pu_qv_q(e^{-i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+e^{i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+e^{-i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}}+e^{i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}})+v_p^2v_q^2(e^{i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+e^{i\mathbf{q}\cdot\mathbf{r}-i\mathbf{p}\cdot\mathbf{r}})]\xi_p^*\xi_p\\&+\Omega^{-2}\sum_{p,q}[u_p^2v_q^2e^{-i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+2u_p^2v_q^2+2v_p^2v_q^2+v_p^2u_q^2e^{i\mathbf{p}\cdot\mathbf{r}+i\mathbf{q}\cdot\mathbf{r}}]\xi_p^*\xi_p+\Omega^{-2}\sum_{p\neq 0}(u_p^4+2v_p^4)\xi_p^*\xi_p\\&+\Omega^{-2}\sum_{\substack{p,q\\p\neq q}}(u_pv_pu_qv_qe^{i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}}+v_p^2v_q^2e^{i\mathbf{p}\cdot\mathbf{r}-i\mathbf{q}\cdot\mathbf{r}})+\Omega^{-2}\sum_{p,q}v_p^2v_q^2+2\Omega^{-2}\sum_{p\neq 0}v_p^4,\end{aligned} \tag{21}$$

where in Eqs. (20) and (21), $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$.

The diagonal part of the matrix elements of the pair distribution function are, therefore, given by the expression

$$[\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2)]_{\text{diag}}=\rho_0^2+\Delta_1+\Delta_2, \tag{22}$$

where Δ_1 and Δ_2 are given by Eqs. (20) and (21), respectively.

We must now find the thermal average of the operator given by Eq. (22) which for brevity we shall denote by $\rho^{(2)}$. Such an average is proportional to the trace of the operator $\rho^{(2)}e^{-\beta H}$, where H is the Hamiltonian of the system given by Eq. (5). The calculation of such an average is performed by averaging over an appropriate grand canonical ensemble.

First we notice that the number of elementary excitations is not arbitrary but it is related to the total number of quasi-particles N and the number of particles in the ground state N_0 through the relation

$$\sum_{p\neq 0}n_p=N-N_0, \tag{23}$$

where n_p is the occupation number of the "quasi-particle" state with momentum p.

We now define a quantity Ξ, which plays the role of the grand partition function, by means of the equation

$$\Xi=\zeta^{N_0}\sum_{N=N_0}^{\infty}\zeta^{N-N_0}Z_N, \tag{24}$$

where ζ is a parameter which must be determined later on, and is not equal to the fugacity of the system be-

cause N is not the total number of particles. Since[6]

$$Z_N = Tre^{-\beta H} \tag{25}$$

and the canonical average of $\rho^{(2)}$ is given by

$$\langle\rho^{(2)}\rangle = Z_N^{-1} Tr\rho^{(2)} e^{-\beta H}, \tag{26}$$

we find from Eqs. (24) and (26) that the grand canonical average of $\rho^{(2)}$ is given by

$$\langle\langle\rho^{(2)}\rangle\rangle = \zeta^{N_0}\Xi^{-1}\sum_{N=N_0}^{\infty}\zeta^{N-N_0}Tr\rho^{(2)}e^{-\beta H}, \tag{27}$$

where $\langle\langle\rho^{(2)}\rangle\rangle$ denotes the grand canonical average of $\rho^{(2)}$.

Let

$$\zeta = e^{-\beta\mu}$$

and let $|n_p,N\rangle$ be an eigenstate of the Hamiltonian H such that Eq. (23) is satisfied. Then, by using the fact that

$$\Xi\zeta^{-N_0} = \sum_{N=N_0}^{\infty}\sum_{\{n_p\}} e^{-\beta[\Sigma' n_p\omega(p)+\mu\Sigma' n_p]}$$

we can write Eq. (27) alternatively as

$$\langle\langle\rho^{(2)}\rangle\rangle = \frac{\sum_{N=N_0}^{\infty}\sum_{\{n_p\}}\langle n_p,N|\rho^{(2)}|n_p,N\rangle\exp\{-\beta[\sum' n_p\omega(p)+\mu\sum' n_p]\}}{\sum_{N=N_0}^{\infty}\sum_{\{n_p\}}\exp\{-\beta[\sum' n_p\omega(p)+\mu\sum' n_p]\}}, \tag{28}$$

where in these last two expressions, $\sum_{\{n_p\}}$ denotes a summation over all possible sets of values of the n_p's satisfying Eq. (23) and $\sum'$ denotes a summation over all possible momenta, except $p=0$. Equation (28) shows explicitly the use of the diagonal elements of the operator $\rho^{(2)}$, which we have previously calculated.

Now, the terms that appear in $\rho^{(2)}$ are either independent of ξ_p and ξ_p^*, they contain these operators in the combination $\xi_p^*\xi_p$, or they contain them in the form $\xi_p^*\xi_p\xi_q^*\xi_q$. Thus, noticing that the double summations appearing in Eq. (28) may be replaced by a single summation over all possible sets of values $\{n_p\}$ without any restriction, we find that this equation gives rise to the three following results:

(a) The terms in $\rho^{(2)}$ independent of ξ_p and ξ_p^* remain the same.

(b) Terms of the type

$$\sum_{q\neq 0} A(q)\xi_q^*\xi_q$$

yield

$$\sum_{q\neq 0} A(q)\langle\langle n_q\rangle\rangle,$$

where

$$\langle\langle n_q\rangle\rangle = \frac{\zeta e^{-\beta\omega(q)}}{1-\zeta e^{-\beta\omega(q)}}$$

is the grand canonical average of the occupation number n_q of the particles having momentum q.

(c) Terms of the type

$$\sum_{q\neq 0}\sum_{p\neq 0} M(p,q)\xi_p^*\xi_p\xi_q^*\xi_q$$

yield, neglecting terms of the order Ω^{-1},

$$\sum_{q\neq 0}\sum_{p\neq 0} M(p,q)\langle\langle n_p\rangle\rangle\langle\langle n_q\rangle\rangle.$$

On combining these results with Eq. (22) and noticing that the density of the system is related to the ground state particle density by the relation

$$\rho_0 = \rho(1-f_0), \tag{29}$$

where

$$f_0 = (N'-N_0)/N' \tag{30}$$

is the fraction of the average number of particles outside the ground state, N' being the average of the total number particles, and keeping only terms up to order $(N')^{-1}$, we find that the pair correlation function averaged over the grand canonical ensemble is given by[7]

$$\begin{aligned}\langle\langle D(\mathbf{r})\rangle\rangle &= \rho^{-2}\langle\langle\rho^{(2)}(\mathbf{r})\rangle\rangle = (1-f_0)^2+[1+F(\mathbf{r})]^2+[1+G(\mathbf{r})]^2\\ &+[1+F_1(\mathbf{r})]^2+[1+H(\mathbf{r})]^2+[1+2G_1(\mathbf{r})]^2\\ &+[1+H(0)]^2+[1+F(0)]^2+[1+F_1(0)]^2\\ &-8-2f_0[F(0)+F_1(0)+H(0)+F(\mathbf{r})+G(\mathbf{r})\\ &+F_1(\mathbf{r})+H(\mathbf{r})+2G_1(\mathbf{r})]+2F(0)[H(0)+F_1(0)]\\ &+2F_1(\mathbf{r})[F(\mathbf{r})+H(\mathbf{r})]+2H(0)F_1(0)\\ &+4G(\mathbf{r})G_1(\mathbf{r})+H(\mathbf{r})F(\mathbf{r})+I(\mathbf{r})F_1(\mathbf{r}),\end{aligned} \tag{31}$$

where

$$F(\mathbf{r}) = \frac{1}{8\pi^3\rho}\int\frac{\alpha^2(p)}{1-\alpha^2(p)}e^{i\mathbf{p}\cdot\mathbf{r}}d^3p$$

$$G(\mathbf{r}) = \frac{1}{8\pi^3\rho}\int\frac{-\alpha(p)}{1-\alpha^2(p)}e^{i\mathbf{p}\cdot\mathbf{r}}d^3p$$

$$G_1(\mathbf{r}) = \frac{1}{8\pi^3\rho}\int\frac{-\alpha(p)}{1-\alpha^2(p)}\langle\langle n_p\rangle\rangle e^{i\mathbf{p}\cdot\mathbf{r}}d^3p$$

$$F_1(\mathbf{r}) = \frac{1}{8\pi^3\rho}\int\frac{\alpha^2(p)}{1-\alpha^2(p)}\langle\langle n_p\rangle\rangle e^{i\mathbf{p}\cdot\mathbf{r}}d^3p$$

$$H(\mathbf{r}) = \frac{1}{8\pi^3\rho}\int\frac{1}{1-\alpha^2(p)}\langle\langle n_p\rangle\rangle e^{i\mathbf{p}\cdot\mathbf{r}}d^3p$$

$$I(\mathbf{r}) = \frac{1}{8\pi^3\rho}\int\frac{1}{1-\alpha^2(p)}e^{i\mathbf{p}\cdot\mathbf{r}}d^3p.$$

[6] The symbol Tr in Eq. (25) must be understood as that acting on the operator $e^{-\beta H}$ when the Hamiltonian H represents the system in a state having precisely N quasi-particles.

[7] This function was called $g(r)$ in I.

The expressions for $F(0)$, $F_1(0)$ and $H(0)$ are the values for $F(\mathbf{r})$, $F_1(\mathbf{r})$ and $H(\mathbf{r})$ when $\mathbf{r}=0$. The α's are related to the coeff u_p and v_p of the canonical transformation defined in Eq. (4) through Eq. (12).

It is worth remarking that if we only restrict ourselves to the average of the operator $\rho^{(2)}$ over the ground state, that is, we consider in Eq. (22) only those terms which are independent of ξ_p and ξ_p^* we get the same result as the one derived by Lee, Huang, and Yang,[5] using the pair theory. In fact, in this case our parameter f_0, the fraction of particles outside the ground state is equal to the parameter f introduced by these authors,

$$f\equiv F(0)=(N')^{-1}\sum_{p\neq 0}\frac{\alpha^2(p)}{1-\alpha^2(p)}=f_0.$$

Hence we find $F_1(\mathbf{r})=G_1(\mathbf{r})=H(\mathbf{r})=0$ and Eq. (31) reduces to[5,8]

$$\langle\langle D(\mathbf{r})\rangle\rangle=[1+G(\mathbf{r})]^2+[1+F(\mathbf{r})]^2-1-2f[G(\mathbf{r})+F(\mathbf{r})]. \quad (32)$$

Equation (31) is the sought for expression for the pair distribution function; it is valid for all distances r and at all temperatures. We shall now proceed to apply it to the case of an ideal Bose gas and then to the hard sphere Bose gas.

3. IDEAL AND HARD SPHERE BOSE SYSTEMS

The pair correlation function for an ideal Bose system at any temperature T is obtained from Eq. (31) in the following way: Since $J(p)=0$ we see from Eqs. (10) or (11), that $\alpha(p)=0$, and hence

$$F(\mathbf{r})=F_1(\mathbf{r})=G(\mathbf{r})=G_1(\mathbf{r})=0.$$

If we keep the terms of order $(N')^{-1}$, which we neglected before, Eq. (31) yields

$$\langle\langle D(\mathbf{r})\rangle\rangle=(1-f_0)^2+2(1-f_0)[H(\mathbf{r})+H(0)]+H^2(0)+H^2(\mathbf{r})-\frac{1}{N'\rho 8\pi^3}\int\langle\langle n_p\rangle\rangle^2 d^3p,$$

where

$$H(0)=\frac{1}{8\pi^3\rho}\int\langle\langle n_p\rangle\rangle d^3p=\frac{1}{\lambda^3\rho}g_{\frac{3}{2}}(z)=f_0$$

$$H(\mathbf{r})=\frac{1}{8\pi^3\rho}\int\langle\langle n_p\rangle\rangle e^{i\mathbf{p}\cdot\mathbf{r}}d^3p=\frac{1}{\lambda^3\rho}g_{\frac{3}{2}}\left[z,\frac{\mathbf{r}}{\lambda}(\pi)^{\frac{1}{2}}\right]$$

and

$$\frac{1}{8\pi^3\rho}\int\langle\langle n_p\rangle\rangle^2 d^3p=g_{\frac{3}{2}}(z)-g_{\frac{3}{2}}(z).$$

In this case, ζ is equal to z, the fugacity of the system, because the diagonal part of the interaction as well as the off diagonal part of it, are identically zero. We then find that

$$\langle\langle D(r)\rangle\rangle=1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}\left(z,\frac{r}{\lambda}\pi^{\frac{1}{2}}\right)\right]^2+\frac{2}{\rho\lambda^3}g_{\frac{3}{2}}\left(z,\frac{r}{\lambda}\pi^{\frac{1}{2}}\right)-\frac{2}{\rho^2\lambda^6}g_{\frac{3}{2}}(z)g_{\frac{3}{2}}\left(z,\frac{r}{\lambda}\pi^{\frac{1}{2}}\right)-\frac{1}{\rho\lambda^3 N'}[g_{\frac{3}{2}}(z)-g_{\frac{3}{2}}(z)]. \quad (33)$$

By using the value of f_0 given in Eq. (30) and $H(0)$ we find

$$f_0=(1/\rho\lambda^3)g_{\frac{3}{2}}(z)=(N'-N_0)/N'.$$

If we introduce a parameter α by means of the relation,

$$z=e^{-\alpha},$$

we see that Eq. (33) can be written as

$$\langle\langle D(r)\rangle\rangle=1+\frac{1}{N'^2}\left[\left\{N_0+\frac{\Omega}{\lambda^3}\sum_{n=1}^{\infty}n^{-\frac{3}{2}}e^{-n\alpha-(x/n)}\right\}^2-N_0^2-N_0+N'-\frac{\Omega}{\lambda^3}\sum_{n=1}^{\infty}n^{-\frac{3}{2}}e^{-\alpha n}\right]\cdots, \quad (34)$$

which is the pair correlation function for an ideal Bose-Einstein system in precisely the form recorded by London.[9] In Eq. (34) $x=\pi r^2\lambda^{-2}$.

For the gaseous phase, (i.e., at temperatures above the condensation point) N_0 is of the order of $(N')^{-1}$ so that f_0 can be taken to be equal to one. Hence, we find that Eq. (33) reduces to

$$\langle\langle D(r)\rangle\rangle=1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}\left(z,\frac{r}{\lambda}\pi^{\frac{1}{2}}\right)\right]^2+0\left(\frac{1}{N'}\right), \quad (35)$$

which agrees with the result obtained in I by the binary collision expansion method.

Next, we want to apply our results to the case of a system of bosons interacting via a hard sphere potential, restricting ourselves only to the gaseous phase. The problem of evaluating the equilibrium properties of a system of this kind has already been thoroughly studied by Lee and Yang,[10] using the pair theory. Since this method is completely equivalent[11] to the quasi-particle method, we shall be able to use some of the results obtained by these authors.

The calculation of the pair correlation function is easily performed. For a hard sphere system of bosons we know that $v(p)=16\pi a$, so from Eq. (6) we get

$$J(p)=16\pi a\rho_0,$$

which is expressed in terms of ρ, with the aid of Eq. (29) as

$$J(p)=16\pi a\rho(1-f_0),$$

where a is the radius of the spheres.

[8] It must be pointed out that the last term of Lee, Huang, and Yang's expression contains a factor $4f$, instead of $2f$, resulting from an error in their calculation.

[9] F. London, J. Chem. Phys. **11**, 203 (1943).

[10] T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958).

[11] J. Peretti, Phys. Fluids **3**, 68 (1960).

On the other hand, let us introduce Lee and Yang's parameter η,[12] which is defined by

$$\eta = N_0/N',$$

so that

$$J(p) = 16\pi a\rho\eta.$$

As they have shown, $\eta=0$ for the gaseous phase, thus $J(p)=0$ and as before $\alpha(p)=0$, and $f_0=1$.

Therefore, Eq. (31) reduces in this case to the following expression:

$$\langle\langle D(r)\rangle\rangle = H^2(0)+H^2(r)=0(1/N'),$$

where ζ is a parameter which has to be determined.

If we use the values found before for $H(0)$ and $H(r)$ with ζ replacing z, and use the fact that to first order in a/λ, (6),

$$\rho = \lambda^{-3}g_{\frac{3}{2}}(\zeta), \tag{36}$$

a result which follows from the condition that $f_0=1$, we find that

$$\langle\langle D(r)\rangle\rangle = 1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}\left(\zeta, \frac{r}{\lambda}\pi^{\frac{1}{2}}\right)\right]^2. \tag{37}$$

The relation between ζ and z[10,13] to first order in a/λ it is found to be

$$\zeta = z(1-(8a/\lambda)g_{\frac{3}{2}}(z)), \tag{38}$$

which substituted into Eq. (37) gives

$$\langle\langle D(r)\rangle\rangle = 1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}\left(z, \frac{r}{\lambda}\pi^{\frac{1}{2}}\right)\right]^2 - \frac{16a}{\rho^2\lambda^7}g_{\frac{3}{2}}(z)g_{\frac{3}{2}}\left(z, \frac{r}{\lambda}\pi^{\frac{1}{2}}\right)g_{\frac{1}{2}}\left(z, \frac{r}{\lambda}\pi^{\frac{1}{2}}\right). \tag{39}$$

This is the pair correlation function for a hard sphere Bose gas up to terms of the order of a/λ. This result does not agree completely with the one obtained in I by the BCE method. The discrepancy between the two results and a relation between them, if any, will be discussed in Sec. 5.

4. COMPARISON WITH THE EXPERIMENT

In this section, we want to compare the values for the pair distribution function, calculated in I by the BCE method and in this paper by the pseudo-potential method, with the experimental values for liquid He^4 given by Goldstein and Reekie.[14] The comparison will be done at a temperature of 4.2°K and a fixed density, namely, that of liquid He^4 at this temperature under the vapor pressure. The selection of this temperature is to assure that we are well above the condensation temperature so that the system is in the "gaseous" phase, i.e., the fugacity is such that $|z|<1$.

One must point out at this stage that the relation between the pair distribution function defined by Goldstein and Reekie, $n(r,T)$, and our definition, $\rho^{(2)}(r,T)$ is such that the following relation holds true,

$$n(r,T) = \rho D(r,T), \tag{40}$$

where ρ is the density at the temperature T.

Let us consider first the pair correlation function calculated from the pseudo-potential method expressed in terms of ζ by Eq. (37). The parameter ζ as we know, is related to z through Eq. (38). We shall see presently that within the approximation considered in this calculation, Eq. (40) is just the pair correlation function for the ideal gas at the same temperature and density. In fact, consider an ideal Bose gas under the same conditions, i.e., with a density equal to that of liquid He^4 at 4.2°K. We know that in this case $D(r)$[15] is given by

$$D(r) = 1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}\left(z_0, \frac{r}{\lambda}\pi^{\frac{1}{2}}\right)\right]^2, \tag{41}$$

where z_0 is the fugacity for the ideal gas. The connection between z_0 and ρ is given by

$$\rho = \lambda^{-3}g_{\frac{3}{2}}(z_0). \tag{42}$$

This equation can be written in an alternative way if we introduce a parameter, T_0, called the "condensation temperature" for the ideal gas. If T_0 is given by

$$T_0 = \frac{h^2}{2\pi mk}\left(\frac{N}{2.612\Omega}\right)^{\frac{2}{3}}, \tag{43}$$

then Eq. (42) reads

$$(T_0/T)^{\frac{3}{2}} = 1/2.612g_{\frac{3}{2}}(z_0). \tag{44}$$

On the other hand, we know that for the hard sphere Bose gas, to first order in a/λ, the density of the system is determined by Eq. (36). Thus it follows that

$$\zeta = z_0,$$

and hence

$$z_0 = z[1-(8a/\lambda)g_{\frac{3}{2}}(z)]. \tag{45}$$

This means that the value for $D(r)$ calculated from Eq. (37) with a value of ζ determined from Eq. (36) is the same as the one calculated from Eq. (39) with a value of z determined from Eq. (45). Thus, we see since $\zeta=z_0$, that to first order in a/λ the pair distribution function obtained from the pseudo-potential method is the same for an ideal gas under the same conditions of temperature and density.

The evaluation of $D(r)$ is straightforward once ζ has

[12] This parameter is called ξ in their paper.

[13] Apparently, ζ would play the role of the fugacity in the gaseous phase since the off diagonal part of the interaction $J(p)$ is proportional to the equilibrium value of η, which is zero in this case, but the diagonal part of the interaction, which is independent of η and included in H_1, in (5), contains a term proportional to the square of the total number of particles and therefore contributes to $\ln z$ by the amount $8a/\lambda g_{\frac{3}{2}}(\zeta)$.[11]

[14] L. Goldstein and J. Reekie, Phys. Rev. **98**, 857 (1955).

[15] From now on, we shall omit the grand canonical ensemble average symbol $\langle\langle\ \rangle\rangle$.

TABLE I.[a]

r	$D(r)$	$n(r,4.2°K)$	r	$D(r)$	$n(r,4.2°K)$
0	2	3.768	5	1.0154	1.91
0.5	1.9715	3.714	6	1.0055	1.89
1	1.8057	3.402	7	1.002	1.886
1.5	1.5935	3.002	8	1.00087	1.885
2	1.3969	2.63	9	1.0004	1.8844
3	1.110	2.09	10	1.00016	1.884
4	1.040	1.96	∞	1	1.884

[a] We give the values for $D(r)$ calculated from Eq. (37) and the corresponding values for $n(r,4.2°K)$ calculated from Eq. (40) with $\rho=1.884\times10^{22}$ atoms/cc r is given in A and $n(V,T)$ in units of 10^{22} atoms/cc.

TABLE II.[a]

r	$D(r)$	$n(r,4.2°K)$	r	$D(r)$	$n(r,4.2°K)$
0	−00	−00	5	1.249	2.35
0.5	−9.11	−17.16	6	1.113	2.097
1	0.1068	0.2012	7	1.052	1.98
1.5	2.614	4.925	8	1.0246	1.93
2	2.953	5.56	9	1.011	1.906
3	2.136	4.02	10	1.0056	1.894
4	1.538	2.89	∞	1	1.884

[a] We give the values for $D(r)$ calculated from Eq. (51) and the corresponding values for $n(r,4.2°K)$ obtained from Eq. (40) with $\rho=1.884\times10^{22}$ atoms/cc r is given in A and $n(r,T)$ in units of 10^{22} atoms/cc.

been determined. If we use Eqs. (42) and (44) we get an equation for ζ, namely

$$g_{\frac{3}{2}}(\zeta)=\sum_{n=1}^{\infty}\frac{\zeta^n}{n^{\frac{3}{2}}}=2.612\left(\frac{T_0}{T}\right)^{\frac{3}{2}}.$$

At $T=4.2°K$ the density of liquid He^4 is 0.12518 g/cm^3 and with these values one finds that $T_0=2.842°K$. Thus, we get that

$$\sum_{n=1}^{\infty}\frac{\zeta^n}{n^{\frac{3}{2}}}=1.48. \tag{46}$$

The functions $g_\sigma(z)$ have been studied and tabulated for some values of z by Truesdell.[16] By using the formula[16]

$$g_{\frac{3}{2}}(z)=\Gamma(-\tfrac{1}{2})(-\ln z)^{\frac{1}{2}}+\sum_{n=0}^{\infty}\zeta(\tfrac{3}{2}-n)\frac{(\ln z)^n}{n!}, \tag{47}$$

where $\zeta(s-n)$[17] is the Riemann zeta function, and an interpolation method we found that the value of ζ satisfying Eq. (46) is equal to 0.8672. Thus, with r expressed in A it is found that Eq. (37) may be written as

$$D(r)=1+0.4731\times\left[\sum_{n=1}^{\infty}\frac{(0.8672)^n}{n^{\frac{3}{2}}}\exp\left(-0.17335\frac{r^2}{n}\right)\right]^2. \tag{48}$$

The evaluation of Eq. (48) was performed by direct summation for values of r up to 3 A and for $r>3$ A; the value of the series was calculated by using Poisson's summation formula. That is, for $r>3$ A we have that

$$g_{\frac{3}{2}}(\zeta,s)=\frac{(\pi)^{\frac{1}{2}}}{s}\sum_{m=-\infty}^{+\infty}\exp[-2s(-\ln\zeta+2\pi im)^{\frac{1}{2}}], \tag{49}$$

where

$$s=r\pi^{\frac{1}{2}}/\lambda. \tag{50}$$

The results are given in Table I, where $n(r,4.2°K)$ calculated with the use of Eq. (40) is expressed in units of 10^{22} atoms/cc.

We shall calculate the values of $n(r,4.2°K)$ by using the result for the pair correlation function obtained in I. We recall that the result is given by

$$D(r)=1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}(z,s)\right]^2-\frac{8a}{\rho^2\lambda^7}g_{\frac{3}{2}}(z)g_{\frac{3}{2}}(z,s)g_{\frac{3}{2}}(z,s)-\frac{8a}{\rho^2\lambda^7}\cdot\frac{\lambda}{r}[g_{\frac{3}{2}}(z,s)]^2, \tag{51}$$

where s is the same variable defined in Eq. (50).

From the expression for the grand potential q obtained by the BCE method to first order in a/λ,[18] it is possible to show that the relation between ρ and z is given by

$$\rho=\lambda^{-3}\left[g_{\frac{3}{2}}(z)-\frac{8a}{\lambda}g_{\frac{3}{2}}(z)g_{\frac{1}{2}}(z)\right]+0(a^2/\lambda^2).$$

However, this equation is the same as Eq. (36) if z and ζ are related by Eq. (45). It is then convenient to express Eq. (51) in terms of ζ and make use of the results obtained in the preceding case. We find that Eq. (51) reads

$$D(r)=1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}(\zeta,s)\right]^2+\frac{8a}{\rho^2\lambda^4}g_{\frac{3}{2}}(\zeta,s)g_{\frac{1}{2}}(\zeta,s)-\frac{8a}{r}\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}(\zeta,s)\right]^2, \tag{52}$$

where in Eq. (52) the first two terms are precisely the value of $D(r)$ obtained from the preceding method. Since $g_{\frac{3}{2}}(\zeta,s)$ is already known, it remains only to evaluate the series $g_{\frac{3}{2}}(\zeta,s)$. Again this was done by direct summation for values of r up to 3 A and by Poisson's summation formula for $r>3$ A. For this case we have

$$g_{\frac{3}{2}}(\zeta,s)=(\pi)^{\frac{1}{2}}\sum_{m=-\infty}^{+\infty}(-\ln\zeta+2\pi im)^{-\frac{1}{2}}\times\exp[-2s(-\ln\zeta+2\pi im)^{\frac{1}{2}}], \tag{53}$$

where s is given in Eq. (50). The results are given in Table II using the same units as in Table I.

[16] C. Truesdell, Ann. Math. **46, 144** (1945).

[17] The symbol $\zeta(s-n)$ should not be confused with the parameter ζ defined by Eq. (24).

[18] K. Huang, T. D. Lee, and C. N. Yang, "Stevens conference on the many body problem" (1957); also, T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1119 (1957).

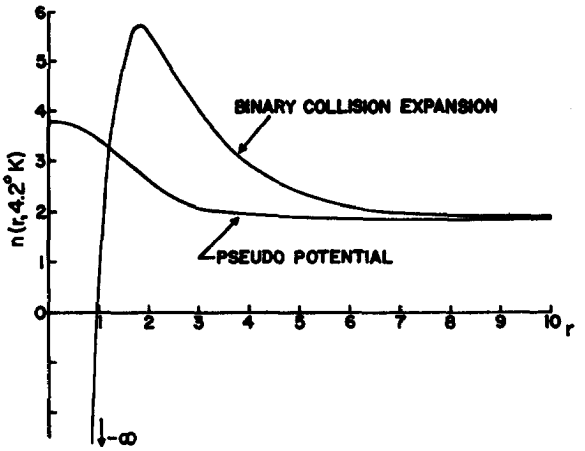

FIG. 1. The curves for the pdf of a hard sphere Bose gas obtained by the pseudo-potential and BCE methods, to first order in "a," are given at a temperature of 4.2°K. $n(Y,4.2°K)$ is given in units of 10^{22} atoms/cc and r is given in A.

In Fig. 1 we have plotted the results obtained by the two methods, the two curves being drawn to the same scale. The comparison with the experimental results cannot be accomplished for those values of r smaller than 2.5 A since the correlation functions for helium obtained from the experimental x-ray scattering intensity data have not been verified for this range.[14] The comparison is thus performed in the range $2.5 \leq r \leq 10$, where, according to Goldstein and Reekie, the experimentally obtained correlation functions should be good approximations to the actual ones for helium. The results are shown in Fig. 2 where the values for the experimental pdf were taken from the paper by Goldstein and Reekie[14] for $r \geq 6$ A and from the paper of Reekie and Beaumont[19] for $r < 6$ A. The agreement is good for large values of r (i.e., $r > 6$ A), but it is poor for small values of r. However, this was to be expected since in the BCE method we have calculated the contribution to the pdf only to the first order in a. With this approximation we have thus neglected terms of the order of $a^2, a^3, \cdots$ and so on, which appear when we take into account not only collisions between more than two particles, but also the contribution to scattering from higher angular momenta. These contributions involve greater values of the relative momenta between the particles and, therefore, they have a greater effect on the pdf at short distances if we are dealing with a system at a finite temperature. Besides, the pdf function would be modified for small values of r if there were an attractive potential outside the hard core considered in our case.

On the other hand, the pseudo-potential method yields a result which to first order in a reduces to the ideal gas case. This is because in the gaseous phase the momentum of the particles is not small and the pseudo-potential is equivalent to a hard core only for small relative momenta. At "high" temperatures, the momenta are large enough to allow the particles to overcome the repulsive action of the pseudo-potential, which is seen to become softer and softer as the temperature increases. Furthermore, the thermodynamical model that we have used here, following Yang and Lee,[10] has besides the above shortcoming, another defect which shall be discussed in Sec. 5.

5. DISCUSSION OF THE RESULTS

In this last section we wish to discuss the two results obtained for the pdf by the BCE and the pseudo-potential methods. However, our considerations will be more extensive than those required for the explanation of the discrepancies between these results. We shall obtain a very precise relation between the two methods which, to first order in a/λ, is able to tell us what we must expect when any equilibrium property of the system is evaluated through their use.

We recall that in the BCE method the general N particle U functions are expressed in terms of the binary kernel U_2 which in turn may be expressed in terms of the binary kernel U_2 which in turn may be expressed as a power series in the particle radius "a" for the case of hard spheres. Such expansion is graphically represented in Fig. 1 of I and may also be expressed as follows,

$$U_2 = aU_2^{(1)} + a^2U_2^{(2)} + \cdots. \tag{54}$$

Since our calculation has been performed to the first order in "a," we have kept in this series only the term represented by $U_2^{(1)}$.

On the other hand, let us calculate the effective interaction between two particles in momentum space if their interaction potential in coordinate space is the pseudo-potential interaction. By using the integral equa-

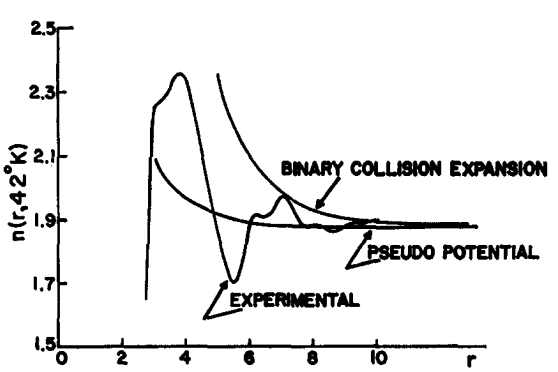

FIG. 2. The results shown in Fig. 1 are compared with the experimental values given by Goldstein and Reekie[14] and Reekie and Beaumont[19] for helium at 4.2°K.

[19] J. Reekie and C. F. A. Beaumont, Proc. Phys. Soc. (London) A228, 363 (1955).

tion for the propagator $K(\mathbf{r}',\beta';\mathbf{r},\beta)$ in r space, i.e.,

$$K(\mathbf{r}',\beta';\mathbf{r},\beta)=K_0(\mathbf{r}',\beta';\mathbf{r},\beta)-\int_\Omega K(\mathbf{r}',\beta';\mathbf{r}'',\beta'')V(\mathbf{r}'')\times K_0(\mathbf{r}''\beta'';\mathbf{r},\beta)d\beta''d^{3N}r'', \quad (55)$$

where $\mathbf{r}=(\mathbf{r}_1,\cdots,\mathbf{r}_N)$ and Eqs. I-(26),[20] we find that

$$K(\mathbf{k}',\beta';\mathbf{k},\beta)=K_0(\mathbf{k}',\beta';\mathbf{k},\beta)-\int_\Omega K(\mathbf{k}',\beta';\mathbf{p}'\beta'')H_I(\mathbf{p},\mathbf{p}')\times K_0(\mathbf{p},\beta'';\mathbf{k},\beta)d^{3N}pd^{3N}p'd\beta'', \quad (56)$$

where $\mathbf{k}=(\mathbf{k}_1,\cdots,\mathbf{k}_N)$ and

$$H_I(\mathbf{p},\mathbf{p}')=(2\pi)^{-3N}\int e^{-i\mathbf{p}'\cdot\mathbf{r}}V(\mathbf{r})e^{i\mathbf{p}\cdot\mathbf{r}}d^{3N}r. \quad (57)$$

For the case that $N=2$ and $V(r)$ is given by

$$V(\mathbf{r})=(16\pi a\hbar^2/2m)\partial(\mathbf{r}).$$

Equation (57) reduces to

$$H_I(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_1,\mathbf{k}_2)=(16\pi a\hbar^2)(2m\Omega)^{-1}\times(2\pi)^{-3}\partial(\mathbf{k}_1'+\mathbf{k}_2'-\mathbf{k}_1-\mathbf{k}_2), \quad (58)$$

which is the desired effective interaction.

Suppose, then, that we now form the series analogous to the one in Eq. (54) for the binary kernel with a pseudo-potential interaction, which we schematically represent by Fig. (3a). It is then easy to show that the diagram represented in Fig. (3b) and which corresponds to $U_2^{(1)}$ in Eq. (54) when calculated with the interaction given by Eq. (58) gives precisely the same result obtained from the BCE method to first order in "a." So far, then, the results obtained by the two methods ought to be the same.

However, in the pseudo-potential method the parameter η defined to be N_0/N' has been shown by Lee and Yang[10] to be equal to zero in the gaseous phase. This means, according to their expression for the Hamiltonian of the system,[21] that the only contribution

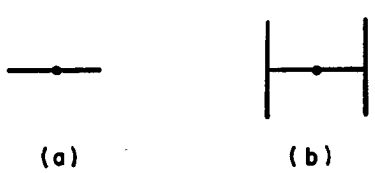

FIG. 3. (a) Schematic representation of the pseudo-potential interaction. (b) Diagram of the order "a" appearing in the power series expansion in "a" of the binary kernel with a pseudo-potential interaction.

[20] The notation I-( ) means Eq. ( ) of I.
[21] See Eq. (14) of footnote 10.

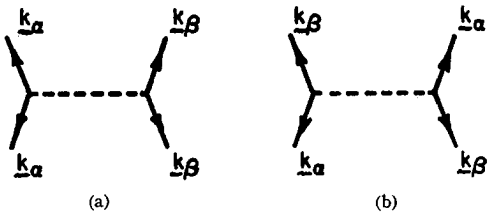

FIG. 4. (a) Direct diagram corresponding to one diagonal element of V'. (b) Exchange diagram corresponding to a diagonal element of V'.

besides the kinetic energy term, comes from the diagonal elements of the interaction potential V'. But since

$$V'=\frac{8\pi a}{\Omega}\sum a_\alpha^*a_\beta^*a_\mu a_\nu\delta^3(\mathbf{k}_\alpha+\mathbf{k}_\beta-\mathbf{k}_\mu-\mathbf{k}_\nu)$$

it is easily seen that these diagonal elements belong to two diagrams only. The first one is that for which $\mathbf{k}_\alpha=\mathbf{k}_\nu$, $\mathbf{k}_\beta=\mathbf{k}_\mu$ corresponding to a zero momentum transfer. This is the so-called direct diagram. The second one is the exchange diagram for which $\mathbf{k}_\alpha=\mathbf{k}_\mu$ and $\mathbf{k}_\beta=\mathbf{k}_\nu$. This diagram may be considered to have zero momentum transfer if we define this quantity to be the difference in momentum between the left (or right) incoming particle in the final and initial states disregarding the exchange effect. This is shown in Figs. (4a) and (4b). Thus, what we shall say from now on will apply to either case.

From the foregoing discussion we see that in the gaseous phase we must restrict ourselves to those diagrams in which the momentum transfer is zero. If we add this restriction to the effective interaction between two particles in momentum space given by Eq. (58), we must multiply this equation by a Krönecker delta $\partial_{\mathbf{k}_1'-\mathbf{k}_1}$. We obtain then

$$H_I(\mathbf{k}_1',\mathbf{k}_2';\mathbf{k}_1,\mathbf{k}_2)=\frac{16\pi a\hbar^2}{2m\Omega}\partial(\mathbf{k}_1'-\mathbf{k}_1)\partial(\mathbf{k}_2'-\mathbf{k}_2). \quad (59)$$

We reach then the last step in our discussion. In order to compare the two results for the pdf we must have a value for the classical binary kernel U_2 for the interaction given by Eq. (59). Since we know that

$$U_2(\mathbf{k}_1',\mathbf{k}_2',\beta;\mathbf{k}_1,\mathbf{k}_2,0)=K(\mathbf{k}_1'\mathbf{k}_2',\beta;\mathbf{k}_1,\mathbf{k}_2,0)-K_0(\mathbf{k}_1'\beta;\mathbf{k}_1,0)K_0(\mathbf{k}_2'\beta;\mathbf{k}_2,0) \quad (60)$$

and the free particle propagators are known [cf. Eq. (I-28)], we have just to solve Eq. (56) with the value of H_I given by Eq. (59). One finds that

$$K(\mathbf{k}_1',\mathbf{k}_2',\beta;\mathbf{k}_1,\mathbf{k}_2,0)=\partial(\mathbf{k}_1'-\mathbf{k}_1)\partial(\mathbf{k}_2'-\mathbf{k}_2)\exp\left[-\frac{\beta\hbar^2}{2m}\left(k_1^2+k_2^2+\frac{16\pi a}{\Omega}\right)\right]$$

and

$$U_2(\mathbf{k}_1',\mathbf{k}_2',\beta;\mathbf{k}_1,\mathbf{k}_2,0)$$
$$=\partial(\mathbf{k}_1'-\mathbf{k}_1)\partial(\mathbf{k}_2'-\mathbf{k}_2)\left\{\exp\left[-\frac{\beta\hbar^2}{2m}\left(k_1^2+k_2^2+\frac{16\pi a}{\Omega}\right)\right]-\exp\left[-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2)\right]\right\}. \quad (61)$$

In order to avoid confusion, from now on we shall call this result $U_{\rm pp}$ and the one obtained by the BCE method $U_{\rm BCE}$. This latter one is found to be given by

$$U_{\rm BCE}=-\frac{a}{\pi^2}\partial(\mathbf{K}'-\mathbf{K})\exp\left(-\frac{\beta\hbar^2}{4m}\mathbf{K}^2\right)(k^2-k'^2)^{-1}\times\left[\exp\left(-\frac{\beta\hbar^2}{2m}k'^2\right)-\exp\left(-\frac{\beta\hbar^2}{2m}k^2\right)\right],$$

where $\mathbf{K}$, $\mathbf{K}'$, $\mathbf{k}$ and $\mathbf{k}'$ are defined in terms of $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_1'$, and $\mathbf{k}_2'$ by means of Eq. (I-33). The momentum transfer is given by $\mathbf{p}=\mathbf{k}_1'-\mathbf{k}_1=\mathbf{k}'-\mathbf{k}$ (since $\mathbf{K}=\mathbf{K}'$), and thus we see that

$$\lim_{p\to 0}U_{\rm BCE}=-\frac{2a}{\pi^2}\frac{\beta\hbar^2}{2m}\partial(\mathbf{K}'-\mathbf{K})\exp[-\beta\hbar^2/2m(k_1^2+k_2^2)].$$

Furthermore, since we have taken $\mathbf{p}=0$ we can multiply this equation by a Kronecker's delta of $\mathbf{p}$, i.e., by

$$\partial_{\mathbf{p}}=\partial_{\mathbf{k}'-\mathbf{k}}=8\pi^3\Omega^{-1}\partial(\mathbf{k}'-\mathbf{k})$$

and get finally that

$$\lim_{p\to 0}U_{\rm BCE}=-\frac{16\pi a}{\Omega}\frac{\beta\hbar^2}{2m}\partial(\mathbf{k}_1'-\mathbf{k}_1)\partial(\mathbf{k}_2'-\mathbf{k}_2)\times\exp\left[-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2)\right]. \quad (62)$$

If we expand Eq. (61) in a powers series in "a," we see that the term of order a is just the same as Eq. (62). Thus, we have shown the following relation

$$\lim_{p\to 0}U_{\rm BCE}=U_{\rm pp}, \quad (63)$$

which is valid up to terms of order a. This equation implies that if we perform the calculation of the pdf for our system using the pseudo-potential method, to first order in a, we are considering only those diagrams for which the momentum transfer vanishes. Physically, it means that the collisions between the particles are elastic, and thus the gas behaves as an ideal one. This is the reason why the pdf given in Eq. (37) reduces to the formula of London.

One may also conclude that if any equilibrium property of a hard sphere Bose system is calculated, up to terms of order a, using the two methods, the results will in general be different. Any relation between them is to be considered as merely fortuitous. This is illustrated by the following example.

The grand potential for a hard sphere Bose gas has been evaluated by using the BCE method[18,22] yielding the following result:

$$\Omega^{-1}q=\lambda^{-3}[g_{\frac{5}{2}}(z)-(4a/\lambda)(g_{\frac{3}{2}}(z))^2]+0(a^2/\lambda^2). \quad (64)$$

This calculation may be repeated using $U_{\rm pp}$, which is seen to differ from the free particle propagator only by the factor

$$f=-(16\pi a/\Omega)(\hbar^2\beta/2m).$$

If the calculation is performed assuming that the correct potential is the sum of the direct and exchange parts of $U_{\rm pp}$, we get precisely Eq. (64). Thus, two different methods lead to the same result, but as we have pointed out before, this is merely fortuitous.

It is perhaps noteworthy to emphasize that for the particular case of the pdf of a hard sphere Bose system the BCE yields a correct answer, independently of the order in a to which the calculation is considered.

ACKNOWLEDGMENTS

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[22] J. Peretti, Tech. Note No. 119, Physics Department, University of Maryland (1958).

On the Pair Distribution Function of a Hard Sphere Bose System*†

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The pair distribution function for a quantum Bose gas is expressed as a power series in terms of the fugacity, the coefficients of which are temperature dependent. For the hard sphere case, these coefficients have been evaluated to the first order in a/λ, (a being the scattering length and λ the thermal wavelength) by using torons with two fixed points, or alternatively U cluster functions. The result gives the first order correction to the ideal gas formula of London and Placzek introduced by the interactions between the particles.

1. INTRODUCTION

SINCE the evaluation of the pair distribution function for an ideal Bose gas by London and Placzek,[1] very little seems to have been done in this connection, particularly when interactions between particles are introduced. The main reason for this has been the lack of an adequate method treating the many-body problem in quantum statistical mechanics. Recently, however, two such methods have appeared, the binary collision expansion of Yang and Lee[2] and the method of "torons" developed by Montroll and Ward.[3] These methods provide powerful tools for the calculation of thermodynamic properties of interacting systems in equilibrium.

In this paper we calculate the pair distribution function for an interacting Bose system using the binary collision-expansion method. We shall apply this method to the hard sphere gas and we shall evaluate the coefficients of the expansion in a power series of the fugacity to the first order in a/λ (a being the scattering length and λ the thermal wavelength). The result will give the first order corrections in "a" to the ideal gas, which are caused by the repulsive core.

2. FORMULATION OF THE PROBLEM

We consider a system of N particles of mass m whose Hamiltonian is

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2m}+V(\mathbf{r}_1,\cdots,\mathbf{r}_N)=T+V, \tag{1}$$

where the potential energy V is of the form,

$$V(\mathbf{r}_1,\cdots,\mathbf{r}_N)=\sum_{i>j}V(|\mathbf{r}_i-\mathbf{r}_j|). \tag{2}$$

The propagator[3] for the system is then defined by

$$K_N(\mathbf{r}',\mathbf{r})=\sum_n \bar{\varphi}_n(\mathbf{r})\varphi_n(\mathbf{r}')e^{-\beta E_n}, \tag{3}$$

where $\{\varphi_n\}$ is a complete orthonormal set of eigenfunctions of the Hamiltonian operator H obtained from Eq. (1), $\beta=(kT)^{-1}$, $\mathbf{r}=(\mathbf{r}_1,\cdots,\mathbf{r}_N)$, E_n are the eigenvalues corresponding to the set $\{\varphi_n\}$ and the summation is to be carried out over all symmetric or antisymmetric wave functions depending on whether the particles satisfy Bose Einstein or Fermi Dirac statistics.

The quantum mechanical distribution function for h particles is defined by the following relation:

$$\rho_N{}^{(h)}(\mathbf{r}_1,\cdots,\mathbf{r}_h)=\frac{1}{Z_N(N-h)!}\int\cdots\int W_N{}^{(q)} \times(\mathbf{r}_1,\cdots,\mathbf{r}_N;\mathbf{r}_1,\cdots\mathbf{r}_N)d^3r_{h+1}\cdots d^3r_N, \tag{4}$$

where Z_N is the partition function of the system and $W_N{}^{(q)}$ is a function which is related to the propagator K_N of the system by

$$W_N{}^{(q)}(\mathbf{r}_1',\cdots,\mathbf{r}_N';\mathbf{r}_1,\cdots,\mathbf{r}_N) =N!K_N(\mathbf{r}_1'\cdots\mathbf{r}_N';\mathbf{r}_1\cdots\mathbf{r}_N). \tag{5}$$

If one defines a quantity $W_{N,0}{}^{(\mathrm{cl})}(\mathbf{r}_1'\cdots\mathbf{r}_N';\mathbf{r}_1,\cdots,\mathbf{r}_N)$ for free particles as follows:

$$W_{N,0}{}^{(\mathrm{cl})}(\mathbf{r}_1'\cdots\mathbf{r}_N';\mathbf{r}_1\cdots\mathbf{r}_N) =K_1(\mathbf{r}_1',\mathbf{r}_1)K_1(\mathbf{r}_2',\mathbf{r}_2)\cdots K_1(\mathbf{r}_N',\mathbf{r}_N), \tag{6}$$

where $K_1(\mathbf{r}_i',\mathbf{r}_i)$ is just the free particle propagator for an interval of temperatures of length β^{-1}, given by

$$K_1(\mathbf{r}_i',\mathbf{r}_i)=\left(\frac{\alpha}{2\pi}\right)^{\frac{3}{2}}\exp\left[-\frac{\alpha}{2}(\mathbf{r}_i'-\mathbf{r}_i)^2\right] \tag{7}$$

and

$$\alpha=(2\pi/\lambda^2)=(m/\hbar^2\beta) \tag{8}$$

then, $W_N{}^{(q)}$ is also given by the relations

$$W_N{}^{(q)}(\mathbf{r}',\mathbf{r})=\sum_{\{P_{r'}\}}(\pm1)^{|P_{r'}|}P_{r'}W_N{}^{(\mathrm{cl})}(\mathbf{r}',\mathbf{r}), \tag{9}$$

where $\sum_{\{P_{r'}\}}$ is a summation over all permutation of the final coordinates, the (+) sign corresponding to bosons and the (−) sign to fermions, and where $W_N{}^{(\mathrm{cl})}(\mathbf{r}',\mathbf{r})$

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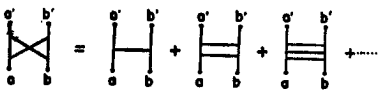

FIG. 1. The binary kernel or total binary interaction, $U_2^{(B)}(a',b';a,b)$.

is defined by the following expansion:

$$W_N^{(\mathrm{cl})}(\mathbf{r}',\mathbf{r}) = \sum_{n=1}^{\infty}(-1)^{n+1}\int_0^{\sum_{i=1}^{n}\beta_i=\beta} W_{N,0}^{(\mathrm{cl})}(\mathbf{r}',\mathbf{r}^1)V(\mathbf{r}^1) \times W_{N,0}^{(\mathrm{cl})}(\mathbf{r}^1,\mathbf{r}^2)\cdots V(\mathbf{r}^{n-1})W_{N,0}^{(\mathrm{cl})}(\mathbf{r}^{n-1},\mathbf{r}) \times d\beta_1\cdots d\beta_N d^3r^1\cdots d^3r^{n-1}. \quad (10)$$

Equation (9) is a very important one. It represents the fact that in calculating the propagator for a system of N quantum interacting particles one may neglect statistics at all intermediate stages. The statistics of the final state is obtained by simply permuting over all the final coordinates of the particles and summing over all these permutations. This equation has been emphasized by Yang and Lee.[2]

Let us denote by $W_N^{(B)}$ the function $W_N^{(q)}$ for a system of N interacting bosons. The pair distribution functions of the system is given by

$$\rho_N^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{Z_N(N-2)!}\int\cdots\int W_N^{(B)}(\mathbf{r}_1\cdots\mathbf{r}_N;\mathbf{r}_1,\cdots\mathbf{r}_N)d^3r_3\cdots d^3r_N. \quad (11)$$

The evaluation of the corresponding quantity $\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ for a grand canonical ensemble, as a power series in z, the fugacity of the system, was performed by Fujita, Isihara, and Montroll[4] by using the method of "torons." An alternate derivation has been presented by the authors[5] using a method which is very similar to the Mayer-Kahn-Uhlenbeck cluster integral expansion of the equation of state for imperfect gases. The result is the following:

$$\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = \rho^2 + F^{(2)}(\mathbf{r}_1,\mathbf{r}_2), \quad (12)$$

where ρ is the thermal average of the particle density of the system and $F^{(2)}$ is a function given by

$$F^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{p=0}^{\infty} z^{p+2}A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2), \quad (13)$$

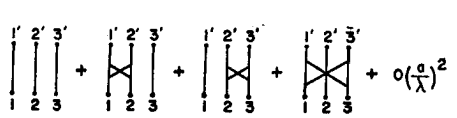

FIG. 2. Diagrammatic representation for the function $W_3^{(\mathrm{cl})}$ obtained by Yang and Lee.

[4] S. Fujita, A. Isihara, and E. W. Montroll, Bull. classe sci. Acad. roy. Belg. 44, 1006 (1958).
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where $A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ is a generalized cluster integral

$$A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{p!}\int\cdots\int U_{p+2}^{(B)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{t}_1,\cdots\mathbf{t}_p)d^3t_1\cdots d^3t_p. \quad (14)$$

The function $U_{p+2}^{(B)}$ appearing in Eq. (14) is the short hand notation for the diagonal part of the generalized cluster function U for $p+2$ particles as defined by Yang and Lee,[2] namely

$$U_{p+2}^{(B)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{t}_1\cdots\mathbf{t}_p;\mathbf{r}_1\mathbf{r}_2,\mathbf{t}_1\cdots\mathbf{t}_p).$$

The problem of evaluating the pair distribution function for an interacting system composed of bosons reduces to the evaluation of the function $F^{(2)}$ defined in Eq. (13) and to this task we shall devote the following sections.

3. DIAGRAMMATIC ANALYSIS OF THE FUNCTION $U_N(\mathbf{r}_1\cdots\mathbf{r}_N)$

The first step in the calculation of $F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ is to find a way of computing the generalized cluster integral

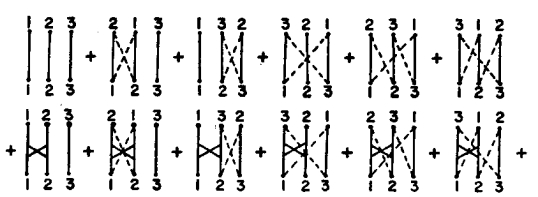

FIG. 3. Diagrammatic form of the function $W_3^{(B)}$ after statistics have been considered in the final states.

$A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ given in Eq. (14). The binary collision expansion method[2] provides a tool for such a computation and we shall obtain a general expression $U_N^{(B)}(\mathbf{r}_1\cdots\mathbf{r}_N)$ in terms of the total binary interaction, which is schematically represented by the diagram in Fig. 1. In this figure, the diagram with n interaction lines corresponds to the $(n+1)$th term in the expansion, Eq. (10), for $N=2$ (the two body problem).

Although the method that we shall describe is quite general, we are interested only in applying it to the calculation of the pair distribution function for a system of hard sphere bosons to the order of a/λ at most. Therefore, we shall only keep those terms which are of this order.

We first express the function $W_N^{(\mathrm{cl})}(r_N)$ in terms of the classical U functions in the same way as is done in Mayer's theory of the imperfect gas. Then, from Eq. (9) we construct $W_N^{(B)}$ for the boson case which in turn yields an expression for $U_N^{(B)}$. This gives us the function $U_N^{(B)}$ for a boson system in terms of the classical U's. The next step is to obtain $U_3^{(\mathrm{cl})}$, $U_4^{(\mathrm{cl})}$, $\cdots$ in terms of $U_2^{(\mathrm{cl})}$ and this has been done by Yang and

Lee.[2] Finally, since we know that $U_2^{(cl)}$ is of the order a/λ, $U_3^{(cl)}$ of the order a^2/λ^2 and so on, we omit all those diagrams containing $U_2^{(cl)}$ two or more times; in principle, we are left with a series of diagrams, all of order a/λ at most, and this is the required expression for $U_N^{(B)}$.

To be more explicit, let us consider the case $N=3$. From the results obtained by Yang and Lee we have in Fig. 2 the expression for $W_3^{(cl)}$.

According to Eq. (10), $W_3^{(B)}$ is obtained from $W_3^{(cl)}$ by adding together all possible permutations of the prime coordinates. In this way, we obtain 24 diagrams of order a/λ at most. We then identify each primed coordinate with the corresponding unprimed one, i.e., $\mathbf{r}_1'=\mathbf{r}_1$, $\mathbf{r}_2'=\mathbf{r}_2$, $\mathbf{r}_3'=\mathbf{r}_3$. The aforementioned permutations, then, give rise to permutations among the unprimed coordinates and these are represented by dotted lines. The result is shown in Fig. 3.

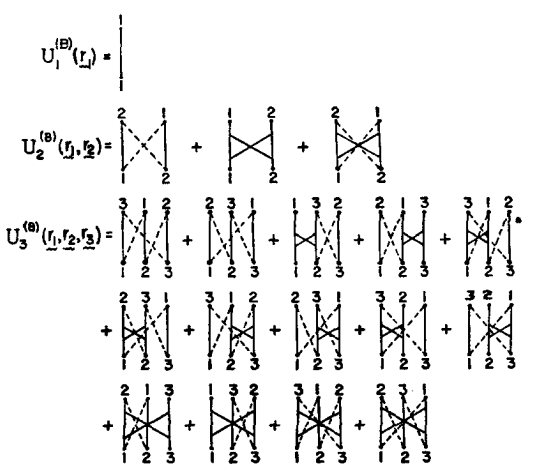

FIG. 4. Diagrammatic representation of the functions $U_N^{(B)}$, $N=1, 2, 3$ obtained from $W_3^{(B)}$.

From the equations relating the $U^{(B)}$ functions with the $W^{(B)}$ functions[6] in the Bose case, we find that the $U_N^{(B)}$ functions for $N=1, 2, 3$ are the ones shown in Fig. 4 where $U^{(B)}(\mathbf{r}_1,\mathbf{r}_3)$ and $U_2^{(B)}(\mathbf{r}_2,\mathbf{r}_3)$ have the same representation as $U_2^{(B)}(\mathbf{r}_1,\mathbf{r}_2)$. The structure of each of the $U_N^{(B)}$ functions is clear from this example and we can, therefore, conclude that for any integer N we can represent this function as a sum of diagrams. This is shown in Fig. 5 where the first summation is over all possible distinct cycles in which all N particles are involved (connected diagrams). The second sum is over all possible diagrams containing two disjoint cycles, the interaction being between two particles in this cycle. The third sum is over all possible diagrams which contain one cycle, the interaction being between two particles in this cycle. Using this expression for $U_N^{(B)}$ we shall proceed in the following sections to evaluate the generalized cluster integral $A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$.

[6] These equations are explicitly written in Eq. (1–6) of footnote 2.

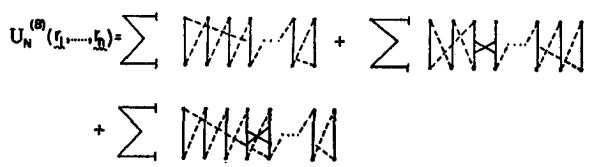

FIG. 5. The function $U_N^{(B)}(\mathbf{r}_1,\cdots\mathbf{r}_N)$ for any integer N, is represented as a sum of three terms, each one being a sum over different kind of diagrams.

4. CALCULATION OF THE FUNCTION $F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ FOR A HARD SPHERE BOSE GAS

A. Contribution of the First Kind of Diagrams

The first term appearing in Fig. 5 will give that contribution to the function $F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ corresponding to the ideal gas. The diagrams that are contained in such term will be called of the first kind. The evaluation of the generalized cluster integral $A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ for this kind of diagrams is readily done, but we must remember that the coordinates of particles 1 and 2 remain constant in the integration.

Let us consider a typical first kind diagram which is shown in Fig. 6a. In this diagram, there are n_1 particles between particles 1 and 2; n_2 particles between 2 and 1 and $n_1+n_2=N$. The integral of this diagram over all coordinates, except 1 and 2, is equal to the product of the propagator for a free particle and a "reciprocal temperature interval" $n_1\beta$ and the propagator for a second free particle and a "reciprocal temperature interval" $n_2\beta$. Let us introduce the convention of representing an integrated diagram of the kind appearing in Fig. 5 by a "toron,"[7] i.e., a closed loop containing as many cycles as particles in the diagram. The integrated diagram corresponding to Fig. 6a is shown in Fig. 6b and its contribution to the generalized cluster integral $A_p^{(2)}$ is given by

$$\left(\frac{\alpha}{2\pi n_1}\right)^{\frac{3}{2}}\left(\frac{\alpha}{2\pi n_2}\right)^{\frac{3}{2}} \times\exp\left[-\frac{\alpha}{2n_1}(\mathbf{r}_1-\mathbf{r}_2)^2-\frac{\alpha}{2n_2}(\mathbf{r}_1-\mathbf{r}_2)^2\right]. \quad (15)$$

As it is shown in Appendix A the total number of diagrams of this kind, for a fixed value of n_1 and n_2 is $(N-2)!$ so that the contribution of the first kind of diagrams to the generalized cluster integral $A_p^{(2)}$ is

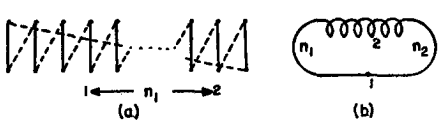

FIG. 6. (a) A typical diagram of the first kind. n_1 is the number of particles between 1 and 2; n_2 the number of particles between 2 and 1; and $n_1+n_2=N$. (b) The integrated diagram shows explicitly points 1 and 2 and the corresponding cycles n_1 and n_2.

[7] See footnote 3 for a discussion of this concept.

after letting $N=p+2$ [8]

$$\sum_{\substack{n_1=1\\{n_1+n_2=p+2\}}}^{p+1}\left(\frac{\alpha}{2\pi n_1}\right)^{\frac{3}{2}}\left(\frac{\alpha}{2\pi n_2}\right)^{\frac{3}{2}}\times\exp\left[-\frac{\alpha}{2n_1}(\mathbf{r}_1-\mathbf{r}_2)^2-\frac{\alpha}{2n_2}(\mathbf{r}_1-\mathbf{r}_2)^2\right], \quad (16)$$

where $\{n_1+n_2=p+2\}$ denotes all possible sets of values of n_1 and n_2 such that their sum is equal to $p+2$. By calling $F_0^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ the function $F^{(2)}$ for the ideal gas, we have after substituting (16) into (13) and setting $z^{p+2}=z^{n_1+n_2}$,

$$F_0^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{n_1+n_2+2=0}^{\infty}\sum_{n_1=1}^{n_1+n_2+1}\left(\frac{\alpha}{2\pi}\right)^3\frac{z_1^{n_1}}{n_1^{\frac{3}{2}}}\times\exp\left[-\frac{\alpha}{2n_1}(\mathbf{r}_1-\mathbf{r}_2)^2\right]\frac{z_2^{n_2}}{n_2^{\frac{3}{2}}}\exp\left[-\frac{\alpha}{2n_2}(\mathbf{r}_1-\mathbf{r}_2)^2\right].$$

By rearranging terms and using the function

$$g_\sigma(z,s)=\sum_{n=1}^{\infty}\frac{z^n}{n^\sigma}\exp(-s^2/n), \quad (17)$$

we obtain

$$F_0^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=\lambda^{-6}\left\{g_{\frac{3}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right]\right\}^2, \quad (18)$$

where $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$.

By writing the pair distribution function $\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ in terms of the pair correlation function $g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$, we have

$$\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=\rho^2 g^{(2)}(\mathbf{r}_1,\mathbf{r}_2), \quad (19)$$

so that

$$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=1+\rho^{-2}F^{(2)}(\mathbf{r}_1,\mathbf{r}_2). \quad (20)$$

Thus, from Eqs. (18) and (20) we get the pair correlation function for an ideal Bose gas

$$g_0^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=1+\frac{1}{\rho^2}\left(\frac{\alpha}{2\pi}\right)^3\left[\sum_{n=1}^{\infty}\frac{z^n}{n^{\frac{3}{2}}}\exp\left(-\frac{\alpha}{2n}r_{12}^2\right)\right]^2, \quad (21)$$

which is the well-known formula of London and Placzek.

B. Transformation Formulas from Coordinate to Momentum Space

The evaluation of the contribution to the function $F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ resulting from the second and third terms in Fig. 5 is most easily performed in momentum space; therefore, in this section, we shall give the necessary formulas to perform such a calculation. Let us consider the eigenstates of the coordinates, the momenta and the energy which we shall denote, respectively, by $|r\rangle$, $|k\rangle$ and $|n\rangle$. These eigenstates are related by

$$\langle r|n\rangle=\varphi_n(r) \quad \langle k|n\rangle=\psi_n(k), \quad (22)$$

where $\varphi_n(r)$ is the properly symmetrized eigenfunction of the Hamiltonian H of the system corresponding to the eigenvalue E_n and $\psi_n(k)$ is its Fourier transform

$$\psi_n(k)=(2\pi)^{-3N/2}\int\varphi_n(r)e^{ik\cdot r}d^{3N}r. \quad (23)$$

It must be emphasized that Eq. (23) is valid true regardless of whether the wave function $\varphi_n(r)$ obeys Fermi-Dirac or Bose-Einstein statistics, provided that it is properly normalized.

Starting from the definition, Eq. (3), of the propagator for the system, it is easily shown that

$$K(\mathbf{r}',\mathbf{r})=\langle\mathbf{r}'|e^{-\beta H}|\mathbf{r}\rangle. \quad (24)$$

Thus, we can define in a similar way a propagator in momentum space by

$$\hat{K}(\mathbf{k}',\mathbf{k})=\langle\mathbf{k}'|e^{-\beta H}|\mathbf{k}\rangle, \quad (25)$$

which is related to $K(\mathbf{r}',\mathbf{r})$ by

$$\hat{K}(\mathbf{k}',\mathbf{k})=(2\pi)^{-3N}\int e^{-ik'\cdot r'+ik\cdot r}K(\mathbf{r}',\mathbf{r})d^{3N}rd^{3N}r' \quad (26a)$$

$$K(\mathbf{r}',\mathbf{r})=(2\pi)^{-3N}\int e^{ik'\cdot r'-ik\cdot r}\hat{K}(\mathbf{k}',\mathbf{k})d^{3N}kd^{3N}k'. \quad (26b)$$

It is also possible to define functions $\hat{W}_N(\mathbf{k}',\mathbf{k})$ and $\hat{U}_N(\mathbf{k}',\mathbf{k})$ in terms of $\hat{K}_N(\mathbf{k}',\mathbf{k})$ just as $W_N(\mathbf{r}',\mathbf{r})$ and $U_N(\mathbf{r}',\mathbf{r})$ have been defined in terms of $K_N(\mathbf{r}',\mathbf{r})$. It follows that the pairs $(U_N,\hat{U}_N)$ and $(W_N,\hat{W}_N)$ satisfy the same duality formulas analogous to Eqs. (26) as the pair $(K,\hat{K})$ does. For example,

$$\hat{U}_N(\mathbf{k}',\mathbf{k})=(2\pi)^{-3N}\int e^{-ik'\cdot r'+ik\cdot r}U^N(\mathbf{r}',\mathbf{r})\times d^{3N}rd^{3N}r' \quad (27a)$$

$$U_N(\mathbf{r}',\mathbf{r})=(2\pi)^{-3N}\int e^{ik'\cdot r'-ik\cdot r}\hat{U}_N(\mathbf{k}',\mathbf{k})\times d^{3N}kd^{3N}k'. \quad (27b)$$

Equations (26a) and (27a) enable us to calculate the free particle propagator and the binary kernel in momentum space from their corresponding expressions in coordinate space. By using Eq. (7) it is easily seen that the free particle propagator in momentum representation is just given by

$$\hat{K}(\mathbf{k}',\mathbf{k})=\delta(\mathbf{k}'-\mathbf{k})\exp(-k^2/2\alpha). \quad (28)$$

Since the binary kernel $U_2^{(B)}(\mathbf{r}_1'\mathbf{r}_2';\mathbf{r}_1\mathbf{r}_2)$ depends on the special kind of interaction which exists amongst the particles in the system, we shall only limit ourselves to the case of hard spheres. For particles having radius "a," the hard sphere interaction is defined by

$$V(|\mathbf{r}_i-\mathbf{r}_j|)=\infty \quad \text{for} \quad |\mathbf{r}_i-\mathbf{r}_j|\leq 2a$$
$$=0 \quad \text{for} \quad |\mathbf{r}_i-\mathbf{r}_j|\geq 2a. \quad (29)$$

[8] Because we need $\int U_{p+2}^{(B)}(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)d^3r_3\cdots d^3r_N$ and we have calculated $\int U_N^{(B)}(\mathbf{r}_1,\cdots,\mathbf{r}_N)d^3r_3\cdots d^3r_N$.

Under these conditions it has been shown[2,9] that the binary kernel in coordinate space, to first order in "a," is given by

$$U_2^{(cl)}(\mathbf{r},\mathbf{r}';\mathbf{R},\mathbf{R}')=-\left(\frac{\alpha}{\pi}\right)^3\frac{a}{8}$$

$$\times\exp[-\alpha(\mathbf{R}-\mathbf{R}')^2]\frac{r+r'}{rr'}\exp[-\alpha(r+r')^2], \quad (30)$$

where $\mathbf{r}$, $\mathbf{r}'$, $\mathbf{R}$, and $\mathbf{R}'$ are the center of mass and relative coordinates of the interacting pair of particles.

By substituting Eq. (30) into Eq. (27a) one obtains

$$\hat{U}_2^{(cl)}(\mathbf{k}_1',\mathbf{k}_2';\mathbf{k}_1,\mathbf{k}_2)$$
$$=\partial(\mathbf{K}_{12}'-\mathbf{K}_{12})\exp\left(-\frac{K_{12}^2}{4\alpha}\right)\frac{\Delta G_0}{\pi^2}, \quad (31)$$

where

$$\Delta G_0=-\frac{a}{k_{12}'^2-k_{12}^2}\left[\exp\left(-\frac{k_{12}^2}{\alpha}\right)-\exp\left(-\frac{k_{12}'^2}{\alpha}\right)\right] \quad (32)$$

and

$$\mathbf{K}_{12}=\mathbf{k}_1+\mathbf{k}_2 \qquad \mathbf{k}_{12}=\tfrac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)$$
$$\mathbf{K}_{12}'=\mathbf{k}_1'+\mathbf{k}_2' \qquad \mathbf{k}_{12}'=\tfrac{1}{2}(\mathbf{k}_1'-\mathbf{k}_2'). \quad (33)$$

Equations (28), (31), and (32) are all the expressions that we shall need in subsequent calculations.

C. Contribution of the Second and Third Kind of Diagrams

Let us consider next the contribution from the diagrams of the second kind appearing in the second sum of the expression for $U_N^{(B)}$. In this case, we have two classes of diagrams which give different contributions, namely, the first class which consists of all those diagrams having particles 1 and 2 in the same cycle, and the second class which consists of those diagrams in which particles 1 and 2 are in different cycles (a special case in this class will be the one where particles 1 and 2 form the interacting pair). A similar classification holds for the third kind of diagrams, appearing in the third sum of the expression for $U_N^{(B)}$, but as we shall see, they may be reduced to either of the two classes for the second kind of diagrams. We shall consider these classes separately.

(i) *First Class of Diagrams*

A typical diagram pertaining to this class is shown in Fig. 7a where the total number of particles N has been divided into two parts, N_1 and N_2. The first one gives the number of particles in the cycle to the left of the interacting pair and the second one the number of particles in the cycle to the right. Thus, $N_1+N_2=N$. The number N_1 is itself subdivided into three numbers: n_3 which gives the number of particles preceding particle 1 and excluding it; n_1 which gives the number of particles between 1 and 2, including 1 and excluding 2;

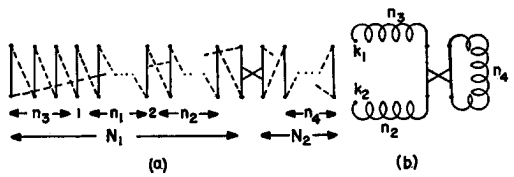

FIG. 7. (a) A typical diagram of the second kind, first class. n_3 is the number of particles preceding particle 1; n_1 the number of particles between 1 and 2 excluding 2; n_2 the number of particles between 2 and the particle preceding the interacting pair; n_4 the number of particles following the particle which is after the interacting pair. (b) The integrated diagram in momentum space. Since $\mathbf{k}_1$ and $\mathbf{k}_2$ are constant in the integration, the number of particles between 1 and 2 do not have to be specified, so we have left the diagram "open."

n_2 gives the number of particles between particle 2, this one included, and the particle preceding the left interacting particle. Therefore, the following relation holds

$$n_1+n_2+n_3+1=N_1.$$

Similarly N_2 is expressed as a sum n_4+1, where n_4 is the number of particles between the right interacting particle, which is excluded, and the last particle. In Appendix A we give another way of visualizing these diagrams when we discuss the combinational factor associated with each one of them.

The integration of this diagram over all momenta of the particles except that of particles 1 and 2 is straightforward. If we label by $\mathbf{k}_3$ and $\mathbf{k}_4$ the initial momenta of the interacting pair and by $\mathbf{k}_5$ and $\mathbf{k}_6$ the final momenta, we see that the integrated diagram is equal to the product of four free particle propagators, in momentum space, over reciprocal temperature intervals of $n_1\beta$, $n_2\beta$, $n_3\beta$ and $n_4\beta$, respectively, times the binary kernel for the interacting pair. That is, we have the following result:

$$\int\partial(\mathbf{k}_1-\mathbf{k}_5)\exp\left(-\frac{k_1^2}{2\alpha}n_3\right)\partial(\mathbf{k}_2-\mathbf{k}_3)$$
$$\times\exp\left(-\frac{k_2^2}{2\alpha}n_2\right)\partial(\mathbf{k}_6-\mathbf{k}_4)\exp\left(-\frac{k_6^2}{2\alpha}n_4\right)$$
$$U_2^{(cl)}(\mathbf{k}_5,\mathbf{k}_6;\mathbf{k}_3,\mathbf{k}_4)d^3k_5d^3k_6d^3k_3d^3k_4 \quad (34)$$

and the integrated diagram is shown in Fig. 7b.

Integration of Eq. (34) over the coordinates $\mathbf{k}_3$, $\mathbf{k}_4$ and $\mathbf{k}_5$ yields the following expression:

$$\exp\left(-\frac{k_1^2}{2\alpha}n_3-\frac{k_2^2}{2\alpha}n_2\right)\int\exp\left(-\frac{k_6^2}{2\alpha}n_4\right)$$
$$U_2^{(cl)}(\mathbf{k}_1,\mathbf{k}_6;\mathbf{k}_2,\mathbf{k}_6)d^3k_6. \quad (35)$$

The integration of Eq. (35) and its subsequent transformation to the space representation are given in Appendix B. If we denote by $D_1(n_1,n_2,n_3,n_4;\mathbf{r}_{12})$ the contribution of the first class of diagrams to the func-

[9] Jean Peretti, Tech. Rept. No. 119 (1958), Physics Dept., University of Maryland.

tion $F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$, we get

$$D_1(n_1,n_2,n_3,n_4;\,\mathbf{r}_{12}) = -\frac{4a}{\lambda^7}\frac{1}{[n_1(N_1-n_1)N_2]^{\frac{3}{2}}}\exp\left(-\frac{N_1}{n_1(N_1-n_1)}S^2\right), \quad (36)$$

where $S^2=(\alpha/2)r_{12}^2$. The numbers n_1, n_2, n_3, n_4 are subject to the following relations and inequalities:

$$\begin{gathered} n_1+n_2+n_3=N_1-1 \quad n_4=N_2-1 \\ N_1+N_2=N \\ 1\leq n_1\leq N_1-1 \quad 0\leq n_2\leq N_1-1 \\ 2\leq N_1\leq N-1 \quad 0\leq N_2\leq N-2 \\ 0\leq n_3\leq N-1. \end{gathered} \quad (37)$$

The total contribution of these diagrams to the generalized cluster integral $A_p^{(2)}$ with a given set of numbers is

$$(1/p!)(N-2)!D_1(n_1,n_2,n_3,n_4;\,\mathbf{r}_{12}), \quad (38)$$

where $N=p+2$ and $(N-2)!$ is the number of such diagrams (c.f. Appendix A) by taking into account the possibility of having the particles 1 and 2 at either side of the interacting pair of particles. Therefore, the contribution to the function $F^{(2)}$ is

$$F_1'^{(2)}(\tilde{\mathbf{r}}_1,\mathbf{r}_2)=\sum_{N=2}^{\infty} Z^N \sum_{\{n_1\cdots n_4\}} D_1(n_1,n_2,n_3,n_4;\,\mathbf{r}_{12}), \quad (39)$$

where the second summation is to be carried out over all possible set of values of n_1, n_2, n_3, n_4 by satisfying Eq. (37).

With the aid of Eqs. (17) and (36) we finally obtain, for the contribution of the first class of diagrams to the function $F^{(2)}$, the following expression:

$$F_{(1)}'^{(2)}=-\frac{4a}{\lambda^7}g_{\frac{3}{2}}(z)g_{\frac{3}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right]g_{\frac{3}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right], \quad (40)$$

where

$$g_{\frac{3}{2}}(z)=\sum_{n=1}^{\infty}\frac{z^n}{n^{\frac{3}{2}}}.$$

The diagrams belonging to the first class of the third kind, give the same contribution as the diagrams of the first class and second kind. In coordinate representation this is shown graphically in Fig. 8. It is easy to see that the propagator for such diagrams could be obtained from the propagator for the first class second kind diagrams by means of the transformation $\mathbf{r}'\rightarrow-\mathbf{r}'$ and $\mathbf{r}\rightarrow-\mathbf{r}$. This transformation leaves the binary kernel invariant and thus the contribution is the same and it is given by Eq. (40). Hence, the combined contribution of the first class, second and third kind, of diagrams is given by

$$F_{(1)}^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = -\frac{8a}{\lambda^7}g_{\frac{3}{2}}(z)g_{\frac{3}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right]g_{\frac{3}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right]. \quad (41)$$

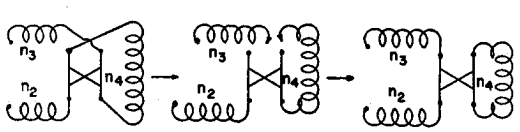

FIG. 8. A graphical representation of the process by means of which a diagram belonging to the first class and third kind is transformed into a diagram of the first class and second kind.

(ii) *Second Class of Diagrams*

A typical diagram of this class is the one shown in Fig. 9a. The numbers n_1, n_2, n_3, n_4, N_1, and N_2 have a meaning similar to the ones in the preceding case and which may be inferred from the figure. They satisfy the following set of relations and inequalities:

$$\begin{gathered} n_1+n_2+1=N_1 \quad n_3+n_4+1=N_2 \\ N_1+N_2=N \\ 0\leq n_1\leq N_1-1 \quad 0\leq n_2\leq N_1-1 \\ 0\leq n_3\leq N_2-1 \quad 0\leq n_4\leq N_2-1. \end{gathered} \quad (42)$$

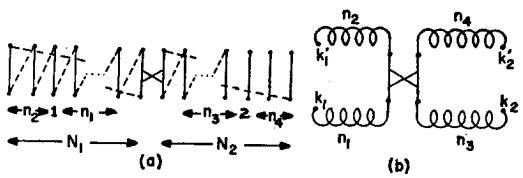

FIG. 9. (a) A typical diagram of the second class and second kind. The numbers n_1, n_2, n_3, n_4, N_1 and N_2 are defined in a similar way as in Fig. 7(a). (b) The integrated diagram in momentum space where the two ends have been left open.

The integration of this diagram over all momenta follows the same pattern as the preceding case. The integrated diagram is shown in Fig. 9b and the result is given by

$$\hat{U}_2(\mathbf{k}_1',\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2) \times\exp\left(-\frac{1}{2\alpha}[n_1k_1^2+n_2k_1'^2+n_3k_2^2+n_4k_2'^2]\right), \quad (43)$$

where we have taken into account the conservation of momentum expressed by the delta function occurring in the free propagator Eq. (29).

The integration of Eq. (43) is given in Appendix C. The contribution of the second class diagrams is then found to be

$$F_{(2)}^{(2)}=-\frac{8a}{\lambda^7}\cdot\frac{\lambda}{r_{12}}\left\{g_{\frac{3}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right]\right\}^2, \quad (44)$$

where we have already multiplied by a factor of 2, which arises from the fact that the contribution to this function from the second class and third kind of diagrams is the same. This can be shown in a way similar to the preceding case.

5. FINAL RESULTS

The total contribution to the function $F^{(2)}$ of the three different kinds of diagrams appearing in Fig. 5 is given by

$$\lambda^6 F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=[g_{\frac{3}{2}}(z,s)]^2-\frac{8a}{\lambda}g_{\frac{3}{2}}(z)g_{\frac{1}{2}}(z,s)g_{\frac{3}{2}}(z,s)-\frac{8a}{\lambda}\cdot\frac{\lambda}{r_{12}}[g_{\frac{3}{2}}(z,s)]^2, \quad (45)$$

where

$$s=\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}. \quad (46)$$

Thus, the pair correlation function of a hard sphere Bose system, is given to first order in a/λ, by the following equation:

$$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=1+\left[\frac{1}{\rho\lambda^3}g_{\frac{3}{2}}(z,s)\right]^2-\frac{8a}{\rho^2\lambda^7}g_{\frac{1}{2}}(z)g_{\frac{1}{2}}(z,s)g_{\frac{3}{2}}(z,s)-\frac{8a}{\rho^2\lambda^7}\cdot\frac{\lambda}{r_{12}}[g_{\frac{3}{2}}(z,s)]^2. \quad (47)$$

Two comments might be added about this result. First, the fact that the series $g_\sigma(z)$ and $g_\sigma(z,s)$ converge only for those values of z such that $|z|<1$, independently of σ, makes this result valid only when the system is in the gaseous phase. Second, the last term in Eq. (47) depends on the inverse interparticle distance, and thus makes the result valid only for large interparticle separations. These short comings shall be corrected in a further calculation.

APPENDIX A

In this appendix we evaluate the combinatorial factor associated with each of the three kinds of diagrams appearing in the expression for $U_N^{(B)}$. We shall label with the numbers 1 and 2 the particles whose coordinates are not integration variables in the evaluation of the generalized cluster integral $A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$.

Let us consider the diagrams of the first kind which include only one cycle without any interaction. To each diagram we associate a box which is constructed in the following way: we subdivide the box in N cells and fix particle 1 in the first cell, particle 2 in another cell in such a way that the number of particle (or cells) between them remains constant. The permutation symbol that corresponds to any such arrangement of the N particles amongst the N cells is the symbol of the cycle. This permutation symbol defines one and only one diagram. Let us call n_1 the number of particles between 1 and 2 including 1 and n_2 the remaining particles, so $n_1+n_2=N$. Then, for instance, if $n_1=3$, $n_2=5$, $N=8$ we have as a possible box the one shown in Fig. 10a and its corresponding diagram is shown in Fig. 10b. The number of diagrams which give the same contribution to the generalized cluster integral $A_p^{(2)}$, for a fixed value of n_1, is simply $(N-2)!$, which is the number of

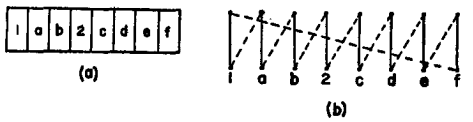

FIG. 10. (a) A possible box for $n_1=3$, $n_2=5$ and $N=8$. (b) The only diagram corresponding to that box. It is defined by the permutation symbol corresponding to the arrangement of the 8 particles in the 8 cells of the box.

arrangements of the $N-2$ remaining particles in the $N-2$ remaining cells. It is noteworthy to point out that with the convention of assigning particle 1 to the first cell, the correspondence between boxes and diagrams *in this case only*, is one to one. Thus, the contribution of these first kind of diagrams to $A_p^{(2)}$ is given in Eq. (16).

Let us consider next the box diagrams belonging to the second kind of diagrams. We first construct our boxes by partitioning the N cells into two groups, one of N_1 particles and another one of N_2 particles. The line between these two partitions will define the interacting pair as being the one composed by the two particles occupying the cells adjacent to it. To each box we associate a diagram in the following way: The permutation symbol defined by the numbers located in the cells to the left of the partition line, will give the first cycle of diagram, whereas the second cycle is given by the permutation symbol defined by the numbers located in the cells to the right of the partition line. It is, however, fairly obvious from the discussion, that since particles 1 and 2 remain unaffected in the integrations, the contribution of each diagram to $A_p^{(2)}$ will depend on the relative positions of these particles with respect to the partition line, so we must consider two classes of boxes:

Class A

The boxes belonging to this class will be such that particles 1 and 2 are always in the same side of the partition line, i.e., on the same cycle. These are the first class diagrams.

Class B

To this class will belong those boxes in which particles 1 and 2 are on different cycles, i.e., on opposite sides of the partition line. These correspond to second class diagrams.

Furthermore, let us assume that in these boxes, particle 1 shall be always written at the left of the partition line; with this convention, the correspondence between boxes and diagrams is one to one.

Consider now the boxes and diagrams belonging to class A. The most general type of box is that shown in Fig. 11 where there are n_3 cells before 1, n_1 cells before 2, n_2 cells between 2 and the cell to the left of the partition line and finally n_4 cells between the cell to the right of this line and the last one. Then,

$$n_1+n_2+n_3+1=N_1; \quad n_4+1=N_2.$$

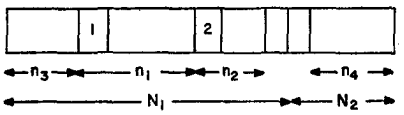

FIG. 11. The general type of box associated with a diagram of the first class and second kind. The partition line is indicated by the dark, broad line.

For a given set of numbers n_1, n_2, n_3 and n_4, the number of boxes corresponding to the set is $(N-2)!$, which is the number of ways in which the remaining $N-2$ particles can be distributed among the remaining $N-2$ cells. As there is one box associated with each diagram, we conclude that for a given value of n_i, $i=1, 2, 3, 4$ there are $(N-2)!$ diagrams of the first class and second kind giving the same contribution to the cluster integral $A_p^{(2)}$.

For the boxes belonging to class B we have for its general term the one shown in Fig. 12. The definition

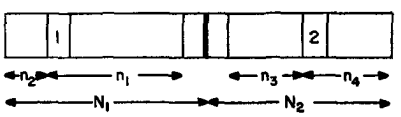

FIG. 12. The most general type of box associated with a diagram of the second kind and second class. This box belongs to class B.

of the numbers n_1, n_2, n_3 and n_4 is similar to their definition in the preceding case, but they now satisfy the relations,

$$n_1+n_2+1=N_1 \quad n_3+n_4+1=N_2.$$

We can immediately see, by a reasoning similar to that used in the first case, that for a given partition N_1 and N_2 and fixed positions of the particles 1 and 2, the number of diagrams of the second class and second kind giving the same contribution to $A_p^{(2)}$ is $(N-2)!$.

Finally, the combinatorial factors associated with the third kind of diagrams is precisely the same as for the second kind of diagrams as can easily be verified.

APPENDIX B

In this appendix we evaluate the contribution of the first class of diagrams to the generalized cluster integral $A_p^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ starting from Eq. (35). Let us denote the quantity Eq. (35) by $D_1(\mathbf{k}_1,\mathbf{k}_2)$. Thus we may write

$$\hat{D}_1(\mathbf{k}_1,\mathbf{k}_2)=\exp\left(-\frac{k_1^2}{2\alpha}n_3-\frac{k_2^2}{2\alpha}n_2\right)\times\int\exp\left(-n_4\frac{k_6^2}{2\alpha}\right)\hat{U}_2^{(\mathrm{cl})}(\mathbf{k}_1,\mathbf{k}_6;\mathbf{k}_2,\mathbf{k}_6)d^3k_6. \quad \text{(B1)}$$

On writing $U_2^{(\mathrm{cl})}$ in terms of $\mathbf{k}_6$, we have

$$U_2^{(\mathrm{cl})}(\mathbf{k}_1,\mathbf{k}_6;\mathbf{k}_2,\mathbf{k}_6)=\partial(\mathbf{k}_1-\mathbf{k}_2)\exp\left[-\frac{(\mathbf{k}_2+\mathbf{k}_6)^2}{4\alpha}\right]\cdot\frac{\Delta G_0}{\pi^2}, \quad \text{(B2)}$$

where ΔG_0 is given by Eq. (32) and may also be written as

$$\Delta G_0=\int_0^1\Delta\Gamma(t)dt, \quad \text{(B3)}$$

where

$$\Delta\Gamma(t)=-\frac{a}{\alpha}\exp\left\{-\frac{1}{4\alpha}[(\mathbf{k}_6-\mathbf{k}_2)^2(1-t)+(\mathbf{k}_6-\mathbf{k}_1)^2t]\right\}. \quad \text{(B4)}$$

If we substitute Eqs. (B2), (B3), and (B4) in Eq. (B1) and integrate with respect to k_6 and t, we find that

$$\hat{D}_1(\mathbf{k}_1,\mathbf{k}_2)=\exp\left[-\frac{k_1^2}{2\alpha}(n_2+n_3+1)\right]\times\partial(\mathbf{k}_1-\mathbf{k}_2)\left(\frac{-a}{2\pi^2\alpha}\right)\left(\frac{2\pi\alpha}{N_2}\right)^{\frac{3}{2}}. \quad \text{(B5)}$$

Thus, in order to obtain $D_1(n_1,n_2,n_3,n_4;\mathbf{r}_{12})$ we substitute Eq. (B5) into Eq. (27b). We therefore find

$$D_1(n_1,n_2,n_3,n_4;\mathbf{r}_{12})=-a\left(\frac{2\alpha}{\pi}\right)^{\frac{3}{2}}N_2^{-\frac{3}{2}}\frac{1}{8\pi^3}\times\int\exp(i\mathbf{k}_1\cdot\mathbf{r}_1-i\mathbf{k}_2\cdot\mathbf{r}_2)\exp\left[-(N_1-n_1)\frac{k_1^2}{2\alpha}\right]\times\partial(\mathbf{k}_1-\mathbf{k}_2)d^3k_1d^3k_2.$$

The integrations are straightforward, the result being

$$D_1(n_1,n_2,n_3,n_4;\bar{r}_{12})=-\frac{4a}{\lambda^7}\frac{1}{[N_2(N_1-n_1)n_1]^{\frac{3}{2}}}\times\exp\left[-\frac{N_1}{2n_1(N_1-n_1)}\alpha\mathbf{r}_{12}^2\right] \quad \text{(B6)}$$

after multiplying by the constant factor $(\alpha/2\pi n_1)^{\frac{3}{2}}\times\exp[-(\alpha/2n_1)\mathbf{r}_{12}^2]$, which is a constant term corresponding to the number of loops between particles 1 and 2 in the space representation of Fig. (7b).[10] Equation (B6) is the desired result.

APPENDIX C

We wish to integrate the expression indicated in Eq. (43) corresponding to the diagram in Fig. 9b. Let us call this quantity $\hat{D}_2(\mathbf{k}_1,\mathbf{k}_1';\mathbf{k}_2,\mathbf{k}_2')$. Then, by Eq. (27b), its Fourier transform, which we shall denote by $D_2(n_1,\cdots,n_4;\mathbf{r}_1',\mathbf{r}_1,\mathbf{r}_2',\mathbf{r}_2)$, corresponds to the diagram shown in Fig. 13. In order to calculate the contribution of the second class diagrams to the generalized cluster integral $A_p^{(2)}$ it is necessary to make in this expression $\mathbf{r}_1=\mathbf{r}_1'$ and $\mathbf{r}_2=\mathbf{r}_2'$. Thus, we are interested in the

[10] The diagram is the same, except that $\mathbf{k}_1$ is substituted by $\mathbf{r}_1$ and $\mathbf{k}_2$ by $\mathbf{r}_2$.

quantity

$$D_2(n_1,n_2,n_3,n_4;\,\mathbf{r}_{12})\equiv D_2(n_1,n_2,n_3,n_4;\,\mathbf{r}_1,\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_2)$$

with

$$D_2(n_1,\cdots,n_4;\,\mathbf{r}_1',\mathbf{r}_1,\mathbf{r}_2',\mathbf{r}_2)$$
$$=(2\pi)^{-6}\int\hat{D}_2(\mathbf{k}_1'\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2)e^{i(\mathbf{k}_1'\cdot\mathbf{r}_1'+\mathbf{k}_2'\cdot\mathbf{r}_2'-\mathbf{k}_1\cdot\mathbf{r}_1-\mathbf{k}_2\cdot\mathbf{r}_2)}\times d^3k_1d^3k_2d^3k_1'd^3k_2', \quad (C1)$$

where

$$\hat{D}_2(\mathbf{k}_1'\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2)=\hat{U}_2(\mathbf{k}_1'\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2)\times\exp\left[-\frac{1}{2\alpha}(n_1k_1^2+n_2k_1'^2+n_3k_2^2+n_4k_2'^2)\right]. \quad (C2)$$

If we use the change of variables, Eq. (33), where we shall drop the index 12, and use the condition $\mathbf{r}_1'=\mathbf{r}_1$, $\mathbf{r}_2'=\mathbf{r}_2$, we have, after integrating over K', the result

$$D_1(n_1,\cdots,n_4;\,\mathbf{r}_{12})=\frac{-a}{\pi^2}(2\pi)^{-6}\times\int\exp(-K^2/4\alpha)\frac{\exp(-k^2/\alpha)-\exp(-k'^2/\alpha)}{k'^2-k^2}\times\exp\left\{-\frac{1}{8\alpha}(n_1+n_2+n_3+n_4)K^2-\frac{1}{2\alpha}\mathbf{K}\times[(n_3-n_1)\mathbf{k}+(n_4-n_2)\mathbf{k}']-\frac{1}{2\alpha}[(n_1+n_3)k^2+(n_2+n_4)k'^2]+i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_{12}\right\}\times d^3Kd^3k'd^3k. \quad (C3)$$

If we integrate over K and introduce the following quantities:

$$\frac{A}{2}=\frac{1}{2\alpha N}\{N(n_1+n_3)-(n_3-n_1)^2\};$$
$$\frac{A'}{2}=\frac{1}{2\alpha N}\{N(n_2+n_4)-(n_2-n_4)^2\} \quad (C4)$$
$$B=-\frac{1}{\alpha N}(n_3-n_1)(n_4-n_2),$$

we get

$$D_2(n_1,\cdots,n_4;\,\mathbf{r}_{12})=(2\pi)^{-6}\frac{-a}{\pi^2}\left(\frac{8\pi\alpha}{N}\right)^{\frac{3}{2}}\times\int\int d^3k'd^3k\frac{\exp(-k^2/\alpha)-\exp(-k'^2/\alpha)}{k'^2-k^2}\times\exp\left\{-\left[\frac{A}{2}k^2+\frac{A'}{2}k'^2+B\mathbf{k}\cdot\mathbf{k}'\right]+i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_{12}\right\}. \quad (C5)$$

In order to perform the integrations over $\mathbf{k}$ and $\mathbf{k}'$ we notice that the integrand remains finite when $\mathbf{k}=\mathbf{k}'$ so that the factor $(k'^2-k^2)^{-1}$ can be replaced by $P(k'^2-k^2)^{-1}$.[11] We then use the following expression for $P(1/x)$:

$$P\frac{1}{x}=\frac{1}{2i}\left[\int_0^\infty e^{ixt}dt-\int_{-\infty}^0 e^{ixt}dt\right]. \quad (C6)$$

Thus, if we substitute (C6) into (C5) we obtain four terms, the first of which is given by

$$J_1=\frac{1}{2i}\int\int d^3kd^3k'\int_0^\infty dt\exp\left\{it(k'^2-k^2)-\frac{k^2}{\alpha}-\left[\frac{A}{2}k^2+\frac{A'}{2}k'^2+B\mathbf{k}\cdot\mathbf{k}'\right]+i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_{12}\right\}, \quad (C7)$$

and which upon integration over $\mathbf{k}$ and $\mathbf{k}'$, becomes

$$J_1=\frac{(2\pi)^3}{2i}\int_{-i(a-a')}^{\infty-i(a-a')}\frac{2d\tau}{\{\tau^2+(a+a')^2-4b^2\}^{\frac{3}{2}}}\times\exp\left(-\frac{2(a+a'+2b)}{\tau^2+(a+a')^2-4b^2}\mathbf{r}_{12}^2\right), \quad (C8)$$

where

$$a=A+\frac{2}{\alpha}\quad a'=A'\quad b=B. \quad (C9)$$

Similarly, the second term resulting from the substitution of (C6) into (C5) is

$$J_2=\frac{(2\pi)^3}{2i}\int_{-\infty-i(a-a')}^{-i(a-a')}\frac{2d\tau}{\{\tau^2+(a+a')^2-4b^2\}^{\frac{3}{2}}}\times\exp\left(-\frac{2(a+a'+2b)}{\tau^2+(a+a')^2-4b^2}\mathbf{r}_{12}^2\right). \quad (C10)$$

From (C8) and (C10) we obtain, after making the change of variable $t=-i\tau$

$$J_1-J_2=2(2\pi)^3\int_0^{(a-a')}\frac{dt}{[(a+a')^2-4b^2-t^2]^{\frac{3}{2}}}\times\exp\left(-\frac{2(a+a'+2b)}{(a+a')^2-4b^2-t^2}\mathbf{r}_{12}^2\right), \quad (C11)$$

an integral which is easily evaluated in terms of the

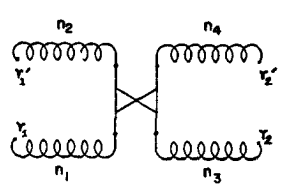

FIG. 13. Space representation of the most general open diagram of the second class and second kind.

error function by using the formula[12,13]

$$\int_0^q \frac{dt}{(p^2-t^2)^{\frac{1}{2}}}\exp\left(-\frac{s^2}{p^2-t^2}\right) = \frac{1}{p|s|}\exp\left(-\frac{s^2}{p^2}\right)Erf\left[\frac{|s|q}{p(p^2-q^2)^{\frac{1}{2}}}\right]. \quad \text{(C12)}$$

According to Eq. (C9) and the definitions of A, A' and B, the three functions a, a' and b of the variables n_1, n_2, n_3 and n_4 are obtained by the substitutions

$$n_1 \to n_1+1; \quad n_2 \to n_2; \quad n_3 \to n_3+1; \quad n_4 \to n_4 \quad \text{(C13)}$$

in the three functions X, X', Y of the same variables, defined as follows:

$$X=\frac{1}{\alpha(N-2)}[(N-2)(n_1+n_3)-(n_3-n_1)^2]$$

$$X'=\frac{1}{\alpha(N-2)}[(N-2)(n_2+n_4)-(n_4-n_2)^2]$$

$$Y=-\frac{1}{\alpha(N-2)}(n_3-n_1)(n_4-n_2)$$

with $N-2=n_1+n_2+n_3+n_4$. Therefore, if we call $P(n_1,n_2,n_3,n_4)$ the function defined by

$$P(n_1,n_2,n_3,n_4)=\int_0^{X-X'}\frac{dt}{[(X+X')^2-4Y^2-t^2]^{\frac{1}{2}}} \times\exp\left(-\frac{2(X+X'+2Y)r_{12}^2}{(X+X')^2-4Y^2-t^2}\right), \quad \text{(C14)}$$

we have that

$$J_1-J_2=2(2\pi)^3P(n_1+1,\, n_2,\, n_3+1,\, n_4). \quad \text{(C15)}$$

In a similar way, we find that the two other terms of Eq. (C5) yield

$$-J_3+J_4=2(2\pi)^3P(n_1,\, n_2+1,\, n_3,\, n_4+1), \quad \text{(C16)}$$

and

$$D_2(n_1,\cdots,n_4;\, \mathbf{r}_{12}) = -\frac{2a}{\pi^2}\frac{1}{(2\pi)^3}\left(\frac{8\pi\alpha}{N}\right)^{\frac{1}{2}}[P(n_1+1,\, n_2,\, n_3+1,\, n_4) -P(n_1,\, n_2+1,\, n_3,\, n_4+1)]. \quad \text{(C17)}$$

[11] P means principal part of.

[12] Equation (C12) is obtained if in the formula in the left, where $0<q\leq p$ we make $t=pw^{\frac{1}{2}}(1+w)^{\frac{1}{2}}$ and the square roots are taken positive. The resulting integral may be expressed as an error function.

[13] A. Erdelyi, W. Magnus, F. Oberhettinger, and F. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, Chap. IX.

Since the combinatorial factor corresponding to these diagrams for a given value of the set n_1, n_2, n_3, n_4, is $(N-2)!$ the contribution of the second class of diagrams to the functions $F^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ is thus

$$-\frac{2a(8\pi\alpha)^3}{8\pi^5}\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\sum_{n_4=0}^{\infty}\frac{z^{n_1+n_2+n_3+n_4+2}}{(n_1+n_2+n_3+n_4+2)^{\frac{1}{2}}} \times[P(n_1+1,\, n_2,\, n_3+1,\, n_4)-P(n_1,\, n_2+1,\, n_3,\, n_4+1)],$$

and after separating the two terms and after proper cancellations have been done we find

$$\frac{2a(8\pi\alpha)^3}{8\pi^5}\left\{\sum_{n_2=0}^{\infty}\sum_{n_4=0}^{\infty}\frac{z^{n_2+n_4}}{(n_2+n_4)^{\frac{1}{2}}}P(0,n_2,0,n_4) -\sum_{n_1=0}^{\infty}\sum_{n_3=0}^{\infty}\frac{z^{n_1+n_3}}{(n_1+n_3)^{\frac{1}{2}}}P(n_2,0,n_3,0)\right\}. \quad \text{(C18)}$$

When $n_1=n_3=0$, we have that $X=0$, $Y=0$, therefore, p^2, q and s occurring in (C12), which is of the same type as (C14), take the values X'^2, $-X'$ and $2X'r_{12}^2$, respectively. Furthermore, since $p^2=q^2$ and $q<0$ the error function in (C12) is independent of s and equal to $-(\pi)^{\frac{1}{2}}/2$. Thus

$$P(0;\, n_2,0,n_4)=-\frac{(\pi)^{\frac{1}{2}}}{2}\frac{1}{\sqrt{2}r_{12}}\frac{1}{X'^{\frac{1}{2}}}\exp\left(-\frac{2r_{12}^2}{X'}\right), \quad \text{(C19)}$$

where

$$X'=\frac{4n_2n_4}{\alpha(n_2+n_4)}.$$

In the same way, when $n_1=n_3=0$, we have $X'=Y=0$, $p^2=X$, $q=X$ and $S^2=2Xr_{12}^2$. Thus, we find

$$P(n_1,0,n_3,0)=\frac{(\pi)^{\frac{1}{2}}}{2}\frac{1}{\sqrt{2}r_{12}}\frac{1}{X^{\frac{1}{2}}}\exp\left(-\frac{2r_{12}^2}{X}\right), \quad \text{(C20)}$$

where

$$X=\frac{4n_1n_3}{\alpha(n_1+n_3)}.$$

On substituting (C19) and (C20) into Eq. (C18) and noticing that the two resultant terms are identical, we find that

$$F_{(2)}{}'^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=-\frac{2a(8\pi\alpha)^{\frac{1}{2}}}{8\pi^5}\frac{(\pi)^{\frac{1}{2}}}{\sqrt{2}r_{12}}\sum_{n_1=0}^{\infty}\sum_{n_3=0}^{\infty}\frac{z^{n_1+n_3}}{(n_1+n_3)^{\frac{1}{2}}} \times\frac{\alpha^{\frac{1}{2}}(n_1+n_3)^{\frac{1}{2}}}{8n_1^{\frac{1}{2}}n_3^{\frac{1}{2}}}\exp\left[-\frac{\alpha}{2}\left(\frac{1}{n_1}+\frac{1}{n_3}\right)r_{12}^2\right],$$

or

$$F_{(2)}{}'^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=-\frac{4a}{\lambda^7}\cdot\frac{\lambda}{r_{12}}\left\{g_{\frac{1}{2}}\left[z,\frac{r_{12}}{\lambda}(\pi)^{\frac{1}{2}}\right]\right\}^2,$$

which is the contribution from the second class of diagrams and second kind to the function $F^{(2)}$.

Formal Solution of Liouville's Equation

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A formal solution of Liouville's equation both for the classical and for the quantum mechanical case is presented. The derivation follows closely the approach employed by Feynman in his papers on the theory of positrons (Phys. Rev. **76**, 749 (1949), *ibid.* **76**, 769 (1949)). A scattering operator S is found which connects the distribution function at time t' with the distribution function at any later time t. Each term of this scattering operator can be represented uniquely and conveniently by a diagram. The topological structure of these diagrams is the same in the classical as well as in the quantum mechanical case. Applications of the method will be given in a forthcoming paper.

1. INTRODUCTION

THE Liouville equation represents a natural starting point for studies of nonequilibrium statistical mechanics.[1] It was soon realized that the many body problem encountered in statistical mechanics may advantageously be handled by the mathematical methods especially developed for the infinite many body problem of quantum field theory.[2] As an example Prigogine and collaborators[3] used the S matrix formalism in some of their papers. Furthermore, the well-known approach by Prigogine and collaborators to the solution of Liouville's equation by means of Fourier transforms and a diagram technique[4] bears much formal resemblance to field theoretical methods. In this paper we present a formal solution of the Liouville equation, which is based on Feynman's approach to the solution of the Schrödinger equation.[5] In Sec. 2 the actual derivation will be given. An integral kernel plays the central role of the development. This kernel is somewhat similar to the phase space transformation function introduced by Ross and Kirkwood[6] although it is a Green's function rather than a solution of the homogeneous Liouville equation. The various contributions of a perturbation expansion of this kernel give rise to corresponding contributions to the distribution function which may be classified by diagrams. The modifications caused by quantum mechanics will also be outlined for the case of the Wigner distribution function.[7] In Sec. 3 the physical significance of the diagrams is clarified by means of an equivalent perturbation expansion of the equations of motion. In a subsequent paper the method described on the following pages will be applied to problems of physical interest.

2. DERIVATION

The classical Liouville equation for an N particle system may be written as

$$\left(\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla_{\mathbf{R}}\right)f(\mathbf{R}\,\mathbf{V},t)=-\mathbf{F}(\mathbf{R},\mathbf{V})\cdot\nabla_{\mathbf{V}}f(\mathbf{R},\mathbf{V},t). \quad (1)$$

We use the abbreviation $\mathbf{R}$ for the set of position coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N$ of the N particles. Similarly, $\mathbf{V}$ is short for $\mathbf{v}_1, \mathbf{v}_2, \cdots \mathbf{v}_N$ the velocities of the particles. $\mathbf{F}\equiv\mathbf{F}_1, \mathbf{F}_2, \cdots \mathbf{F}_N$, where $\mathbf{F}_j$ is the force acting on particle j divided by its mass. We allow $\mathbf{F}$ to be a function of both position and velocity. The symbol $\mathbf{V}\cdot\nabla_R$, for instance, is an abbreviation for

$$\mathbf{V}\cdot\nabla_{\mathbf{R}}=\sum_{i=1}^{N}\mathbf{v}_i\cdot\nabla_{\mathbf{r}_i}.$$

We now introduce a kernel $G(\mathbf{R},\mathbf{V},t;\mathbf{R}',\mathbf{V}',t')$ which allows us to express the distribution function $f(R,V,t)$ for $t>t'$ by

$$f(\mathbf{R},\mathbf{V},t)=\int dR'dV'G(\mathbf{R},\mathbf{V},t;\mathbf{R}',\mathbf{V}',t)f(\mathbf{R}',\mathbf{V}',t'), \quad (2)$$

if it is known at an earlier time t'. The integration runs over the complete phase space

$$dR'dV'=d^3r_1'd^3r_2'\cdots d^3v_1'd^3v_2'\cdots.$$

The kernel G has the following properties:

$$\left(\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla_{\mathbf{R}}+\mathbf{F}\cdot\nabla_{\mathbf{V}}\right)G(\mathbf{R},\mathbf{V},t;\mathbf{R}',\mathbf{V}',t')$$
$$=\delta(\mathbf{R}-\mathbf{R}')\delta(\mathbf{V}-\mathbf{V}')\delta(t-t') \quad (3)$$

$$\lim_{t\to t'}G(\mathbf{R},\mathbf{V},t;\mathbf{R}',\mathbf{V}',t')=\delta(\mathbf{R}-\mathbf{R}')\delta(\mathbf{V}-\mathbf{V}'). \quad (4)$$

[1] J. G. Kirkwood, J. Chem. Phys. **15**, 72 (1947); J. Ross and J. G. Kirkwood, J. Chem. Phys. **22**, 1094 (1954); H. Mori, S. Ono, Progr. Theoret. Phys. (Japan) **8**, 327 (1952); H. S. Green, Proc. Phys. Soc. (London) **A64**, 325 (1953); R. Brout and I. Prigogine, Physica **22**, 621 (1956); I. Prigogine and J. Philippot, Physica **23**, 569 (1957); A. W. Saenz, Phys. Rev. **105**, 546 (1957).

[2] See for instance B. S. de Witt, "The operator formalism in quantum perturbation theory," University of California, Berkeley, California (September, 1955).

[3] I. Prigogine and F. Hènin, Bull. Acad. Sci. Belg. **11**, 814 (1957); P. Resibois, Physica **25**, 725 (1959).

[4] I. Prigogine, "Statistical mechanics and thermodynamics of irreversible processes," Free University of Brussels, Techn. Rept EORDC PR 59-18.

[5] See, for instance, the account of this approach in S. S. Schweber, H. A. Bethe, and F. de Hoffman, *Mesons and Fields* (Row Peterson and Company, 1956), Vol. 1, p. 54.

[6] J. G. Ross and J. G. Kirkwood, J. Chem. Phys. **22**, 1094 (1954); J. Ross, J. Chem. Phys. **24**, 375 (1956).

[7] E. P. Wigner, Phys. Rev. **40**, 749 (1932).

Equation (3) shows that G is a Green's function of the Liouville equation. Equation (4) is necessary for Eq. (2) to be consistent. Equations (2)–(4) are strongly reminiscent to Feynman's approach to the solution of Schrödinger's equation. In fact, replacing the operator $\mathbf{V}\cdot\nabla_R+\mathbf{F}\cdot\nabla_V$ by the Hamiltonian H and the distribution function f by the wave function ψ, Eqs. (2), (3), and (4) are identical with Feynman's theory.[5]

We now propose to solve Eq. (3) by an iteration method assuming weak interactions. We obtain

$$G=G_0+G_1+G_2+\cdots \tag{5}$$

$$\left(\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla_{\mathbf{R}}\right)G_0=\delta(\mathbf{R}-\mathbf{R}')\delta(\mathbf{V}-\mathbf{V}')\delta(t-t') \tag{6}$$

$$\left(\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla_{\mathbf{R}}\right)G_n=-\mathbf{F}\cdot\nabla_{\mathbf{V}}G_{n-1}\quad n\geq 1. \tag{7}$$

The solution of Eq. (6) is immediately written down[8]

$$G_0(\mathbf{R}\mathbf{V}t;\mathbf{R}'\mathbf{V}'t')=\delta(\mathbf{V}-\mathbf{V}')\times\delta[(\mathbf{R}-\mathbf{R}'-\mathbf{V}'(t-t')]S(t-t'), \tag{8}$$

where we introduced the step function

$$S(x)=\begin{cases}1 & \text{for}\quad x>0\\ 0 & \text{for}\quad x<0.\end{cases} \tag{9}$$

It is easily seen that Eq. (4) is satisfied for expression (8). From Eq. (7) we have

$$G_n(\mathbf{R},\mathbf{V},t;\mathbf{R}',\mathbf{V}',t')=-\int dt''dR''dV''G_0(\mathbf{R}\mathbf{V}t;\mathbf{R}''\mathbf{V}''t'')\times\mathbf{F}(\mathbf{R}'',\mathbf{V}'')\cdot\nabla_{\mathbf{V}''}G_{n-1}(\mathbf{R}'',\mathbf{V}'',t'';\mathbf{R}'\mathbf{V}'t'). \tag{10}$$

Successive application of Eq. (10) reveals after straightforward calculation that

$$\begin{aligned}G_n(\mathbf{R}\mathbf{V}t;\mathbf{R}'\mathbf{V}'t')&=\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\cdots\int_{t'}^{t_{n-1}}dt_n\int dV_2dV_3\cdots dV_n\\&\times(-1)^n\delta[(\mathbf{R}-\mathbf{V}(t-t_1)-\sum_{j=2}^{n}\mathbf{V}_j(t_{j-1}-t_j)\\&-\mathbf{V}'(t_n-t')]\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1),\mathbf{V})\cdot\nabla_{\mathbf{V}}\delta(\mathbf{V}-\mathbf{V}_2)\\&\times\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1)-\mathbf{V}_2(t_1-t_2),\mathbf{V}_2)\cdot\nabla_{\mathbf{V}_2}\\&\times\delta(\mathbf{V}_2-\mathbf{V}_3)\cdots\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1)\\&-\sum_{j=2}^{n}\mathbf{V}_j(t_{j-1}-t_j),\mathbf{V})\cdot\nabla_{\mathbf{V}_n}S(\mathbf{V}_n-\mathbf{V}').\end{aligned} \tag{11}$$

[8] The solution Eq. (8) is the retarded Green's function. The advanced Green's function is found by replacing $S(t-t')$ by $-S(t'-t)$. We take the retarded Green's function of course since we are interested in the future knowing the present, i.e., the distribution function at time t'.

By inserting the expressions (8) and (11) into Eq. (2) and by performing the phase space integrations as indicated we get the following result. The distribution function at time t is connected with the initial distribution function at time t' through a scattering operator S,

$$f(\mathbf{R},\mathbf{V},t)=Sf(\mathbf{R}-\mathbf{V}(t-t'),\mathbf{V},t'), \tag{12}$$

where

$$S=\sum_{n=0}^{\infty}S_n\quad S_0=1, \tag{13}$$

and (for $n\geq 1$)

$$S_n=(-1)^n\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\cdots\int_{t'}^{t_{n-1}}dt_n\times\prod_{\alpha=1}^{n}F(\mathbf{R}-\mathbf{V}(t-t_\alpha),\mathbf{V})\cdot\mathbf{P}_\alpha \tag{14}$$

with

$$\begin{aligned}\mathbf{P}_\alpha&=\nabla_{\mathbf{V}}-(t_\alpha-t')\nabla_{\mathbf{R}}-\sum_{\beta=\alpha+1}^{n}[\nabla_{\mathbf{V}}-(t_\alpha-t_\beta)\nabla_{\mathbf{R}}]\\&=\mathbf{P}_\alpha,+\sum_{\beta=\alpha+1}^{n}\mathbf{P}_{\alpha\beta}.\end{aligned} \tag{15}$$

The grad ∇_V in expressions (15) is always connected with a grad ∇_R in the specific configuration

$$\mathbf{P}_{\alpha\beta}=\nabla_{\mathbf{V}}-(t_\alpha-t_\beta)\nabla_R. \tag{16}$$

The operator $\mathbf{P}_{\alpha\beta}$ is defined to act only on that function of $\mathbf{R}$ and $\mathbf{V}$, which contains the same time label β. Furthermore, $\nabla_{\mathbf{V}}$ does not act on the argument $\mathbf{R}-\mathbf{V}(t-t_\beta)$. In other words,

$$\mathbf{P}_{\alpha\beta}\mathbf{F}[\mathbf{R}-\mathbf{V}(t-t_\gamma),\mathbf{V}]=\delta_{\beta\gamma}\{\nabla_{\mathbf{V}}\,\mathbf{F}[\mathbf{R}-\mathbf{V}(t-t_\gamma),\mathbf{V}\,]-(t_\alpha-t_\beta)\nabla_R\,\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_\gamma),\mathbf{V})\} \tag{17}$$

with $\nabla_{\mathbf{V}}$ operating only on the second argument of F. By inserting Eq. (15) into (14) we see that S_n can be expressed by a sum of terms of the following structure:

$$S_n=(-1)^n\sum_{\lambda}\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\cdots\int_{t'}^{t_{n-1}}dt_n\times\prod_{\alpha=1}^{n}\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_\alpha),\mathbf{V})\cdot\mathbf{P}_{\alpha\gamma_\alpha}. \tag{18}$$

In Eq. (18) it is $\gamma_\alpha>\alpha$, but otherwise arbitrary and the sum runs over all $n!$ possibilities to pick a set of $\gamma_\alpha>\alpha$. Any particular term of the sum (18) may be represented by a diagram. We define the diagrams in the following way: An nth order diagram consists of $n+1$ vertices labeled with a time coordinate t_α starting with the latest time t_1 on the left (Fig. 1a) and ending with a vertex associated with the earliest time t' the initial time on the right. From each vertex α (except the one associated with t') one and only one directed

solid line starts which ends at any arbitrary vertex β with an earlier time including the last vertex (Fig. 1b). The last vertex associated with the initial time t' is called the external vertex (each diagram has only one external vertex) all the others are called internal vertices. A solid line starting from any internal vertex and ending at any other internal vertex is called an internal line. If it ends on the external vertex however it is called an external line. Fig. 1 (c) shows a possible 5th order diagram with 2 external and 3 internal lines, similarly Fig. 1d shows one with 3 external and 2 internal lines. The number of lines is equal to the number of internal vertices, i.e., the order of the diagram. There are $n!$ different diagrams of order n corresponding to the $n!$ different ways of connecting any two of the $n+1$ vertices by a solid line such that only one solid line starts from any internal vertex. We associate with each vertex α the factor $-\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_\alpha),\mathbf{V})$ and with an internal line the operator $\mathbf{P}_{\alpha\beta}$, which acts on the $-\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_\beta),\mathbf{V})$ associated with vertex β in the manner specified by (17). Furthermore, associated with an external line starting at the vertex α is the

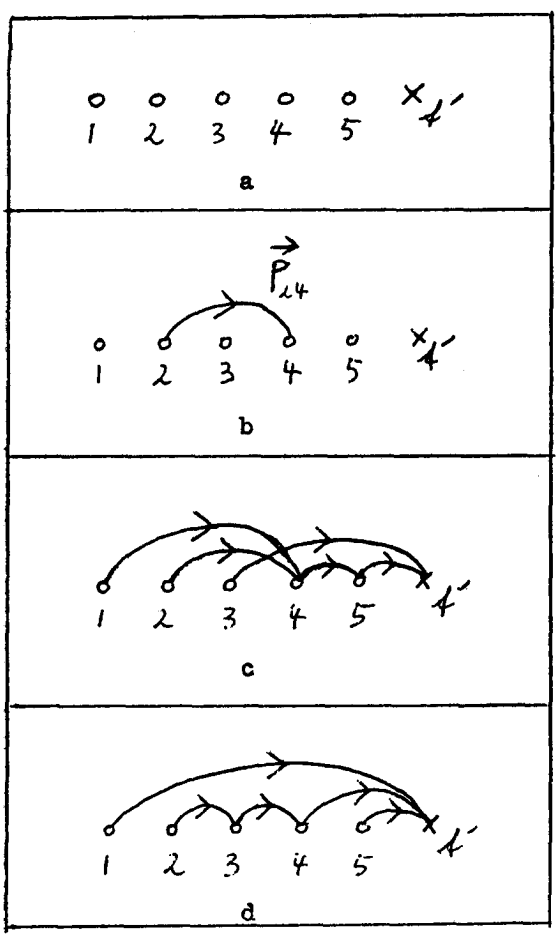

FIG. 1. (a), (b) construction of a diagram. (c), (d) two possible 5th order diagrams.

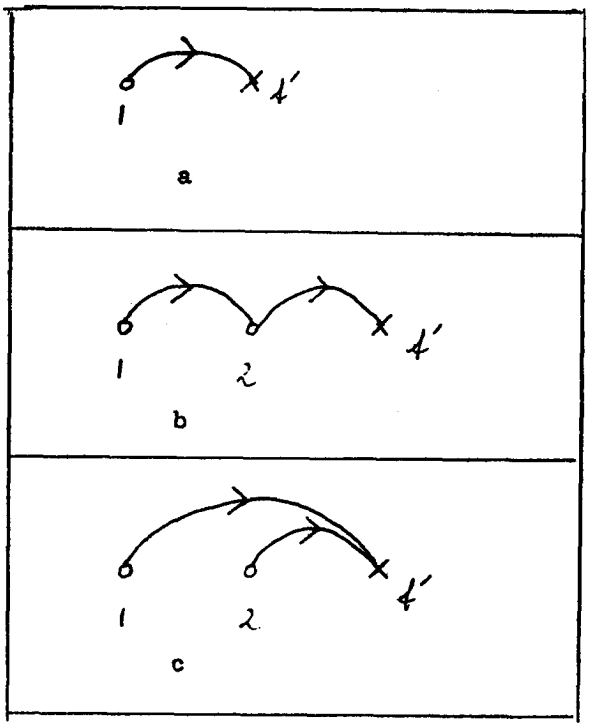

FIG. 2. (a) first order diagram. (b), (c) the two second order diagrams.

operator

$$\mathbf{P}_{\alpha'}=\nabla_V-(t_\alpha-t')\nabla_R, \tag{16a}$$

which acts on the initial distribution function represented by the external vertex. We now see that any given diagram (Fig. 1c, d for example) represents uniquely one term of the sum (18). As an example, Fig. 2 shows the three lowest order diagrams. According to the rules outlined above the first-order contribution (Fig. 2a) is given by

$$\begin{aligned} S_1&=-\int_{t'}^{t} dt_1\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1),\mathbf{V})\cdot\mathbf{P}_1,\\ &=-\int_{t'}^{t} dt_1\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1),\mathbf{V})\cdot(\nabla_{\mathbf{V}}-(t_1-t')\nabla_{\mathbf{R}}). \end{aligned} \tag{19}$$

The second-order contribution Fig. 2b is given by

$$S_2=\int_{t'}^{t} dt_1\int_{t'}^{t_1} dt_2\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1),\mathbf{V}) \cdot\mathbf{P}_{12}\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_2),\mathbf{V})\cdot\mathbf{P}_{2'}. \tag{20}$$

Here $\mathbf{P}_{12}$ acts on the succeeding $\mathbf{F}$, whereas $\mathbf{P}_{2'}$ acts on the initial distribution function as explained in the foregoing. The other second-order contribution Fig. 2c is given by

$$S_2'=\int_{t'}^{t} dt_1\int_{t'}^{t_1} dt_2\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_1),\mathbf{V}) \cdot\mathbf{P}_1\mathbf{F}(\mathbf{R}-\mathbf{V}(t-t_2),\mathbf{V})\cdot\mathbf{P}_{2'}, \tag{21}$$

where both $\mathbf{P}$ act on the initial distribution function. Turning now to the quantum mechanical Liouville equation for the Wigner distribution function[7] we restrict ourselves to the case in which the force $\mathbf{F}$ is derived from a potential $\mathbf{F}(R)=-\nabla_{\mathbf{R}}\phi(R)$. The Liouville equation for the Wigner distribution function $f^{(W)}$ is well known to be[9]

$$\left(\frac{1}{\partial t}+\mathbf{V}\cdot\nabla_{\mathbf{R}}\right)f^{(W)}=\frac{2}{\hbar}\sin\left(\frac{\hbar}{2M}\nabla_{\mathbf{R}}\cdot\nabla_{\mathbf{V}}\right)\phi(\mathbf{R})f^{(W)}. \quad (22)$$

Here the operator $\nabla_{\mathbf{R}}$ acts only on the potential $\phi(\mathbf{R})$. The sin operator is defined by its power series expansion. It is easily seen that the scattering operator S for $f^{(W)}$ may still be determined by the same diagrams as in the classical case. Only the rules of associating an internal vertex and an internal line to a given mathematical quantity have to be changed. An internal vertex α represents now

$$\frac{2}{\hbar}\sin\left(\frac{\hbar}{2M}\nabla_{\mathbf{R}}\cdot\cdots\right)\phi[\mathbf{R}-\mathbf{V}(t-t_\alpha)]. \quad (23)$$

An internal solid line connecting the vertices α and β represents

$$\mathbf{P}_{\alpha\beta}'=-(t_\alpha-t_\beta)\nabla_{\mathbf{R}}, \quad (24)$$

where $\nabla_{\mathbf{R}}$ acts on the potential associated with vertex β. By the way the operator $\mathbf{P}_{\alpha\beta}$ Eq. (16) is also replaced by $\mathbf{P}_{\alpha\beta}'$ Eq. (24) in the classical case if the forces do not depend explicitly on the velocity as is seen from Eq. (17). The complete expression for the part of the diagram shown in Fig. 1b is according to (23) and (24)

$$\cdots\frac{2}{\hbar}\sin\left(\frac{\hbar}{2M}\nabla_{\mathbf{R}}\cdot\mathbf{P}_{24}'\right)\phi(\mathbf{R}-\mathbf{V}(t-t_2))\cdots. \quad (25)$$

An external solid line is still represented by (15a). As an example let us consider the diagram Fig. 2b. It represents

$$S_2'=\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\frac{2}{\hbar}\sin\left(\frac{\hbar}{2M}\nabla_{\mathbf{R}}\cdot\mathbf{P}_{12}'\right)\times\phi[\mathbf{R}-\mathbf{V}(t-t_1)]\frac{2}{\hbar}\sin\left(\frac{\hbar}{2M}\nabla_{\mathbf{R}}\cdot\mathbf{P}_{21}'\right)\times\phi[\mathbf{R}-\mathbf{V}(t-t_2)].$$

3. DISCUSSION

Having established the rules which generate the scattering operator S we like to discuss some of the consequences at this point. First of all we notice that the nth order term of the series for S consists of a sum over n diagrams with a various number of internal and external lines. The physical significance of an internal or external line will be made clear by the following considerations. In zeroeth order the motion of the particles is undisturbed. They proceed along straight lines. In fact, the scattering operator being $S_0=1$ to zeroth order we have from Eq. (12)

$$f(\mathbf{R},\mathbf{V},t)=f(\mathbf{R}-\mathbf{V}(t-t'),\mathbf{V},t').$$

To see how precisely the higher order terms of the scattering operator introduce deviations from the unperturbed straight lines of the zeroeth order approximation, we outline here a perturbation scheme applied directly to the equations of motion, which is completely equivalent to the perturbation analysis for the scattering operator described in Sec. 2. By confining ourselves to the classical equations of motion and to forces which depend only on the position we have

$$d^2\mathbf{R}/dt^2=\lambda\mathbf{F}(\mathbf{R}) \quad (27)$$

together with the initial conditions

$$\mathbf{R}(t')=\mathbf{R}'\ (d\mathbf{R}/dt)(t')=\mathbf{V}. \quad (27a)$$

We introduced a small expansion parameter λ and write

$$\mathbf{R}=\mathbf{R}_0+\lambda\mathbf{R}_1+\lambda^2\mathbf{R}_2+\cdots. \quad (28)$$

By inserting (28) into (27) we have the successive approximations

$$\begin{aligned}&d^2\mathbf{R}/dt^2=0\\&d^2\mathbf{R}/dt^2=\mathbf{F}(\mathbf{R}_0)\\&d^2\mathbf{R}/dt^2=\mathbf{R}_1\cdot\nabla_{\mathbf{R}_0}F(\mathbf{R}_0),\quad\text{etc.},\end{aligned} \quad (29)$$

and the initial conditions are

$$\begin{aligned}&\mathbf{R}_0(t')=\mathbf{R}'\ (d\mathbf{R}/dt)(t')=\mathbf{V}\\&\mathbf{R}_1(t')=(d\mathbf{R}/dt)(t')=0\\&\mathbf{R}_2(t')=(d\mathbf{R}/dt)(t')=0,\quad\text{etc.}\end{aligned} \quad (29a)$$

It follows from (29) and (29a) that the successive approximations to the acceleration are given by

$$d^2\mathbf{R}/dt^2=0 \quad (30a)$$

$$d^2\mathbf{R}/dt^2=\mathbf{F}[\mathbf{R}'-\mathbf{V}(t'-t)] \quad (30b)$$

$$d^2\mathbf{R}/dt^2=\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\mathbf{F}[\mathbf{R}'-\mathbf{V}(t'-t_2)]\cdot\nabla_{\mathbf{R}}\mathbf{F}[\mathbf{R}'-\mathbf{V}(t'-t)],\quad\text{etc.} \quad (30c)$$

A glance back to Eqs. (19) (20) and (21) and a comparison with Eqs. (30b) and (30c) reveals that Eq. (19) the first-order scattering operator takes into account a deviation from the unperturbed straight paths of the particles to exactly the same degree of approximation on which Eq. (30b) is based. Expression (20) corresponding to the diagram with one internal line (Fig. 2b) takes into account a first order correction to the first-order effect given by (19) (it is therefore of second

[9] J. M. Irving and R. W. Zwanzig, J. Chem. Phys. **19**, 1173 (1951).

order). The exact analog to this correction expressed by an internal line is Eq. (30c). But this is not all that might happen in second order! Actually, a new 'scattering' may be introduced at some other time between t' and t. But Eq. (21) corresponding to the diagram with two external lines (Fig. 2c) represents precisely the contribution from this event again to the correct order of magnitude. These findings may now immediately be generalized to an nth order contribution. Suppose we have a specific nth order diagram which represents one of the $n!$ nth order contributions to the scattering operator. This diagram generates $n+1$ diagrams of the $(n+1)$st order. By adding a new internal vertex to the left of the nth order diagram and connecting it with either of the n other internal vertices we obtain n new possible diagrams with one more internal line. By connecting it with the external vertex we obtain one new diagram with one more external line. From the previous discussion it is clear that the $(n+1)$st order diagrams generated from a specific nth order diagram take into account a correction to the path of any one particle in the sense of Eq. (30c). This is possible in n different ways corresponding to the n different new internal lines. Whereas the possibility of a new 'scattering' is represented by the addition of a new external line. In short, internal lines represent corrections to already existing scatterings and external lines represent the introduction of new scatterings. Of course, it should be realized that this explanation is more or less heuristic since we did not introduce scattering cross sections explicitly. The scattering operator rather gives the detailed time dependence of the distribution function and is therefore completely equivalent to the exact knowledge of the orbits of all the particles involved. This is far too much information to be useful. In fact, in order to extract useful information one has to have recourse to averaging procedures. One may introduce singlet doublet, etc., distribution functions, and subsequently use Kirkwoods coarse graining device,[10] 'Stosszahl ansatz', etc; But this is beyond the scope of the present paper.

[10] J. G. Kirkwood, J. Chem. Phys. 14, 180 (1946).

Solution of the Collisionless Boltzmann Equation using a Diagram Technique

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The diagram technique recently developed by the author (see footnote 1) for the solution of Liouville's equation is extended and suitably modified to cover the case of the collisionless Boltzmann equation for a plasma. The usefulness of the method is demonstrated by two problems. These are: first, the influence of a plane polarized electric wave on the electron distribution function of a low-temperature plasma, and second, the propagation of a (small) initial disturbance for the case of a plasma which is governed by the Vlasov equation (see footnote 8).

1. INTRODUCTION

IN another paper[1] a solution of the Liouville equation for an N particle system was found essentially by expanding the associated Green's function into a Sturm Liouville series. The result obtained may be stated as follows: The distribution function f at time t is uniquely connected with an arbitrarily prescribed initial distribution function f_0 at time t' through a scattering operator thus

$$f(\mathbf{R},\mathbf{V},t)=Sf_0(\mathbf{R}-\mathbf{V}(t-t'),\mathbf{V},t'). \tag{1}$$

The scattering operator in turn is given by the series

$$S=\sum_{n=0}^{\infty} S_n \tag{2}$$

with $S_0=1$ and each S_n for $n\geq 1$ turned out to be a sum of contributions consisting of various products of forces and gradients. The structure of these terms can be expressed by diagrams and each contribution may be written down easily according to the rules given in I.

However, it is to be remarked that a complete solution according to this scheme is more or less useless if it is not supplemented by statistical considerations. Of course, an exact solution of Liouville's equation is equivalent to an exact solution of the equations of motion of the N particle system, which is as everybody knows a prohibitive venture.

The case we wish to consider here is the case of the so-called collisionless Boltzmann equation for a plasma. This equation describes a system of charged particles in which only the influence of the long range forces is taken into account. It can be shown[2] that the collision less Boltzmann equation is obtained from Liouville's equation with only *one* statistical assumption. This assumption is that the distribution function for the N particles factorizes into a product of distribution functions for each individual particle[3]

$$f(\mathbf{R},\mathbf{V},t)=f(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_N;\,\mathbf{v}_1\mathbf{v}_2\cdots\mathbf{v}_N t)$$
$$\equiv\mathbf{f}(\mathbf{r}_1,\mathbf{v}_1 t)\mathbf{f}(\mathbf{r}_2,\mathbf{v}_2 t)\cdots\mathbf{f}(\mathbf{r}_N,\mathbf{v}_N t). \tag{3}$$

Considering f as the probability density for finding particle 1 at $\mathbf{r}_1\mathbf{v}_1$, particle 2 at $\mathbf{r}_2\mathbf{v}_2$ etc., Eq. (3) is an expression for the assumption that the particles are uncorrelated (the joint probability is equal to the product of the individual probabilities). This assumption introduces of course errors. It is intuitively clear that assumption (3) should break down under any circumstances if two or more particles come close to each other. At low enough densities the encounter of more than two particles is a rare event and the close encounter of two particles finds its expression in the collision integral.[4] Therefore, to maintain assumption (3) for *all* values of $\mathbf{r}_j$ and $\mathbf{v}_j$ simply means to neglect the collision integral altogether. This would be a bad approximation if any appreciable forces would only be exerted during close encounters as it is the case in a neutral gas for instance. But the situation is different with a plasma. Here we have predominantly the long range Coulomb forces between the particles so that the error made by neglecting collisions may presumably be within tolerable limits.

In Sec. 2 we are going to derive the solution of the initial value problem for the collisionless Boltzmann equation. The method of solution will be patterned after the approach given in I. However, owing to the nonlinear character of the basic equation the scheme to be developed will be more complex than that given in I. But the diagram representation of I can be extended naturally to cover this case. The advantage of the diagram method will be demonstrated in Sec. 3. Once the rules of the game, i.e., the connection between the topological structure of a diagram and the mathematical structure of its algebraic counterpart are known it is only a matter of comparatively simple algebra to obtain explicit expressions for the solution of the collisionless Boltzmann equation in many cases, that is in cases where the number of possible diagrams representing nonvanishing contributions is not forbiddingly high. The real advantage of a diagram expansion is here as elsewhere (for instance, Feynman diagrams) to keep track of a large number of possible contributions so that nothing is forgotten and to see immediately

[1] O. von Roos, J. Math. Phys. 1, 107 (1960). Hereafter referred to as I.

[2] N. Rostocker, General Atomics Rept. GAMD-663 (July 10, 1959) (unpublished).

[3] The presence of transverse photons does not change this statement. Only the distribution function has to be suitably modified to include the additional degrees of freedom.

[4] See, for instance, J. G. Kirkwood, J. Chem. Phys. 15, 72 (1947).

whether a certain contribution actually vanishes as the case may be. Here, as elsewhere, a diagram by itself does not have any physical significance other than that of the algebraic expression it stands for.

2. DERIVATION

The collisionless Boltzmann equation in its most general form may be written as[2,5]

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla_r\right)f_j(\mathbf{r},\mathbf{v},t)=\mathbf{A}_j(\mathbf{r},\mathbf{v},t)\cdot\nabla_v f_j(\mathbf{r},\mathbf{v},t)$$
$$+\int_{-\infty}^{t}dt'\int d^3r'd^3v'\sum_i \mathbf{B}_{ji}(\mathbf{r},\mathbf{v},t;\,\mathbf{r}',\mathbf{v}',t')$$
$$\times f_i(\mathbf{r}',\mathbf{v}',t')\cdot\nabla_v f_j(\mathbf{r},\mathbf{v},t). \quad (4)$$

In this equation the meaning of the various terms is as follows: $f_j(\mathbf{r},\mathbf{v},t)$ is the distribution function for particles of kind j (electrons ions etc.). The vector $\mathbf{A}_j$ represents an externally applied force acting on the particles of kind j. The integral kernel $\mathbf{B}_{ji}$ stands for the interaction of the particles among each other and is essentially given by a complete solution of Maxwell's equations.[5] The retardation is properly accounted for by the integral over all times t' earlier than t. If retardation is neglected $\mathbf{B}_{ji}$ contains a factor $\delta(t-t')$. Equation (4) is now solved with the following "ansatz," which is nothing else than an ordinary perturbation expansion with respect to $\mathbf{A}$ and $\mathbf{B}$.

$$f_j=f_j^{(0)}+f_j^{(1)}+\cdots \quad (5)$$

so that

$$[(\partial/\partial t)+\mathbf{v}\cdot\nabla_r]f_j^{(0)}=0 \quad (6)$$

$$[(\partial/\partial t)+\mathbf{v}\cdot\nabla_r]f_j^{(1)}$$
$$=\mathbf{A}_j\cdot\nabla_v f_j^{(0)}+\int_{-\infty}^{t}dt'\int d^3r'd^3v'\sum_i \mathbf{B}_{ji}(\mathbf{r},\mathbf{v},t;\,\mathbf{r}',\mathbf{v}',t')$$
$$\times f_i^{(0)}(\mathbf{r}',\mathbf{v}',t')\cdot\nabla_v f_j^{(0)}, \quad (6a)$$

and, in general,

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla_r\right)f_j^{(n)}=\mathbf{A}_j\cdot\nabla_v f_j^{(n-1)}$$
$$+\int_{-\infty}^{t}dt'\int d^3r'd^3v'\sum_i \mathbf{B}_{ji}(\mathbf{r},\mathbf{v},t;\,\mathbf{r}',\mathbf{v}',t')$$
$$\times\sum_{m=0}^{n-1} f_i^{(m)}(\mathbf{r}',\mathbf{v}',t')\cdot\nabla_v f_j^{(n-1-m)}. \quad (7)$$

Let us assume that we know the distribution functions f_j for some initial time τ

$$f_j(\mathbf{r},\mathbf{v},\tau)=f_j^*(\mathbf{r},\mathbf{v},\tau). \quad (8)$$

[5] W. E. Brittin, Phys. Rev. **106**, 843 (1957).

We also specify the initial electromagnetic fields

$$\left.\begin{aligned}\mathbf{E}&=\mathbf{E}_0(\mathbf{r},\mathbf{v})\\ \mathbf{H}&=\mathbf{H}_0(\mathbf{r},\mathbf{v})\end{aligned}\right\}\quad \text{for}\quad t=\tau. \quad (9)$$

This, of course, is tantamount to assuming that we not only know the distribution function at $t=\tau$, but also for earlier times since

$$-\frac{e_j}{m_j}\left(\mathbf{E}_0+\frac{1}{c}\mathbf{v}\times\mathbf{H}_0\right)$$
$$=\int_{-\infty}^{\tau}dt'\int d^3r'd^3v'\mathbf{B}_{ji}(\mathbf{r},\mathbf{v},t;\,\mathbf{r}'\mathbf{v}'t')f_i(\mathbf{r}',\mathbf{v}',t'). \quad (10)$$

Without retardation, $\mathbf{E}_0$ and $\mathbf{H}_0$ are uniquely given by the initial distribution function f^* alone.

The solution of Eq. (6) together with (8) is given by

$$f_j^{(0)}=f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\,\mathbf{v},\,\tau)\quad\text{for}\quad t\geq\tau, \quad (11)$$

so that the equation for the first order contribution $f_j^{(1)}$ Eq. (6a) reads

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla_r\right)f_j^{(1)}=\mathbf{A}_j\cdot\nabla_v f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\,\mathbf{v},\,\tau)$$
$$-\frac{e_j}{m_j}\left(\mathbf{E}_0+\frac{1}{c}\mathbf{v}\times\mathbf{H}_0\right)\cdot\nabla_v f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\,\mathbf{v},\,\tau)$$
$$+\int_{\tau}^{t}dt'\int d^3r'd^3v'\sum_i \mathbf{B}_{ji}(\mathbf{r},\mathbf{v},t;\,\mathbf{r}',\mathbf{v}',t')$$
$$\times f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau),\,\mathbf{v}',\,\tau)\cdot\nabla_v f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\,\mathbf{v},\,\tau). \quad (12)$$

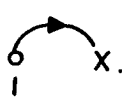
From now on we will incorporate the second term on the right-hand side of Eq. (12) into the first one without specific change of notation. Equation (12) is easily solved with the aid of the Green's function introduced in I [see I, Eq. (3)] and the first-order contribution is

$$f_j^{(1)}=\int_{\tau}^{t}dt_1\Big\{\mathbf{A}_j(\mathbf{r}-\mathbf{v}(t-t_1),\,\mathbf{v},\,t_1)$$
$$+\int_{\tau}^{t_1}dt'\int d^3r'd^3v'\sum_i \mathbf{B}_{ji}(\mathbf{r}-\mathbf{v}(t-t_1),\,\mathbf{v},t_1;\,\mathbf{r}',\mathbf{v}',t')$$
$$\times f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau),\,\mathbf{v}',\,\tau)\Big\}\cdot[\nabla_v-(t_1-\tau)\nabla_r]$$
$$\times f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\,\mathbf{v},\,\tau). \quad (13)$$

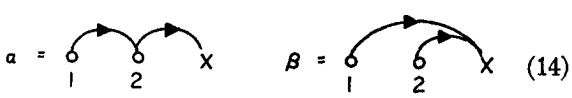
We note that the term involving the external forces $\mathbf{A}$ is exactly equal to the corresponding term in the expansion of Liouville's equation given in I.[6] Of course,

[6] The properties of the operator $\nabla_v-(t_1-\tau)\nabla_r$ are explained in I. We note here that ∇_v only operates on the second argument $\mathbf{v}$ in $f^*(\mathbf{r}-\mathbf{v}(t-\tau),\,\mathbf{v},\,\tau)$.

this is to be expected since Eq. (4) without the nonlinear term is just the (one particle) Liouville equation. Now, inserting Eq. (13) back into the equation which expresses $f_j^{(2)}$ by $f_j^{(0)}$ and $f_j^{(1)}$ one is easily able to determine $f_j^{(2)}$. On continuing along this line, expressions may be found for $f_j^{(3)} f_j^{(4)}$, etc. In principle, the distribution function is therefore known for all times $t > \tau$ provided it is known together with the initial fields for $t = \tau$. However, it must be said that owing to the nonlinear character of the basic Eq. (4) the higher order terms become rapidly more and more involved so that in practice we are as far from a general solution as if we had confined ourselves to simply write down Eq. (4) and let it go at that. Fortunately, the outlook is not so dim in many cases of interest, namely in cases where some kind of approximations are allowed. But in order to see how exactly any given approximation influences higher order terms $f_j^{(n)}$ we have to study the mathematical structure of a term of arbitrary order. This we do conveniently by means of a diagram technique which allows us to express any contribution to f_j in a concise way. In another paper[1] we already developed a diagram scheme which is applicable to the present problem in its entirety. Provided that the non linear term of Eq. (4) is missing the scheme developed in I is completely sufficient and all contributions to any order are given by those diagrams. The first-order contribution for instance is given by (13) if we drop the nonlinear (**B** containing) term. It is represented by the diagram



The reader is referred to I for details. The second-order contributions



(14)

can immediately be written down with the help of the rules given in I, and we find

$$\alpha = \int_\tau^t dt_1 \int_\tau^{t_1} dt_2 \mathbf{A}(\mathbf{r} - \mathbf{v}(t-t_1), \mathbf{v}, t_1) \cdot \mathbf{P}_{12} \mathbf{A}(\mathbf{r} - \mathbf{v}(t-t_2), \mathbf{v}, t_2) \cdot \mathbf{P}_{2\tau} f^* \quad (15)$$

$$\beta = \int_\tau^t dt_1 \int_\tau^{t_1} dt_2 \mathbf{A}(\mathbf{r} - \mathbf{v}(t-t_1), \mathbf{v}, t_1) \cdot \mathbf{P}_{1\tau} \mathbf{A}(\mathbf{r} - \mathbf{v}(t-t_2), \mathbf{v}, t_2) \cdot \mathbf{P}_{2\tau} f^*. \quad (16)$$

In these expressions the gradient operations $\mathbf{P}_{\alpha\beta}$ are defined by

$$\mathbf{P}_{\alpha\beta} = \nabla_v - (t_\alpha - t_\beta)\nabla_r \quad (17)$$

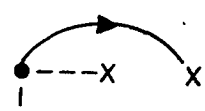
and act on that function of **v** and **r**, on which their representative lines in the corresponding diagram end. In (15) $\mathbf{P}_{12}$ acts on the succeeding **A** vector, whereas $\mathbf{P}_{1\tau} = \nabla_v - (t_1 - \tau)\nabla_r$ acts on the last (external) vertex, i.e., on the initial distribution function. From now on, we will call a vertex representing an **A** vector (external force vector) an A vertex. The diagrams shown so far contain only A vertices. A vertex associated with the initial distribution function (the external vertex of I) will be called an f vertex. The diagrams shown so far each contain one f vertex. We now turn to an inspection of the contributions resulting from the nonlinear integral term of Eq. (4). The first-order contribution caused by the nonlinear integral term is shown in Eq. (13). We observe that it may be generated from the first contribution (the one represented by an A vertex) by replacing $\mathbf{A}(\mathbf{r} - \mathbf{v}(t-t_1), \mathbf{v}, t_1)$ by

$$\sum_i \int_\tau^{t_1} dt' \int d^3r' d^3v' \mathbf{B}_{ji}(\mathbf{r} - \mathbf{v}(t-t_1), \mathbf{v}, t_1; \mathbf{r}', \mathbf{v}', t') \times f_i^*(\mathbf{r}' - \mathbf{v}'(t'-\tau), \mathbf{v}', \tau). \quad (18)$$

Furthermore, we notice that the first set of variables of the integral kernel $B(\mathbf{r},\mathbf{v},t;\mathbf{r}',\mathbf{v}',t')$ is treated in exactly the same way as the set of variables of the corresponding A vertex. The vector **B** is also multiplied by $f^*(\mathbf{r}' - \mathbf{v}(t'-\tau), \mathbf{v}', \tau)$. Obviously, the zero-order contribution to the distribution function is given by Eq. (11). It may be represented by a simple f vertex

$$x \equiv f_j^*(\mathbf{r} - \mathbf{v}(t-\tau), \mathbf{v}, \tau). \quad (19)$$

We see that in replacing the $\mathbf{r}\mathbf{v}t$ variables of the zero-order term (19) by the second set of variables $\mathbf{r}'\mathbf{v}'t'$ of the integral kernel and then integrating over all phase space $d^3r'd^3v'$ and over the time t' from τ to t_1 and finally sum over all distribution functions **i** as indicated in (18) we obtain an expression, which is mathematically completely equivalent to $\mathbf{A}(\mathbf{r} - \mathbf{v}(t-t_1), \mathbf{v}, t_1)$ in as far as the further steps of calculation are concerned. A diagram which reproduces these facts is



(20)

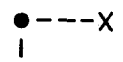
A "filled dot" is called a B vertex. A B vertex at position α is the representative of the following operator:

$$\sum_i \int_\tau^{t_\alpha} dt' \int d^3r' d^3v' \mathbf{B}_{ji}(\mathbf{r} - \mathbf{v}(t-t_\alpha), \mathbf{v}, t_\alpha; \mathbf{r}', \mathbf{v}'t') \cdots. \quad (21)$$

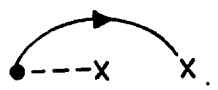
The diagram (20) shows a B vertex at position 1. This B vertex is connected with an f vertex by a dotted line. The meaning of this is now clear. The single f vertex, which is connected with the B vertex, contains the primed variables $\mathbf{r}'\mathbf{v}'t'$ over which the integration indicated in (21) takes place. Therefore, in first order, we have two contributions. The first one is familiar from I

and is given by

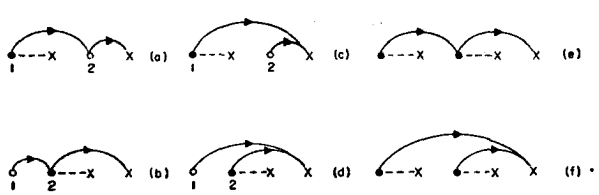
The second one is obtained from the first one by replacing the A vertex by



which is precisely expression (18). Therefore, it is given by



We are now ready to investigate the second-order contributions. The corresponding diagrams can only contain either two A vertices, two B vertices or one A and one B vertex. The diagrams with two A vertices are shown in (14). Their contributions are easily obtained by using the rules given in I. The replacing of either one or both of the A vertices by a B vertex with attached zero-order diagram yields 6 new possibilities. They are

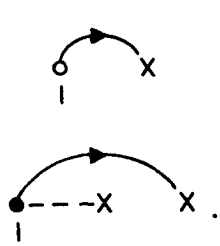


(22)

As an example, let us write down the contribution resulting from diagram (22d). It is

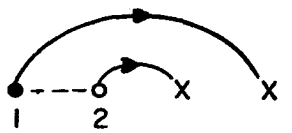
$$\int_\tau^t dt_1 \int_\tau^{t_1} dt_2 \mathbf{A}_j(\mathbf{r}-\mathbf{v}(t-t_1), \mathbf{v}, t_1)\cdot \mathbf{P}_{1\tau} \int_\tau^{t_2} dt' \int d^3r' d^3v'$$
$$\times \sum_i \mathbf{B}_{ji}(\mathbf{r}-\mathbf{v}(t-t_2), \mathbf{v}, t_2; \mathbf{r}', \mathbf{v}', t') f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau), \mathbf{v}', \tau)$$
$$\times \mathbf{P}_{2\tau} f_j^*(\mathbf{r}-\mathbf{v}(t-\tau), \mathbf{v}, \tau). \quad (23)$$

The eight contributions so far considered are not all in second order. Actually, there are two more. A B vertex may have attached to it (by dotted line) a first-order diagram. Since the B vertex counts as first order, the B vertex with an attached first-order diagram is of second order. Now, there are two first-order diagrams,



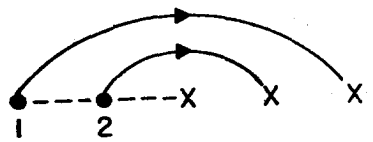
and

Therefore, we have



(24a)

and



(24b)

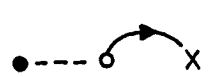
as possible second-order diagrams. Earlier we gave a prescription for an f vertex, which was connected with a B vertex by a dotted line. It said: multiply the kernel represented by the B vertex with the zero-order diagram in which $\mathbf{rv}$ and t are replaced by the integration variables $\mathbf{r}'\mathbf{v}'$ and t', and then integrate as indicated. Therefore, we suspect that in order to obtain the correct expression for the diagram (24a), for instance, we merely have to multiply the integral kernel represented by the B vertex with the expression corresponding to the first-order diagram in which only the variables $\mathbf{rv}$ and t are changed into the integration variables $\mathbf{r}'\mathbf{v}'$ and t'. This is true in fact. We call a diagram which is attached to a B vertex by a dotted line an internal diagram. It is necessarily of lower order than the complete diagram. (24) shows the two possible cases in which a second-order diagram is constructed by means of B vertices and internal diagrams of the first order. The internal diagram of (24a) is given by (on replacing already $\mathbf{r}$, $\mathbf{v}$, t by $\mathbf{r}'$, $\mathbf{v}'$, t')

$$\int_\tau^{t'} dt_2 \mathbf{A}_j(\mathbf{r}'-\mathbf{v}'(t'-t_2), \mathbf{v}', t_2)\cdot \mathbf{P}_{2\tau} f_j^*(\mathbf{r}'-\mathbf{v}'(t'-\tau), \mathbf{v}', \tau).$$

Therefore, this is the expression with which the kernel (the B vertex) has to be multiplied. By applying our prescriptions to (24a) we see that it represents

$$\int_\tau^t dt_1 \sum_i \int_\tau^{t_1} dt' \int d^3r' d^3v' \mathbf{B}_{ji}(\mathbf{r}-\mathbf{v}(t-t_1), \mathbf{v}, t_1; \mathbf{r}', \mathbf{v}', t')$$
$$\times \int_\tau^{t'} dt_2 \mathbf{A}_i(\mathbf{r}'-\mathbf{v}'(t'-t_2), \mathbf{v}', t_2)$$
$$\times \mathbf{P}_{2\tau} f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau), \mathbf{v}', \tau)$$
$$\times \mathbf{P}_{1\tau} f_j^*(\mathbf{r}-\mathbf{v}(t-\tau), \mathbf{v}, \tau). \quad (25)$$

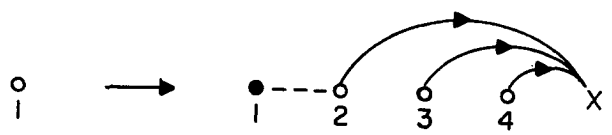
We note here that the expression



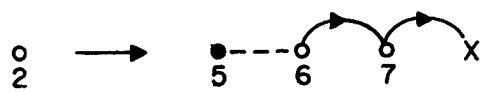
may be considered as a replacement for an A vertex so that the rules governing the connection of A vertices

by solid lines as outlined in I still apply in its entirety if we replace a simple A vertex by a more complicated structure (a B vertex with an attached internal diagram). For instance, from the two possible second-order diagrams with only A vertices (14)

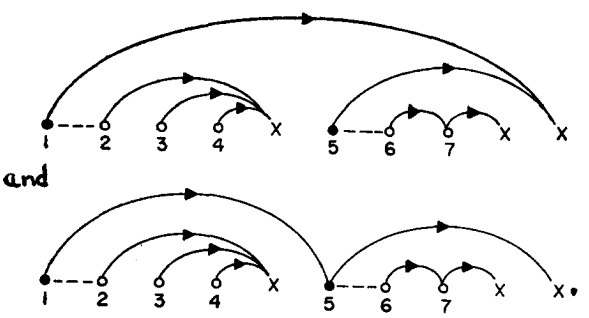
we obtain by replacing



and



two possible seventh-order diagrams, viz.,



If one turns back to diagram (24b) we obtain the expression it represents by noting that the internal diagram it contains is given by (13) or

$$\int_\tau^t dt_2 \int_\tau^{t_2} dt' \int d^3v' d^3v' \sum_i \mathbf{B}_{ji}(\mathbf{r}-\mathbf{v}(t-t_2), \mathbf{v}, t_2; \mathbf{r}', \mathbf{v}', t')$$

$$\times f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau), \mathbf{v}', \tau) \cdot \mathbf{P}_{2\tau} f_j^*(\mathbf{r}-\mathbf{v}(t-\tau), \mathbf{v}, \tau).$$

We only have to replace $\mathbf{r}\mathbf{v}t$ in the foregoing expression by $\mathbf{r}''\mathbf{v}''t''$, the integration variables of the first B vertex of diagram (24b), multiply and integrate thus:

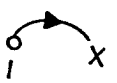
$$\int_\tau^{t_1} dt'' \int d^3r'' d^3v'' \sum_j \mathbf{B}_{kj}(\mathbf{r}-\mathbf{v}(t-t_1), \mathbf{v}, t_1; \mathbf{r}'', \mathbf{v}'', t'')$$

$$\times \int_\tau^{t''} dt_2 \int_\tau^{t_2} dt' \int d^3r' d^3v'$$

$$\times \sum_i \mathbf{B}_{ji}(\mathbf{r}''-\mathbf{v}''(t''-t_2), \mathbf{v}'', t_2; \mathbf{r}', \mathbf{v}', t')$$

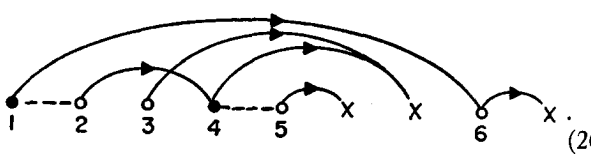
$$\times f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau), \mathbf{v}', \tau) \cdot \mathbf{P}_{2\tau} f_j^*(\mathbf{r}''-\mathbf{v}''(t''-\tau), \mathbf{v}'', \tau)$$

to obtain the expression which replaces the simple A vertex of the diagram



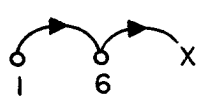
thereby converting it into diagram (24b).

For the sake of completeness let us illustrate the rules of associating any given diagram with its corresponding contribution to the distribution function with the following example:



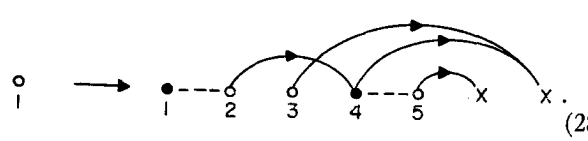
(26)

This is a six-order diagram which contains 2 internal diagrams. It is generated from the simple second-order diagram



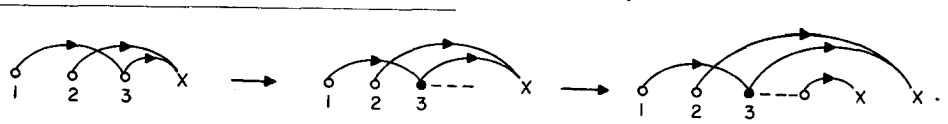
(27)

by replacing the first A vertex with a B vertex with an attached internal diagram of the fourth-order in this manner



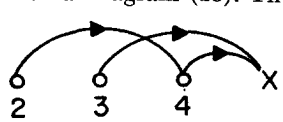
(28)

The fourth-order diagram in turn is obtained from a third-order diagram by replacing the third A vertex with a B vertex with attached first-order diagram in the following way:



(29)

To write down the contribution to the distribution function f represented by diagram (26) we have first to work out the internal diagram (28). The diagram



(30)

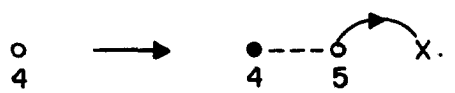
gives (on applying the rules of I)

$$\int_\tau^t dt_2 \int_\tau^{t_2} dt_3 \int_\tau^{t_3} dt_4 \mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_2), \mathbf{v}, t_2)$$

$$\cdot \mathbf{P}_{24} \mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_3), \mathbf{v}, t_3) \cdot \mathbf{P}_{3\tau} \mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_4), \mathbf{v}, t_4)$$

$$\cdot \mathbf{P}_{4\tau} f_j^*(\mathbf{r}-\mathbf{v}(t-\tau), \mathbf{v}, \tau).$$

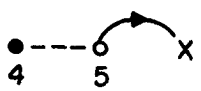
We now have to replace the A vertex number 4 by a B vertex with attached first-order diagram



To do this we write down the first-order diagram

$$\equiv\int_\tau^t dt_5\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_5),\mathbf{v},t_5)\cdot\mathbf{P}_{5\tau}f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\mathbf{v},\tau).$$

Therefore,



is given by (according to Eq. 21)

$$\int_\tau^{t_4}dt'\int d^3r'd^3v'\sum_i\mathbf{B}_{ji}(\mathbf{r}-\mathbf{v}(t-t_4),\mathbf{v},t_4;\mathbf{r}',\mathbf{v}',t')\times\int_\tau^{t'}dt_5\mathbf{A}(\mathbf{r}'-\mathbf{v}'(t'-t_5),\mathbf{v}',t_5)\cdot\mathbf{P}_{5\tau}'f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau),\mathbf{v}',\tau).$$

This then is the expression which replaces the A vertex number 4 in (30). In other words, the complete internal diagram (29) is given by

$$\begin{aligned}&\alpha_j(\mathbf{r},\mathbf{v},t)\\&=\int_\tau^t dt_2\int_\tau^{t_2}dt_3\int_\tau^{t_3}dt_4\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_2),\mathbf{v},t_2)\cdot\mathbf{P}_{24}\\&\times\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_3),\mathbf{v},t_3)\cdot\mathbf{P}_{3\tau}\int_\tau^{t_4}dt'\int d^3r'd^3v'\\&\times\sum_i\mathbf{B}_{ji}(\mathbf{r}-\mathbf{v}(t-t_4),\mathbf{v},t_4;\mathbf{r}',\mathbf{v}',t')\int_\tau^{t'}dt_5\\&\times\mathbf{A}(\mathbf{r}'-\mathbf{v}'(t'-r_5),\mathbf{v}',t_5)\cdot\mathbf{P}_{5\tau}'f_i^*(\mathbf{r}'-\mathbf{v}'(t'-\tau),\mathbf{v}',\tau)\\&\cdot\mathbf{P}_{4\tau}f_j^*(\mathbf{r}-\mathbf{v}(t-\tau),\mathbf{v},\tau).\end{aligned}$$

Again applying rule (21) this time to (28) yields the expression

$$\int_\tau^{t_1}dt''\int d^3r''d^3v''\sum_j\mathbf{B}_{kj}(\mathbf{r}-\mathbf{v}(t-t_1),\mathbf{v},t_1;\mathbf{r}'',\mathbf{v}'',t'')\alpha_j(\mathbf{r}'',\mathbf{v}'',t''),$$

which replaces the first A vertex of diagram (27). Since diagram (27) is given by

$$\int_\tau^t dt_1\int_\tau^{t_1}dt_6\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_1),\mathbf{v},t_1)\cdot\mathbf{P}_{16}\times\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_6),\mathbf{v},t_6)\cdot\mathbf{P}_{6\tau}f_k^*(\mathbf{r}-\mathbf{v}(t-\tau),\mathbf{v},\tau),$$

we finally find for diagram (26)

$$\text{diagram (26)}\equiv\int_\tau^t dt_1\int_\tau^{t_1}dt_6\int_\tau^{t_1}dt''\int d^3r''d^3v''\times\sum_j\alpha_j(\mathbf{r}'',\mathbf{v}'',t'')\mathbf{B}_{kj}(\mathbf{r}-\mathbf{v}(t-t_1),\mathbf{v},t_1;\mathbf{r}'',\mathbf{v}'',t'')\cdot\mathbf{P}_{16}\times\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_6),\mathbf{v},t_6)\cdot\mathbf{P}_{6\tau}f_k^*(\mathbf{r}-\mathbf{v}(t-\tau),\mathbf{v},\tau).\quad(31)$$

Although we now have a concise idea as to what contributions to expect for any given order n we will give here a formula for the number N_n of diagrams of order n.[7] Let n be the order for which we wish to know the number of possible diagrams N_n. We then write

$$n=\alpha_0+2\alpha_1+3\alpha_2+\cdots n\alpha_{n-1},\quad(32)$$

and determine all possible ways by which Eq. (32) can be satisfied with positive integers $\alpha_1\alpha_2\cdots\alpha_{n-1}$. For instance, for $n=4$ we would have the five possible solutions:

$\alpha_0=4$	$\alpha_1=\alpha_2=\alpha_3=0$		
$\alpha_0=2$	$\alpha_1=1$	$\alpha_2=\alpha_3=0$	
$\alpha_0=1$	$\alpha_1=0$	$\alpha_2=1$	$\alpha_3=0$
$\alpha_0=0$	$\alpha_1=2$	$\alpha_2=\alpha_3=0$	
$\alpha_0=0$	$\alpha_1=\alpha_2=0$		$\alpha_3=1.$

If there are M solutions in the general case, we have M sets of positive integers $\alpha_i^{(\epsilon)}$ (including the zero) $1\leq\epsilon\leq M$. The number N_n is then given by the expression

$$N_n=\sum_{\epsilon=1}^{M}\frac{[(\sum_{i=0}^{n-1}\alpha_i^{(\epsilon)})!]^2}{\prod_{i=0}^{n-1}(\alpha_i^{(\epsilon)})!}2^{\alpha_0^{(\epsilon)}}\prod_{\gamma=0}^{n-1}(N_\gamma)^{\alpha_\gamma^{(\epsilon)}}.\quad(33)$$

The sum goes over all possible solutions of Eq. (32). To give an idea of how rapidly N_n increases we list N_n for the first few orders. For large n N_n goes approximately as $2^n\,n!$

n	N_n
0	1
1	2
2	10
3	74
4	690

[7] The author is grateful to H. Wahlquist for the derivation of formula (33).

3. APPLICATIONS

Therefore, although the number of diagrams and the number of contributions increases tremendously with increasing n there are many cases which can be handled advantageously by the diagram method. We will give here two examples confining ourselves to the Vlasov equation.[8] Its linearized version has been treated by several authors.[9] The Vlasov equation is applicable to a moderately low density fully ionized electron ion plasma, in which the ions have negligible velocities (they form an immovable uniform background of positive charges). Only the electrons are considered to move at liberty but again they are slow enough so that all effects of retardation for the electromagnetic fields are negligible ($v/c \to 0$). Equation (1) of Sec. 2 becomes Vlasov's equation if we drop the index of the distribution function (we only have to worry about the electron distribution) and if we put

$$\mathbf{B}(\mathbf{r},\mathbf{v},t;\,\mathbf{r}',\mathbf{v}',t') \equiv -\frac{e^2N}{m}\delta(t-t')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}. \tag{34}$$

Here N is the number density of electrons.

The first problem we are considering here is the following: At $t=\tau=0$ a plane polarized light wave is switched on. Initially, the electron distribution function $f(\mathbf{r},\mathbf{v},t)$ was maxwellian $f^*=f^*(\mathbf{v})\sim e^{-\alpha v^2}$. How does the light wave disturb the plasma?

The light-wave may be described by

$$\mathbf{E}_{\text{ext}}=\mathbf{a}\cos(\mathbf{k}\cdot\mathbf{r}-\omega t) \tag{35}$$

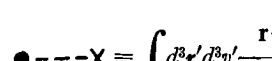
with

$$\mathbf{a}\cdot\mathbf{k}=0. \tag{36}$$

Vlasov's equation reads then (for $t>0$)

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla_r\right)f=-\frac{e}{m}\mathbf{a}\cdot\nabla_v f\cos(\mathbf{k}\cdot\mathbf{r}-\omega t)$$
$$-\frac{e^2N}{m}\int d^3r'd^3v'\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}f(\mathbf{r}',\mathbf{v}',t)\cdot\nabla_v f \tag{37}$$

$f(\mathbf{r},\mathbf{v},t)$ for $t>0$ is given by the sum of all possible diagrams according to Sec. 2. It is immediately noticed that a great simplification arises from the fact that the initial f is solely a function of velocity. Because then all diagrams containing a zero-order internal diagram vanish and



$$\equiv\int d^3r'd^3v'\frac{\mathbf{r}-\mathbf{v}(t-t_1)-\mathbf{r}'}{|\mathbf{r}-\mathbf{v}(t-t_1)-\mathbf{v}'|^3}f^*(\mathbf{v}')\equiv 0. \tag{38}$$

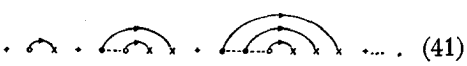
Without the external force (35) we can write

(39)

and we see that all diagrams vanish and the general solution is

$$f(\mathbf{r},\mathbf{v},t)=f^*(\mathbf{v}) \tag{40}$$

independent of time provided it was only a function of velocity initially. Let us now look for the effect of the external force switched on at $t=0$. If the light wave is sufficiently small we may neglect all higher order terms but the first. In other words, only one A vertex representing the light wave Eq. (35) is allowed in any diagram. The only diagrams which do not vanish off hand to this order [because of (38)] are



(41)

The actual evaluation is easy enough and we have

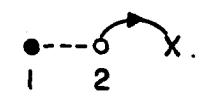
$$=\int_0^t dt_1\mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_1),\,\mathbf{v},\,t_1)\cdot\mathbf{P}_{1\tau}f^*(\mathbf{v})$$
$$\equiv-\frac{e}{m}\int_0^t dt_1\cos\{\mathbf{k}\cdot[\mathbf{r}-\mathbf{v}(t-t_1)]-\omega t_1\}$$
$$\times\mathbf{a}\cdot\nabla_v f^*(\mathbf{v}), \tag{42}$$

or

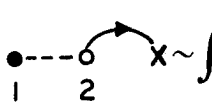
$$=-\frac{e}{m}\mathbf{a}\cdot\nabla_v f^*(\mathbf{v})F(\mathbf{k}\cdot\mathbf{v},\,\mathbf{r},\,t) \tag{43}$$

$$F(\mathbf{k}\cdot\mathbf{v},\,\mathbf{r},\,t)=\frac{\sin(\mathbf{k}\cdot\mathbf{r}-\omega t)-\sin\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}t)}{\mathbf{k}\cdot\mathbf{v}-\omega}. \tag{44}$$

In order to evaluate the remaining terms of the series (41) we determine the always occurring combination



According to the rules of Sec. 2 we have



$$\sim\int d^3r'd^3v'\frac{\mathbf{r}-\mathbf{v}(t-t_1)-\mathbf{r}'}{|\mathbf{r}-\mathbf{v}(t-t_1)-\mathbf{r}'|^3}$$
$$\times F(\mathbf{k}\cdot\mathbf{v}',\,\mathbf{r}',\,t_1)\mathbf{a}\cdot\nabla_{v'}f^*(\mathbf{v}'), \tag{45}$$

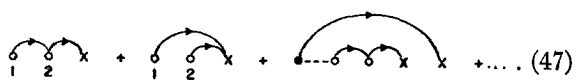
where F is that part of expression (43) which depends explicitly on the scalar product $\mathbf{k}\cdot\mathbf{v}$. But by partial integration the integral over $\mathbf{v}'$ can be converted into

$$\int d^3v'F(\mathbf{k}\cdot\mathbf{v}',\,\mathbf{r}',\,t_1)\mathbf{a}\cdot\nabla_{v'}f^*(\mathbf{v}')$$
$$=-\mathbf{a}\cdot\mathbf{k}\int d^3v'f^*(\mathbf{v}')\left(\frac{dF(u,\mathbf{r}',t_1)}{du}\right)_{u=\mathbf{k}\cdot\mathbf{v}'}\equiv 0, \tag{46}$$

[8] A. Vlasov, J. Phys. U.S.S.R. **9**, 25 (1945).

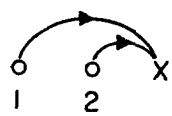
[9] L. Landau, J. Phys. U.S.S.R. **10**, 25 (1946); N. G. van Kampen, Physica **21**, 949 (1955); K. M. Case, Ann. Phys. **7**, 349 (1959).

which gives zero by virtue of (36). So we see that to 1st order only Eq. (42) contributes to 41. In 2nd order we would have contributions from the following series:



(47)

The first diagram of (47) vanishes again because of (36) and the second yields



$$\equiv \frac{1}{2}\left(-\frac{e}{m}\right)^2 \{F(\mathbf{k}\cdot\mathbf{v},\mathbf{r},t)\}^2 \times(\mathbf{a}\cdot\nabla_v)^2 f^*(\mathbf{v}). \quad (48)$$

If we consider (48) as a possible candidate for an internal diagram we see that by the same reasoning as before no contribution arises. This is easily extended to all higher orders and we have as solution for f

$f(\mathbf{r},\mathbf{v},t)=f^*(\mathbf{v})+$  (49)

all other diagrams vanish. It is not difficult to sum these diagrams up. In fact, the general nth order term is

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_1),t_1)\cdot\nabla_v \times \mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_2),t_2)\cdot\nabla_v \cdots \mathbf{A}(\mathbf{r}-\mathbf{v}(t-t_n),t_n)\cdot\nabla_v f^*(\mathbf{v}),$$

which is simply

$$\frac{1}{n!}\left\{\int_0^t d\tau \mathbf{A}(\mathbf{r}-\mathbf{v}(t-\tau),\tau)\cdot\nabla_v\right\}^n f^*(\mathbf{v}).$$

Therefore, the series (49) yields

$$f(\mathbf{r},\mathbf{v},t)=\exp\left\{\int_0^t d\tau \mathbf{A}(\mathbf{r}-\mathbf{v}(t-\tau),\tau)\cdot\nabla_v\right\} f^*(\mathbf{v}) = f^*\left\{\mathbf{v}+\int_6^t d\tau \mathbf{A}[\mathbf{r}-\mathbf{v}(t-\tau),\tau]\right\}. \quad (50)$$

If we insert expression (42) into (50) we obtain finally the desired result

$$f(\mathbf{r},\mathbf{v},t) = f^*\left(\mathbf{v}-\frac{e}{m}\mathbf{a}\frac{\sin(\mathbf{k}\cdot\mathbf{r}-\omega t)-\sin\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}t)}{\mathbf{k}\cdot\mathbf{v}-\omega}\right). \quad (51)$$

It is easily verified that Eq. (51) is in fact a solution of Eq. (37). The second case we are considering here is treated several times in the literature.[9] It is the following problem: Suppose that initially the distribution function is split into two parts

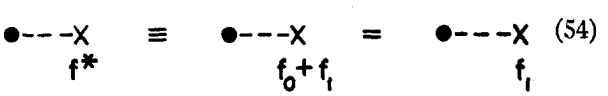
$$f^*(\mathbf{r},\mathbf{v},\tau)=f_0(\mathbf{v})+f_1(\mathbf{r},\mathbf{v}), \quad (52)$$

where the space dependent part f_1, is considered small compared to the uniform background which we assume to be Maxwellian

$$f_0(\mathbf{v})=\left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} e^{-\alpha v^2} \quad \alpha=\frac{m}{2kT}. \quad (53)$$

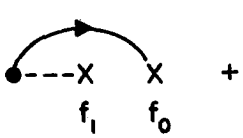
The question is: How does the initial disturbance f_1, propagate in time? Since we do not have any external forces the solution is entirely given by diagrams consisting of B vertices. We assume furthermore that all higher order terms of f_1 may be neglected. This is equivalent to using the linearized version of the Vlasov equation. Let us now look at the basic vertex

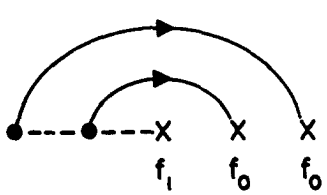
From (38) and (52) we see that



(54)

so that only f_1 survives as a zero-order internal diagram. Therefore, we obtain a complete description of the time development of the distribution function through the following series:

$f=f_0+f_1(\mathbf{r}-\mathbf{v}t,\mathbf{v})+$ 

$+$ 

$+\cdots$; (55)

all other diagrams either vanish or give a higher order contribution with respect to f_1. For f_1 let us take

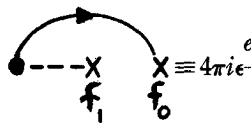
$$f_1=\epsilon\delta(\mathbf{v})e^{i\mathbf{k}\cdot\mathbf{r}} \quad (56)$$

ϵ measures the strength of the anisotropy. Expression (56) really is only a Fourier component of the arbitrary density fluctuation

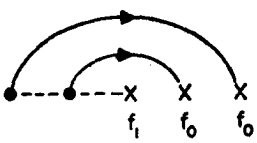
$$\rho(\mathbf{r})=(2\pi)^{-3}\int \rho(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}d^3k,$$

but since the series (55) is linear in f_1 we may first sum

it and then integrate over $\mathbf{k}$ to obtain the result for an arbitrary $\rho(\mathbf{r})$. The particles represented by f_1 are also considered to be at rest initially. After some calculation it is found that

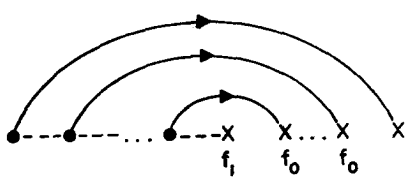


$$\equiv 4\pi i\epsilon\frac{e^2N}{m}\int_0^t dt_1 e^{i\mathbf{k}\cdot[\mathbf{r}-\mathbf{v}(t-t_1)]}\frac{\mathbf{k}\cdot\nabla_v f_0(\mathbf{v})}{\mathbf{k}^2} \tag{57}$$



$$\equiv (4\pi i)^2\epsilon i\left(\frac{e^2N}{m}\right)^2\int_0^t dt_1\int_0^{t_1} dt_2 e^{i\mathbf{k}\cdot[\mathbf{r}-\mathbf{v}(t-t_1)]} \times(t_1-t_2)g((t_1-t_2)\mathbf{k})\frac{\mathbf{k}\cdot\nabla_v f_0(\mathbf{v})}{\mathbf{k}^2}, \tag{58}$$

and in general,



$$\equiv -i\epsilon\left(-\frac{4\pi e^2N}{m}\right)^n\int_0^t dt_1\cdots\int^{t_{n-1}} dt_n$$

$$\times e^{i\mathbf{k}\cdot[\mathbf{r}-\mathbf{v}(t-t_1)]}(t_1-t_2)g((t_1-t_2)\mathbf{k})(t_2-t_3)g((t_2-t_3)\mathbf{k})\cdots$$

$$\times(t_{n-1}-t_n)g[(t_{n-1}-t_n)\mathbf{k}]\frac{\mathbf{k}\cdot\nabla_v f_0(\mathbf{v})}{\mathbf{k}^2}, \tag{59}$$

where $g(\mathbf{k})$ is defined as the Fourier transform of the background distribution function

$$g(t\mathbf{k})=\int d^3v f_0(\mathbf{v})e^{-it\mathbf{k}\cdot\mathbf{v}}=\exp\left(-\frac{\mathbf{k}^2}{4\alpha}t^2\right) \tag{60}$$

from (53). The general expression (59) can be simplified considerably by noting that the time integrals are nothing else than a number of convolution integrals "nested" into each other. If we define the Laplace transform of $\exp(-it\mathbf{k}\cdot\mathbf{v})$ and $g(t\mathbf{k})$ by

$$\mathfrak{L}(e^{-it\mathbf{k}\cdot\mathbf{v}})=\int_0^\infty e^{-st}e^{-it\mathbf{k}\cdot\mathbf{v}}dt=(s+i\mathbf{k}\cdot\mathbf{v})^{-1}=\alpha(s) \tag{61}$$

$$\mathfrak{L}(g(t\mathbf{k}))=\int_0^\infty e^{-st}g(t\mathbf{k})dt=\beta(s)$$

$$=\frac{(\pi\alpha)^{\frac{1}{2}}}{k}\exp(\alpha s^2/k^2)\left\{1-\phi\left[\frac{(\alpha s)^{\frac{1}{2}}}{k}\right]\right\}, \tag{62}$$

we see that the Laplace transform of the general term (59) is

$$\mathfrak{L}(\text{Eq. (59)})=-i\epsilon\left(-\frac{4\pi e^2N}{m}\right)^n e^{i\mathbf{k}\cdot\mathbf{r}} \times\frac{\mathbf{k}\cdot\nabla_v f_0(\mathbf{v})}{\mathbf{k}^2}\frac{\alpha(s)}{s}\left(\frac{2\alpha}{\mathbf{k}^2}\right)^n(1-s\beta(s))^{n-1}. \tag{63}$$

It is therefore easy to sum the Laplace transform of the series (55) and the result is

$$\mathfrak{L}(f-f_0-f_1)=i\epsilon\frac{4\pi e^2N}{m}e^{i\mathbf{k}\cdot\mathbf{r}} \times\frac{\mathbf{k}\cdot\nabla_v f_0(\mathbf{v})}{\mathbf{k}^2}\frac{\alpha(s)}{s}\{1+(\mathbf{k}\lambda_D)^{-2}[1-s\beta(s)]\}^{-1}, \tag{64}$$

where we introduced the Debye-Hückel length

$$\lambda_D=(kT/4\pi e^2N)^{\frac{1}{2}}. \tag{65}$$

Expression (64) can easily be shown to be identical with the result obtained by Landau[9] and Berz.[10]

[10] F. Berz, Proc. Phys. Soc. (London) **B69**, 939 (1956).

Variational Method for Studying the Motion of Classical Vibrating Systems*

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A quantity Z (essentially the action integral) is shown to be stationary for small periodic deviations from the actual motion. By choosing approximations to the motion containing the frequency and some other parameters, it is possible to make this variational principle the basis of an approximate determination of the motion.

Quite simple trial functions are found to give surprisingly accurate values for the frequency and the Fourier components of the motion. Comparison between the exact solution and ours for some systems is given.

I. INTRODUCTION

IN recent years, variational techniques have come into wide use as a method of obtaining numerical results when exact solutions are not available, or not convenient for computation. The purpose of this brief note is to point out the existence of a very simple variational procedure which is of use in studying the motion of a classical vibrating system with one degree of freedom. The method was developed by Luttinger and used by Luttinger and Goodman[1] to study a problem which arose in the theory of cyclotron resonance for degenerate bands. The accuracy of the numerical results obtained there was so encouraging that it was thought worth while to publish the method independently, along with some simple illustrative examples. As is seen from the results given below, relatively simple choices for trial functions give quite accurate values for the frequency and Fourier components of the motion of the system. The latter we regard as perhaps the more important contribution of the method, since it seems rather difficult to get a hold on these coefficients by direct means. We may mention that in studying (say) the absorption of radiation by such a system, it is these Fourier coefficients which play a determining role.

In Sec. II, the general method is presented, and in Sec. III some illustrative examples are given and compared with the exact solutions.

II. GENERAL FORMULATION OF THE METHOD

Suppose we have a classical system with one degree of freedom, which is described by a generalized coordinate q. Let the system have a Lagrangian $L(q,\dot{q})$, where $\dot{q}=dq/dt$. Consider the quantity defined by

$$Z=\int_0^T (L(q,\dot{q})+E)dt, \tag{1}$$

where E is the energy of the motion and T is the period of $q(t)$. What we shall show is that if $q(t)$, T differ by small quantities of first order from $q_0(t,E)$, $T_0(E)$ (the exact solutions of the equations of motion for the system with Lagrangian L), then Z differs from Z_0 by quantities of the second order. That is, the quantity Z is stationary for small periodic deviation from the actual motion.

To see this we write

$$q=q_0+\delta q. \tag{2}$$

Then

$$\begin{aligned}
Z&=\int_0^T (L(q_0+\delta q,\dot{q}_0+\delta\dot{q}_0)+E)dt\\
&=\int_0^T \left(L(q_0,\dot{q}_0)+\frac{\partial L_0}{\partial q_0}\delta q+\frac{\partial L_0}{\partial \dot{q}_0}\delta\dot{q}\right)dt+ET\\
&=\int_0^T \left(L(q_0,\dot{q}_0)+\left[\frac{\partial L_0}{\partial q_0}-\frac{d}{dt}\left(\frac{\partial L_0}{\partial \dot{q}_0}\right)\right]\delta q\right)dt\\
&\qquad +\frac{\partial L_0}{\partial \dot{q}_0}\delta q\Big|_{t=0}^{t=T}+ET\\
&=\int_0^T L(q_0,\dot{q}_0)dt+\frac{\partial L_0}{\partial \dot{q}_0}\delta q\Big|_0^T+ET
\end{aligned} \tag{3}$$

on using the Lagrangian equations of motion. We may rewrite (3) to the first order as

$$\begin{aligned}
Z&=\int_0^{T_0} (L_0+E)dt+\int_{T_0}^T L_0dt\\
&\qquad +\frac{\partial L_0}{\partial \dot{q}_0}\delta q\Big|_0^{T_0}+E(T-T_0)\\
&=Z_0+(L_0(t=T_0)+E)(T-T_0)\\
&\qquad +\frac{\partial L_0(t=T_0)}{\partial \dot{q}_0}[\delta q(T_0)-\delta q(0)],
\end{aligned} \tag{4}$$

where we have used the fact that q_0 has the periodicity T_0. Clearly,

$$\begin{aligned}
\delta q(T_0)&=q(T_0)-q_0(T_0)=q(T+(T_0-T))-q_0(T_0)\\
&=q(T)-q_0(T_0)+\dot{q}(T)(T_0-T)+\cdots\\
&=\delta q(0)+\dot{q}_0(T_0)(T_0-T)+\cdots,
\end{aligned} \tag{5}$$

* Supported in part by the Office of Naval Research.

[1] J. M. Luttinger and R. R. Goodman, Phys. Rev. **100**, 673 (1955).

to the first order. Therefore, (4) becomes

$$Z=Z_0+[L_0-\dot{q}_0(\partial L_0/\partial\dot{q}_0)+E]_{t=T_0}(T-T_0). \quad (6)$$

However, the Hamiltonian of the system is given by

$$H=\dot{q}(\partial L/\partial\dot{q})-L. \quad (7)$$

For the exact motion, q_0 this is conserved and equal to E at all times. Therefore, we get

$$Z=Z_0+\text{second-order terms}, \quad (8)$$

which we wanted to prove.

The same method of proof shows that

$$Z'=\int_0^T (p\dot{q}-H(q,p)+E)dt \quad (9)$$

is stationary in the same sense as Z.

The stationary property of (1) or (9) is utilized as follows. A guess for the motion $q(t)$ is made. This will in general contain an unknown period T (or frequency ω), and some other parameters A_i. With this choice we compute Z. To make the $q(t)$ we have chosen as close as possible to the $q_0(t)$, we then choose the frequency and the A_i such that Z is also stationary under small changes in q, just as it would for the real motion. That means that ω and A_i are to be determined by the conditions that

$$\partial Z/\partial\omega=0 \quad (10)$$

$$\partial Z/\partial A_i=0, \quad i=1, 2, \cdots N. \quad (11)$$

Equation (10) actually has a simple and plausible physical content. Put $\omega t=x$. $q=q(\omega t)=q(x)$,

$$\begin{aligned}
Z&=\int_0^T (L(q,\dot{q})+E)dt\\
&=\frac{1}{\omega}\int_0^{2\pi} (L(q(x),\omega q'(x))+E)dx\\
q'(x)&=\frac{dq(x)}{dx}\\
\frac{\partial Z}{\partial\omega}&=-\frac{2\pi}{\omega^2}E+\frac{1}{\omega}\int_0^{2\pi}\left(-\frac{L}{\omega}+\frac{\partial L}{\partial\dot{q}}q'\right)dx\\
&=\frac{2\pi}{\omega^2}\left[-E+\frac{1}{2\pi}\int_0^{2\pi}\left(-L+\frac{\partial L}{\partial\dot{q}}\dot{q}\right)dx\right]\\
&=\frac{2\pi}{\omega^2}\left[-E+\frac{1}{2\pi}\int_0^{2\pi} Hdx\right]=0.
\end{aligned} \quad (12)$$

Therefore, going back to time variables,

$$E=\frac{1}{T}\int_0^T Hdt=\bar{H}. \quad (13)$$

This means that although the approximate solution does not conserve energy exactly, it must be chosen in such a way that it conserves energy *on the average* during one period.

The technique described in the forgoing gives rather surprisingly good values for the frequency, using relatively simple trial functions $q(t)$. Some insight into this may be obtained as follows. From (13) and (7) we have at once that

$$\begin{aligned}
Z&=\int_0^T \dot{q}\frac{\partial L}{\partial\dot{q}}dt\\
&=\int_0^T p\dot{q}dt\\
&=\int_0^T pdq=\oint pdq,
\end{aligned} \quad (14)$$

which is just the action integral of the system. Now, if we had the exact motion then from the theory of action-angle variables, we know that

$$\partial Z_0/\partial E=2\pi/\omega_0. \quad (15)$$

A relationship of the same form holds for the Z, which we compute to within second-order terms. To show this we first note that Z will be of the form,

$$Z=Z(E,\omega,A_1,A_2\cdots A_N). \quad (16)$$

On taking the total derivative of Z with respect to E we obtain, by using (10) and (11),

$$\begin{aligned}
\frac{dZ}{dE}&=\frac{\partial Z}{\partial E}+\frac{\partial Z}{\partial\omega}\frac{d\omega}{dE}+\sum_{i=1}^{N}\frac{\partial Z}{\partial A_i}\frac{dA_i}{dE}\\
&=\frac{\partial Z}{\partial E}\\
&=\frac{\partial}{\partial E}\oint\frac{1}{\omega}(\omega pq'(x)-H+E)dx\\
&=\frac{1}{\omega}\oint dx=\frac{2\pi}{\omega}.
\end{aligned} \quad (17)$$

This is quite reasonable since the Z which we compute is, for small errors, equal to Z_0 within second order terms and we would expect that ω is equal to ω_0 also within second order terms. Therefore, we would expect the frequency to be given rather more accurately than properties of the system (Fourier coefficients, say), and this turns out to be the case.

III. USE OF THE VARIATIONAL PRINCIPLE

The Lagrangian or Hamiltonian function characterizing some vibratory motion is given. We wish to find approximate values of the frequency and Fourier components of the motion. To do this a trial function

of ωt and one or more amplitude parameters is selected which has the approximate form of the exact motion. By using this trial function Z is computed and obtained as an explicit function of the frequency, amplitude parameters, and energy. Z is then made stationary with respect to the frequency and amplitude parameters. Sufficient relations are thereby obtained to provide an expression for each which depends only on the energy.

Our first concern when dealing with a particular problem is the choice of a suitable trial function. Linear combinations of harmonic functions of ωt will, of course, provide an approximation of the motion. If we take our initial condition such that the amplitude is zero at $t=0$ only sines having for their arguments odd multiples of ωt need be included in any trial function, provided the Lagrangian is an *even* function of q. To see why this is so we look at the most general harmonic trial function satisfying the initial condition $q(0)=0$,

$$q=\sum_{n=1}^{N} A_n \sin n\omega t. \tag{18}$$

At one quarter period, $\omega t=\pi/2$, $\dot{q}$ must be zero for a symmetric potential. This will be true only if we exclude terms in (18) having even integers n.

Some difficulty may be encountered in performing the required integration using harmonic functions. This difficulty may in some cases be circumvented by making use of a quadratic or even linear trial function having the form

$$q=A\left(\omega t-\frac{\omega^2 t^2}{\pi}\right) \tag{19}$$

$$q=A(2/\pi)\omega t \tag{20}$$

in the first quarter period. We could of course include two different amplitudes in the quadratic function. We have in fact chosen the constant factors in these expressions so that A has the physical significance of an amplitude. The method is applied to several simple systems.

1. The Harmonic Oscillator

The Lagrangian for the harmonic oscillator is

$$L=\tfrac{1}{2}(\dot{q}^2-q^2), \tag{21}$$

taking the force constant and the particle mass to be unity. After taking the trial function

$$q=A\sin\omega t, \tag{22}$$

Z is computed to be

$$Z=\tfrac{1}{2}A^2\pi\left(\omega-\frac{1}{\omega}\right)+\frac{2\pi E}{\omega}. \tag{23}$$

If we make Z stationary with respect to A, we find

$$\frac{\partial Z}{\partial A}=A\pi\left(\omega-\frac{1}{\omega}\right)=0,$$

which implies

$$\omega=1. \tag{24}$$

On making Z stationary with respect to ω and by using (23), we find that

$$\frac{\partial Z}{\partial \omega}=2\pi\left(\frac{A^2}{2}-E\right)=0,$$

which implies

$$E=A^2/2. \tag{25}$$

The results (24) and (25) are seen to be exactly correct for a system described by the Lagrangian (21). This must be so since the trial function (22) has in fact the form of the exact solution.

If Z is computed for the harmonic oscillator by using the quadratic approximation (19)

$$Z=\frac{A^2\omega\pi}{3}+\frac{2\pi E}{\omega}-\frac{A^2\pi^3}{30\omega}. \tag{26}$$

The ratio of the period computed from (26) to the exact period is very close to one, 1.0064. The first Fourier amplitude has the value $1.413(E)^{\frac{1}{2}}$ as compared with the exact value $(2E)^{\frac{1}{2}}$.

2. Power Potentials

The general expression for the exact period of motion in the potential

$$V=\tfrac{1}{2}|q|^n \tag{27}$$

is given by

$$T(n)=\frac{4}{(2E)^{(n-2)/2n}}\frac{\pi^{\frac{1}{2}}}{n}\frac{\Gamma(1/n)}{\Gamma(1/n+\frac{1}{2})} \tag{28}$$

in terms of the Gamma function for $n>0$. It is interesting to compare the periods predicted by formula (28) with those found by the variational method for various trial functions. In Figs. (1) and (2) we have plotted the percentage error in the period computed for the first two harmonic trial functions. Power potentials for n up to 4 have been included. If only the first harmonic is used the error is less than 1%. The inclusion of the third harmonic in the trial function reduces this error by a factor of ten.

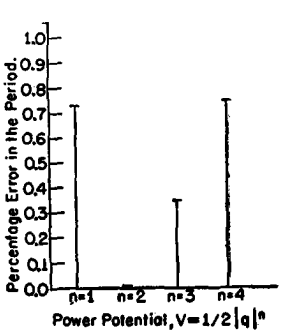

FIG. 1. Percentage error in the period computed for the power potentials $V=\frac{1}{2}|q|^n$ by using the trial function $q=A_1\sin\omega t$.

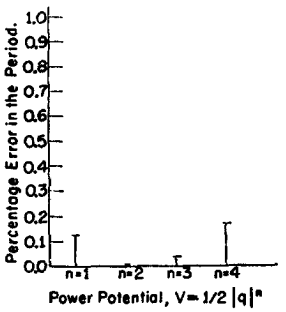

FIG. 2. Percentage error in the period computed for the power potentials $V=\frac{1}{2}|q|^n$ by using the trial function $q=A_1\sin\omega t+A_3\sin 3\omega t$.

Computations for these same potentials were carried out using linear and quadratic trial functions (20) and (19). Figure (3) shows that the linear approximation becomes progressively better as n becomes larger. The explanation for this lies in the fact that the linear solution is in fact the exact solution in the limit of very large n. The quadratic trial function, Fig. (4) gives results comparable with those obtained using a single harmonic as might be expected from their similarity.

Two cases, $n=1$ and $n=\infty$, are of particular interest since the motion itself can be obtained in terms of functions with known Fourier expansions. For $n=1$ we have just the constant force with the well known quadratic dependence on time. In Fig. (5) we have plotted the percentage error in the computed Fourier components for the first three harmonic approximations. The predictions are about 1% or less in error with a progressive decrease in error for each component in succeeding approximations.

The limiting case where n approaches infinity is also of interest. It is seen that the potential $V=\lim_{n\to\infty}\times\frac{1}{2}|q|^n$ becomes simply a pair of potential walls at $q=\pm 1$ with $V=0$ for $|q|<1$. If we again take the first harmonic as our trial function

$$Z=\tfrac{1}{2}A^2\omega\pi+\frac{2\pi E}{\omega}-\frac{\pi^{\frac{1}{2}}A^n}{\omega}\frac{\Gamma[(n+1)/2]}{\Gamma[(n/2)+1]} \tag{29}$$

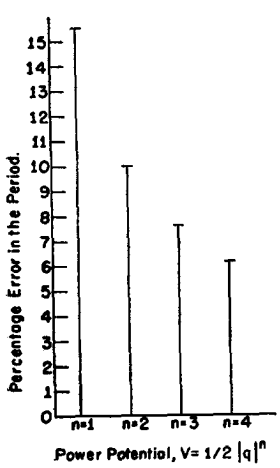

FIG. 3. Percentage error in the period computed for the power potentials $V=\frac{1}{2}|q|^n$ by using the trial function $q=A(2/\pi)\omega t$.

for arbitrary n. In the limit of very large n, this predicts a period $\pi/(E)^{\frac{1}{2}}$ and an amplitude $A=1$. The potential wall problem can be solved exactly to obtain the simple linear dependence on time with its well-known Fourier expansion. Trial functions containing terms up to the fifth harmonic were applied to this problem. The percentage error in the components predicted by each of these trial functions is shown in Fig. (6). The 10% error in the period found after using the first harmonic is reduced to about 3% when the 3rd and 5th harmonics are included. Large errors are to be expected when the potential well is treated by using only a few harmonics since a Fourier representation of the discontinuous motion requires a large share of the higher harmonics. The application of all harmonic and polynomial trial functions to the power potential leads to expressions for the period having the same energy dependence as the exact expression (28). This is also found to be true for the amplitude expressions. Fractional errors involved in these quantities are therefore independent of energy.

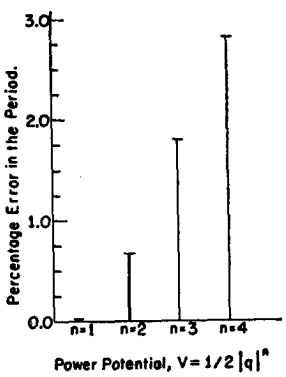

FIG. 4. Percentage error in the period computed for the power potentials $V=\frac{1}{2}|q|^n$ by using the trial function $q=A(\omega t-\omega^3 t^3/\pi)$.

3. Simple Pendulum

The exact period of the simple pendulum characterized by the potential

$$V=gl(1-\cos\theta) \tag{30}$$

is given by

$$T(\theta_0)=4(l/g)^{\frac{1}{2}}F(\pi/2,\sin\theta_0/2) \tag{31}$$

in terms of the elliptic integral of the first kind $F(\pi/2, k)$. θ is the angular amplitude which determines the energy of the system. l is the length of the pendulum and g is the acceleration of gravity.

Z was computed by using two trial function; the first harmonic, and the quadratic. In each case we encounter a transcendental equation for the amplitude parameter which must be solved before this quantity can be eliminated in the expression for the period. In Fig. (7) we have plotted the percentage errors computed using the first harmonic and quadratic trial functions. For an angular amplitude $\theta_0<\pi/2$, they are seen to be only a few parts per thousand.

The exact equation of motion for the simple pendulum can be expressed in terms of the Sn function by

$$\theta=2\sin^{-1}\{kSn(t(g/l)^{\frac{1}{2}},k)\}, \tag{32}$$

where $k=\sin\theta_0/2$. It would be desirable to express θ as a Fourier sine series, but there does not seem to be any elementary way to accomplish this. We can, however, take as our variable

$$\eta=\sin\theta/2, \tag{33}$$

as suggested by Eq. (31). The exact equation of motion then becomes

$$\eta=kSn(t(g/l)^{\frac{1}{2}},k). \tag{33}$$

η can now be expressed in terms of its Fourier components by making use of the known expansion of the Sn function[2]

$$\eta=\frac{2\pi}{K}\left\{\frac{q^{\frac{1}{2}}}{1-q}\sin\frac{\pi}{2K}\left(\frac{g}{l}\right)^{\frac{1}{2}}t+\frac{q^{\frac{3}{2}}}{1-q^3}\sin\frac{3\pi}{2K}\left(\frac{g}{l}\right)^{\frac{1}{2}}t+\frac{q^{\frac{5}{2}}}{1-q^5}\sin\frac{5\pi}{2K}\left(\frac{g}{l}\right)^{\frac{1}{2}}t+\cdots\right\}, \tag{34}$$

where

$$q=e^{-\pi K'/K}$$
$$k=\sin\theta_0/2=(1-k'^2)^{\frac{1}{2}}$$
$$K=F(\pi/2,k)$$
$$K'=F(\pi/2,k').$$

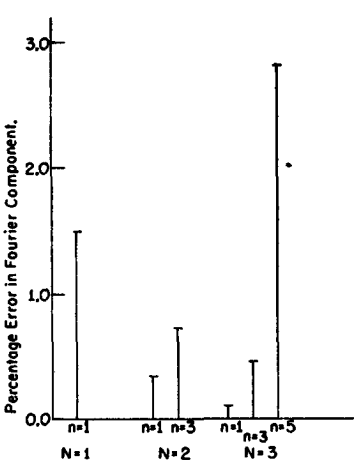

FIG. 5. Percentage error in the Fourier components of motion in the potential $V=\frac{1}{2}|q|$ using trial functions $q=\sum_{n=1}^{N}A_n\sin n\omega t$. $n=i$th harmonic and N =number of harmonics included in trial function.

We can now proceed in the same manner as before since it is evident from (34) that η is also periodic. Expressed in the variable η, the Lagrangian for the simple pendulum becomes

$$L=\frac{2l^2}{1-\eta^2}\left(\frac{d\eta}{dt}\right)^2-2gl\eta^2. \tag{35}$$

By using the first harmonic as a trial function, Z is

[2] H. Hancock, *Theory of Elliptic Functions* (John Wiley & Sons, Inc., New York), p. 256.

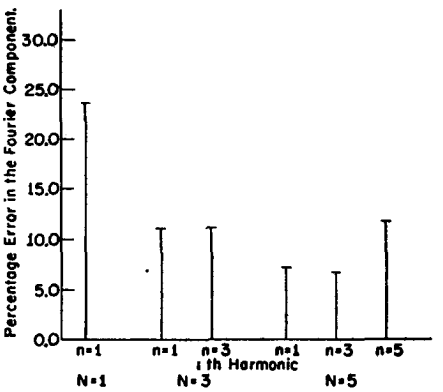

FIG. 6. Percentage error in the Fourier components of motion between infinite potential walls by using trial functions $q=\sum_{n=1}^{N}A_n\times\sin n\omega t$. N=number of harmonics taken in trial function.

found to be

$$Z=\frac{2\pi E}{\omega}+4l^2\omega\pi\{1-(1-A^2)^{\frac{1}{2}}\}-\frac{2gl\pi A^2}{\omega} \tag{36}$$

for the Lagrangian (35). The first Fourier amplitudes found from (36) are 0.387 and 0.745 for θ_0 equal to $\pi/4$ and $\pi/2$, respectively. These compare remarkably well with the exact values 0.386 and 0.733 computed from (34).

4. Anharmonic Oscillator

Numerous linear combinations of the various power potentials can be formed and treated by our variational procedure. One such potential is that associated with the anharmonic oscillator. It has the form

$$V=\tfrac{1}{2}\{\alpha q^2+\beta q^4\}, \tag{37}$$

where α and β are constants. The exact period for this

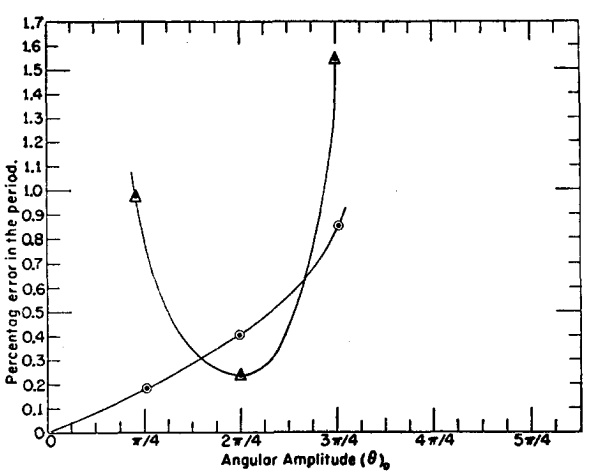

FIG. 7. Percentage error in the period computed for the potential $V(\theta)=gl(1-\cos\theta)$ at various angular amplitudes by using the trial functions $n=\phi\sin\omega t$ and $n=\phi(\omega t-\omega^3t^3/\pi)$.

potential can be written as

$$T(\alpha,\beta,E)=\frac{4}{[2E(\mu+\epsilon)]^{\frac{1}{2}}}F\left[\frac{\pi}{2},\left(\frac{\epsilon}{\epsilon+\mu}\right)^{\frac{1}{2}}\right], \quad (38)$$

where

$$\mu=\frac{\alpha+(\alpha^2+8E\beta)^{\frac{1}{2}}}{4E}$$

$$\epsilon=\frac{2\beta}{\alpha+(\beta^2+8E\beta)^{\frac{1}{2}}}.$$

Z is the easily computed to be

$$Z=\tfrac{1}{2}A^2\omega\pi+\frac{2\pi E}{\omega}-\frac{\alpha A^2\pi}{2\omega}-\frac{3}{16}\frac{\beta A^4\pi}{\omega} \quad (39)$$

by using the first harmonic as a trial function. (39) yields the angular frequency

$$\omega=\left[\frac{\alpha}{3}+\frac{2}{3}\alpha\left(1+\frac{9\beta E}{\alpha^2}\right)^{\frac{1}{2}}\right]^{\frac{1}{2}}. \quad (40)$$

The ratio of the computed to the exact period found from (38) is 1.0003 for the case where $\alpha=\beta=E=1$.

Another interesting combination

$$V=\tfrac{1}{2}\{\alpha|q|+\beta q^2\}, \quad (41)$$

having the exact period

$$T(\alpha,\beta,E)=\frac{4}{\sqrt{3}}\left\{\frac{\pi}{2}-\sin^{-1}\frac{\alpha}{(\alpha^2-8E\beta)^{\frac{1}{2}}}\right\}, \quad (42)$$

also can be treated by the same methods.

5. Luttinger-Goodman System

As a final example, we wish to treat briefly the system having for its Hamiltonian

$$H=\tfrac{1}{2}\{\alpha(q^2+p^2)\pm[\beta^2(q^2+p^2)^2+\lambda^2q^2p^2]\}. \quad (43)$$

The investigation of this and similar systems led initially to the development of the procedure presented in this note. The exact period for the Hamiltonian (43) can be written in terms of complete elliptic integrals of the third kind, but no closed expressions for the Fourier components may be obtained.

By taking for our trial functions

$$q=A\sin\omega t$$

$$p=A\cos\omega t,$$

a Z can be computed, which yields the expression

$$\omega_\pm=\alpha\pm\frac{1}{\pi}(4\beta^2+\lambda^2)^{\frac{1}{2}}\cdot E\left(\frac{\pi}{2},k\right)$$

for the angular frequency in terms of the elliptic integral of the second kind, where

$$k^2=\lambda^2/(4\beta^2+\lambda^2).$$

Note that as in the harmonic oscillator the frequency of this system is independent of energy. For the case where $\alpha=2\sqrt{2}$, $\beta=\sqrt{3}$ and $\lambda=2\sqrt{3}$, the variational angular frequencies are $\omega_+=4.9346$ and $\omega_-=0.7222$, which bear the ratios 1.0026 and 1.1453 to the exact values, respectively.

Electrical Conduction in Deformed Isotropic Materials

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The current density in a deformed conductor is assumed to be a function of the electric field and the deformation gradients. The form of the relationship is restricted by invariance under changes in orientation of the physical system. Material symmetries impose further restrictions. The resulting form for isotropic materials is given. Simplifications are obtained in the cases of small deformation and large homogeneous deformation. Generalizations and further applications are pointed out.

1. INTRODUCTION

IN a previous paper[1] the manner in which constitutive equations in continuum physics may be formulated is discussed in general terms. In the present paper, we apply the procedures of the previous paper to formulate constitutive equations for electrical conduction in a material which is subjected to an initial deformation.

We take as our starting point the assumption that the current density vector at any instant of time is a single-valued function of the electric field and deformation gradients at that instant. We then determine the restrictions on the form of the constitutive equation imposed by the consideration that it is unaltered by a simultaneous rotation of the physical system and the coordinate system. The further restrictions imposed on the form of the constitutive equation by the assumption that it is isotropic and possesses a center of symmetry are then determined.

Next, we consider the manner in which the resulting constitutive equation can be simplified by the assumption that the deformation to which the body is subjected is small. In Sec. 6 we consider the case when the deformation is pure homogeneous, but not necessarily small. Finally, in Sec. 7, it is pointed out that the constitutive equations derived in the paper can be applied to other areas of continuum physics than electrical conduction in deformed materials, in which we are concerned with the dependence of a vector on the deformation gradients and another vector. Also, it is pointed out that constitutive equations of similar form, in which however the scalar coefficients depend on time, can be applied to certain classes of time-dependent problems in the continuum physics of isotropic materials. However, in all these cases we assume that the phenomena with which we are concerned are quasi-static in character, so that complicating effects due to such phenomena as magnetic induction and moving electric currents may be neglected.

2. SOME FUNDAMENTAL CONSIDERATIONS

Let us suppose that a body is deformed in such a way that a particle initially at X_i in a rectangular Cartesian coordinate system x moves to x_i in the same system. Suppose an electric field exists in the deformed body with components e_i in the coordinate system x, and let us assume that the components of the current density vector J_i in the system x are functions of e_p and of the deformation gradients $\partial x_p/\partial X_q$, thus

$$J_i = f_i(\partial x_p/\partial X_q, e_p). \tag{2.1}$$

It follows from the results of a previous paper[1] that the dependence of J_i on the arguments $\partial x_p/\partial X_q$ and e_p must be of the form

$$J_i = (\partial x_i/\partial X_j)F_j(G_{pq}, G^{-\frac{1}{3}}, E_p), \tag{2.2}$$

where

$$G_{pq} = (\partial x_r/\partial X_p)(\partial x_r/\partial X_q), \quad G = |G_{pq}|$$

and

$$E_p = (\partial x_r/\partial X_p)e_r. \tag{2.3}$$

If, in (2.1), f_i is a single-valued function of its arguments, so is F_j in (2.2). If f_i is a polynomial function of its arguments, so is F_j.

3. EFFECT OF SYMMETRY

If the material considered has some symmetry, when undeformed and no electric field exists in the material, then the functions F_j are subject to further restrictions. Let $\bar{x}$ be a rectangular Cartesian coordinate system which, in view of the particular symmetry possessed by the material, is equivalent to the system x. We denote the components, in the coordinate system $\bar{x}$, of the current density and electric field vectors by $\bar{J}_i$ and $\bar{e}_i$, respectively. We define $\bar{E}_i$ and $\bar{G}_{ij}$, in a manner analogous to E_i and G_{ij}, by

$$\bar{E}_i = (\partial \bar{x}_j/\partial \bar{X}_i)\bar{e}_j \quad \text{and} \quad \bar{G}_{ij} = (\partial \bar{x}_k/\partial \bar{X}_i)(\partial \bar{x}_k/\partial \bar{X}_j), \tag{3.1}$$

where $\bar{X}_i$ are the coordinates in the system $\bar{x}$ of a point with coordinates X_i in the system x. Since the transformation relating the reference systems x and $\bar{x}$ is orthogonal, we have

$$\bar{G} = |\bar{G}_{ij}| = |G_{ij}| = G. \tag{3.2}$$

Since the coordinate system $\bar{x}$ is equivalent to the system x, we have, from (2.2),

$$\bar{J}_i = (\partial \bar{x}_i/\partial \bar{X}_j)F_j(\bar{G}_{pq}, \bar{G}^{-\frac{1}{3}}, \bar{E}_p). \tag{3.3}$$

Let the orthogonal transformation relating the co-

[1] A. C. Pipkin and R. S. Rivlin, Arch. Ratl. Mech. Anal. 4, 129 (1959).

ordinate systems x and $\bar{x}$ be

$$\bar{x}_i = s_{ij}x_j, \tag{3.4}$$

with

$$s_{ij}s_{ik} = s_{ji}s_{ki} = \delta_{jk}. \tag{3.5}$$

It is easily seen that

$$\begin{aligned} &\bar{X}_i = s_{ij}X_j, \quad \bar{J}_k(\partial\bar{X}_i/\partial\bar{x}_k) = s_{ij}J_k(\partial X_j/\partial x_k), \\ &\bar{G}_{ij} = s_{ip}s_{jq}G_{pq} \quad \text{and} \quad \bar{E}_i = s_{ij}E_j. \end{aligned} \tag{3.6}$$

From (2.2), (3.3), (3.4), and (3.6), we obtain

$$F_i(\bar{G}_{pq}, \bar{G}^{-\frac{1}{3}}, \bar{E}_p) = s_{ij}F_j(G_{pq}, G^{-\frac{1}{3}}, E_p). \tag{3.7}$$

Let $\bar{\psi}_i$ and ψ_i be the components in the coordinate systems $\bar{x}$ and x respectively of an arbitrary vector. Then,

$$\psi_j = s_{ij}\bar{\psi}_i. \tag{3.8}$$

From (3.7), we obtain, multiplying throughout by $\bar{\psi}_i$ and employing (3.8)

$$\begin{aligned} \bar{\psi}_iF_i(\bar{G}_{pq}, \bar{G}^{-\frac{1}{3}}, \bar{E}_p) &= \psi_iF_i(G_{pq}, G^{-\frac{1}{3}}, E_p) \\ &= F(\text{say}). \end{aligned} \tag{3.9}$$

We have, of course, from (3.9)

$$F_i(G_{pq}, G^{-\frac{1}{3}}, E_p) = \partial F/\partial\psi_i. \tag{3.10}$$

Now (3.9) implies that F is a scalar invariant, under the group of orthogonal transformations $\{S\}$, say, characterizing the symmetry of the material, of the vectors ψ_p and E_p, and the symmetric second-order tensor G_{pq}. We note from (3.2) that $\bar{G}^{-\frac{1}{3}} = G^{-\frac{1}{3}}$. Thus, F must be expressible as a polynomial in $G^{-\frac{1}{3}}$ and the elements of an integrity basis, under the transformation group $\{S\}$, for the vectors ψ_p and E_p and the symmetric tensor G_{pq}. Since F is linear in the components of the vector ψ_p, we may express it in the form

$$F = \sum_{R=1}^{M} P_RA_R, \tag{3.11}$$

where $A_R(R=1,2,\cdots,M)$ are the elements of the integrity basis which are linear in the vector ψ_p and $P_R(R=1,2,\cdots,M)$ are polynomials in $G^{-\frac{1}{3}}$ and the elements of the integrity basis which do not involve the vector ψ_p at all.

4. ISOTROPIC MATERIAL POSSESSING A CENTER OF SYMMETRY

If, when it is undeformed and the field strength is zero, the material is isotropic and possesses a center of symmetry, the appropriate transformation group expressing its symmetry is the full orthogonal group. The elements of an integrity basis for the vectors ψ_p and E_p and the symmetric tensor G_{pq}, which are linear in ψ_p, may be taken[1] as

$$\psi_pE_p, \quad \psi_pG_{pq}E_q, \quad \psi_pG_{pq}G_{qr}E_r. \tag{4.1}$$

Those which are independent of the vector ψ_p may be taken as

$$\begin{aligned} &E_pE_p, \quad E_pG_{pq}E_q, \quad E_pG_{pq}G_{qr}E_r, \\ &G_{pp}, \quad G_{pq}G_{qp}, \quad G_{pq}G_{qr}G_{rp}. \end{aligned} \tag{4.2}$$

On replacing $A_R(R=1,2,\cdots,M)$ in (3.11) by (4.1), we obtain

$$F = P_1\psi_pE_p + P_2\psi_pG_{pq}E_q + P_3\psi_pG_{pq}G_{qr}E_r, \tag{4.3}$$

where P_1, P_2 and P_3 are polynomials in the quantities (4.2) and $G^{-\frac{1}{3}}$.

On introducing (4.3) into (3.10), we obtain

$$F_j(G_{pq}, G^{-\frac{1}{3}}, E_p) = (P_1\delta_{jk} + P_2G_{jk} + P_3G_{jp}G_{pk})E_k. \tag{4.4}$$

On introducing (4.4) into (2.2) and bearing in mind the definitions (2.3) of G_{pq} and E_p, we obtain

$$J_i = (P_1g_{ij} + P_2g_{ip}g_{pj} + P_3g_{ip}g_{pq}g_{qj})e_j, \tag{4.5}$$

where g_{ij} is defined by

$$g_{ij} = (\partial x_i/\partial X_k)(\partial x_j/\partial X_k). \tag{4.6}$$

We now use the Hamilton-Cayley theorem for the matrix $\mathbf{g} = \|g_{ij}\|$. This may be stated as

$$\begin{aligned} \mathbf{g}^3 - \mathbf{g}^2tr\mathbf{g} + \tfrac{1}{2}[(tr\mathbf{g})^2 - tr\mathbf{g}^2]\mathbf{g} - \tfrac{1}{6}[(tr\mathbf{g})^3 \\ - 3tr\mathbf{g}tr\mathbf{g}^2 + 2tr\mathbf{g}^3]\mathbf{I} = 0, \end{aligned} \tag{4.7}$$

where $\mathbf{I}$ is the unit matrix. We bear in mind that

$$\mathbf{g}^3 = \|g_{ip}g_{pq}g_{pj}\| \quad \text{and} \quad \mathbf{g}^2 = \|g_{ip}g_{pj}\|, \tag{4.8}$$

and that

$$tr\mathbf{G} = tr\mathbf{g}, \quad tr\mathbf{G}^2 = tr\mathbf{g}^2, \quad tr\mathbf{G}^3 = tr\mathbf{g}^3 \quad \text{and} \quad G = g, \tag{4.9}$$

where

$$\mathbf{G} = \|G_{ij}\| \quad \text{and} \quad g = |g_{ij}|. \tag{4.10}$$

On employing (4.7) to (4.10) in (4.5), we see that

$$J_i = (Q_1\delta_{ij} + Q_2g_{ij} + Q_3g_{ik}g_{kj})e_j, \tag{4.11}$$

where δ_{ij} denotes the Kronecker delta and Q_1, Q_2 and Q_3 are polynomials in (4.2) and $G^{-\frac{1}{3}}$.

If we use (2.3) and (4.6), we note that

$$\begin{aligned} &E_pE_p = e_pg_{pq}e_q, \quad E_pG_{pq}E_q = e_pg_{pq}g_{qr}e_r \\ &\text{and} \\ &E_pG_{pq}G_{qr}E_r = e_pg_{pq}g_{qr}g_{rs}e_s. \end{aligned} \tag{4.12}$$

If we use (4.7), we see that E_pE_p, $E_pG_{pq}E_q$ and $E_pG_{pq}G_{qr}E_r$ are expressible as polynomials in

$$\begin{aligned} &tr\mathbf{g}, \quad tr\mathbf{g}^2, \quad tr\mathbf{g}^3, \\ &e_pe_p, \quad e_pg_{pq}e_q \quad \text{and} \quad e_pg_{pq}g_{qr}e_r. \end{aligned} \tag{4.13}$$

With this result and (4.9), we see that, in (4.11), Q_1, Q_2 and Q_3 are expressible as polynomials in $g^{-\frac{1}{3}}$ and the quantities (4.13).

By using the vector notation $\mathbf{J}$ and $\mathbf{e}$ for the current density and electric field strength, respectively, Eq. (4.11) may be rewritten as

$$\mathbf{J} = Q_1\mathbf{e} + Q_2\mathbf{ge} + Q_3\mathbf{g}^2\mathbf{e}, \tag{4.14}$$

and the quantities (4.13) may be written as

$$\begin{gathered} tr\mathbf{g},\quad tr\mathbf{g}^2,\quad tr\mathbf{g}^3 \\ \mathbf{ee},\quad \mathbf{ege}\quad \text{and}\quad \mathbf{eg}^2\mathbf{e}. \end{gathered} \tag{4.15}$$

If the conduction is ohmic, then in (4.14) Q_1, Q_2 and Q_3 are polynomials in g^{-1}, $tr\mathbf{g}$, $tr\mathbf{g}^2$ and $tr\mathbf{g}^3$ only.

Another special case arises if we consider the body to be undeformed, so that $g_{ij}=\delta_{ij}$. We then obtain, from (4.11)

$$J_i=Qe_i, \tag{4.16}$$

where Q is a polynomial in e_pe_p. This is the law governing nonohmic conduction in an undeformed isotropic material.

5. SMALL DEFORMATIONS

Let u_i be the displacement components in the coordinate system x undergone by the body in the deformation. Then,

$$x_i=X_i+u_i. \tag{5.1}$$

If we make the assumption that the displacement gradients are small compared with unity, then substituting from (5.1) in (4.6) and neglecting terms of the second degree in the displacement gradients, we obtain

$$g_{ij}=\delta_{ij}+2\epsilon_{ij}, \tag{5.2}$$

where

$$\epsilon_{ij}=\tfrac{1}{2}(\partial u_i/\partial X_j+\partial u_j/\partial X_i). \tag{5.3}$$

After introducing (5.2) into (4.11) and (4.13), it is easily seen that

$$J_i=(R_1\delta_{ij}+R_2\epsilon_{ij}+R_3\epsilon_{ik}\epsilon_{kj})e_j, \tag{5.4}$$

where R_1, R_2 and R_3 are expressible, with the notation $\epsilon=\|\epsilon_{ij}\|$, as polynomials in

$$\begin{gathered} tr\boldsymbol{\epsilon},\quad tr\boldsymbol{\epsilon}^2,\quad tr\boldsymbol{\epsilon}^3, \\ e_pe_p,\quad e_p\epsilon_{pq}e_q,\quad e_p\epsilon_{pq}\epsilon_{qr}e_r. \end{gathered} \tag{5.5}$$

If we make the more stringent assumption that (5.4) can be linearized with respect to the displacement gradients, we obtain[2]

$$J_i=[(S_1+S_2\epsilon_{kk}+S_3e_p\epsilon_{pq}e_q)\delta_{ij}+S_4\epsilon_{ij}]e_j, \tag{5.6}$$

where S_1, S_2, S_3 and S_4 are expressible as polynomials in e_pe_p. If the conductivity is ohmic, $S_3=0$ and S_1, S_2 and S_4 are constants.

6. THE CASE OF PURE, HOMOGENEOUS DEFORMATION

If the deformation to which the body is subjected is a pure homogeneous deformation with principal directions parallel to the axes of the coordinate system x, then the deformation may be described by

$$x_1=\lambda_1X_1,\quad x_2=\lambda_2X_2,\quad x_3=\lambda_3X_3. \tag{6.1}$$

[2] We note, as an example, that (5.4) may provide a good approximation for J_i, while (5.6) does not if $\epsilon_{ij}\ll 1$ while $R_3\gg R_2$.

We obtain, from (4.6)

$$\begin{gathered} g_{11}=\lambda_1^2,\quad g_{22}=\lambda_2^2,\quad g_{33}=\lambda_3^2 \\ \text{and}\quad g_{ij}=0\quad (i\neq j). \end{gathered} \tag{6.2}$$

By introducing (6.2) into (4.11), we obtain

$$\begin{aligned} J_1&=(Q_1+Q_2\lambda_1^2+Q_3\lambda_1^4)e_1, \\ J_2&=(Q_1+Q_2\lambda_2^2+Q_3\lambda_2^4)e_2 \end{aligned} \tag{6.3}$$

and

$$J_3=(Q_1+Q_2\lambda_3^2+Q_3\lambda_3^4)e_3.$$

Q_1, Q_2 and Q_3 are, or course, polynomials in the quantities (4.13). We shall denote these quantities in the order in which they appear in (4.13) by $\alpha_1, \alpha_2, \cdots, \alpha_6$. Expressions for these quantities in the case when the deformation is pure homogeneous may be obtained by introducing (6.2) into (4.13).

For simplicity we shall first consider that the conduction is ohmic. Then Q_1, Q_2 and Q_3 are polynomials in α_1, α_2 and α_3 only, which are given by

$$\begin{aligned} \alpha_1&=tr\mathbf{g}=\lambda_1^2+\lambda_2^2+\lambda_3^2, \\ \alpha_2&=tr\mathbf{g}^2=\lambda_1^4+\lambda_2^4+\lambda_3^4 \end{aligned} \tag{6.4}$$

and

$$\alpha_3=tr\mathbf{g}^3=\lambda_1^6+\lambda_2^6+\lambda_3^6.$$

We may in principle determine completely the dependence of Q_1, Q_2 and Q_3 on α_1, α_2 and α_3 in this case by performing the following experiments. For a given pure homogeneous deformation, and hence, from (6.4), for given values of α_1, α_2 and α_3 we measure the ratios J_1/e_1, J_2/e_2 and J_3/e_3, i.e., the resistivities in the three principal directions. We thus obtain, provided λ_1, λ_2 and λ_3 are all unequal, three independent simultaneous equations for the determination of the values of Q_1, Q_2 and Q_3 corresponding to these values of α_1, α_2 and α_3. This experiment may then be repeated for various values of α_1, α_2 and α_3.

7. APPLICATION OF THE RESULTS TO OTHER PHYSICAL PROBLEMS

The constitutive equations obtained in the preceding sections are applicable to other physical problems than those concerning electrical conduction in deformed materials. For example, by interpreting the vectors $\mathbf{J}$ and $\mathbf{e}$ in (4.14) as the heat flux vector and temperature gradient, respectively, in a deformed material, we obtain a constitutive equation for thermal conduction in a deformed isotropic material possessing a center of symmetry, in which the "thermal conductivity" depends on the deformation at the instant of measurement. By interpreting $\mathbf{J}$ and $\mathbf{e}$ in other ways, Eq. (4.14) may be applied to the description of other physical phenomena than electrical or thermal conduction, which involve a relation between a vector on the one hand and a second vector and the deformation gradients on the other.

We now consider that a body is deformed at time $t=0$ and is then held in a constant state of deformation. Simultaneously, an electric field is applied. We assume that the current density vector $\mathbf{J}$ at time t depends on the field $\mathbf{e}$, the constant deformation gradients $\partial x_p/\partial X_q$ and the time t after the deformation is applied, thus

$$J_i=f_i(\partial x_p/\partial X_q, e_p, t). \tag{7.1}$$

Then, proceeding in a manner similar to that adopted in the preceding sections, we see that if the material is initially isotropic, the current density vector $\mathbf{J}$ must be expressible in the form (4.14), where Q_1, Q_2 and Q_3 are functions of the quantities (4.15) and of t.

We now consider a material in some state of deformation and assume that the current $\mathbf{J}$ in it at time t is a polynomial function of the deformation gradients and electric field at time t and is a continuous functional of the electric field $\mathbf{e}(\tau)$ in the interval $0\leq\tau\leq t$. We now suppose that $\mathbf{e}$ varies with time in some specified manner, so that

$$\mathbf{e}(\tau)=f(\tau)\mathbf{e}^*, \tag{7.2}$$

where $\mathbf{e}^*$ is independent of time and $f(\tau)$ is a specified function of time. If we follow an argument outlined in a previous paper[3] and the analysis given in the present paper, it can be shown that provided we limit ourselves to situations for which $\mathbf{e}$ varies in accordance with (7.2) the constitutive equation may be written in the form

$$\mathbf{J}=Q_1\mathbf{e}^*+Q_2\mathbf{g}\mathbf{e}^*+Q_3\mathbf{g}^2\mathbf{e}^*, \tag{7.3}$$

where Q_1, Q_2 and Q_3 are polynomials in

$$tr\mathbf{g},\quad tr\mathbf{g}^2,\quad tr\mathbf{g}^3,\quad g^{-\frac{1}{2}},$$
$$\mathbf{e}^*\mathbf{e}^*,\quad \mathbf{e}^*\mathbf{g}\mathbf{e}^*\quad\text{and}\quad \mathbf{e}^*\mathbf{g}^2\mathbf{e}^*, \tag{7.4}$$

and are single-valued functions of t.

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Convergence of the Born Expansion

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The convergence of the iterated Born series for the Green's function in nonrelativistic potential scattering is studied in n dimensions, thus generalizing a recent study of Zemach and Klein. For spherically symmetrical potentials the series is proved to converge at sufficiently high energies for a rather general class of potentials.

I. INTRODUCTION

A SIMPLE proof of the convergence of the Born Series for the scattering of a particle by a potential in nonrelativistic quantum mechanics was given in a previous paper by Klein and Zemach[1] for a rather general class of potentials. Our purpose will be to extend this proof to a particle with n spatial dimensions. While the problem considered is largely of academic interest, one is nevertheless able to illustrate several interesting properties of the Born expansion, and to gain further insight into its structure. The authors intend this effort to serve as a preliminary to the investigation of physical problems involving many dimensional Green's functions, for example, neutron-deuteron scattering. In the integral formulation of the scattering problem, a wave function $\psi(r)$ is sought which satisfies

$$\begin{aligned}\psi&=\psi_0+G_0V\psi,\\&=\psi_0+GV\psi_0,\end{aligned}\tag{1}$$

where the (outgoing wave) Green's function $G(\mathbf{r},\mathbf{r}')$ obeys the equation

$$G=G_0+G_0VG.\tag{2}$$

The Born series is defined by iteration of Eqs. (1) and (2)

$$\psi=\sum_{n=0}^{\infty}\psi_n\tag{3}$$

$$G=\sum_{n=0}^{\infty}G_n,\tag{4}$$

where

$$\psi_{n+1}(\mathbf{r})=\int G_0(\mathbf{r},\mathbf{s})V(\mathbf{s})\psi_n(\mathbf{s})\mathbf{ds}\tag{5}$$

and

$$G_{n+1}(\mathbf{r},\mathbf{r}')=\int G_0(\mathbf{r},\mathbf{s})V(\mathbf{s})G_n(\mathbf{s},\mathbf{r}')\mathbf{ds}.\tag{6}$$

From the last equation the more general relation

$$G_{n+m+1}(\mathbf{r},\mathbf{r}')=\int G_n(\mathbf{r},\mathbf{s})V(\mathbf{s})G_m(\mathbf{s},\mathbf{r}')\mathbf{ds}\tag{7}$$

follows directly. It is useful to introduce an associated set of functions

$$\begin{aligned}g_0(\mathbf{r},\mathbf{r}')&=1\\g_n(\mathbf{r},\mathbf{r}')&=G_n(\mathbf{r},\mathbf{r}')/G_0(\mathbf{r},\mathbf{r}'),\\g(\mathbf{r},\mathbf{r}')&=G(\mathbf{r},\mathbf{r}')/G_0(\mathbf{r},\mathbf{r}'),\end{aligned}\tag{8}$$

and to consider in place of Eq. (5) the series

$$g(\mathbf{r},\mathbf{r}')=\sum_{n=0}^{\infty}g_n(\mathbf{r},\mathbf{r}').\tag{9}$$

With the notation

$$D_{r,r'}(\mathbf{s})=\frac{G_0(\mathbf{r},\mathbf{s})G_0(\mathbf{s},\mathbf{r}')}{G_0(\mathbf{r},\mathbf{r}')},\tag{10}$$

Eq. (7) assumes the form

$$g_{n+m+1}(\mathbf{r},\mathbf{r}')=\int g_n(\mathbf{r},\mathbf{s})D_{rr'}(\mathbf{s})Vg_m(\mathbf{s},\mathbf{r}')\mathbf{ds}.\tag{11}$$

A norm may be assigned to the function g as follows:

$$\|g_i\|=\max_{r,r'}|g_i(\mathbf{r},\mathbf{r}')|,\tag{12}$$

i.e., the norm $\|g_i\|$ is the maximum numerical value obtained by $g_i(r,r')$ as r and r' vary. The norm is well defined for any function of two variables and is either a nonnegative real number or infinity. We shall consider only spherically symmetric potentials which satisfy certain conditions at the origin and infinity. From Eq. (11) we obtain

$$g_1(\mathbf{r},\mathbf{r}')=\int D_{r,r'}(\mathbf{s})V(\mathbf{s})\mathbf{ds}.\tag{13}$$

The general form of G_0 (outgoing) for $p+2$ dimensions is[2]

$$G(\mathbf{r})=\frac{\pi}{\Omega}\left(\frac{k}{2}\right)^{p}\left(\frac{2}{kr}\right)^{p/2}H_{p/2}^{(1)}(kr)/ip\Gamma\left(\frac{p}{2}\right),\tag{14}$$

where Ω is the solid angle in $p+2$ dimensions, Γ the gamma function, and $H^{(1)}$ the Hankel function. From the foregoing relations it follows directly that if $\|g_i\|$ is to be less than infinity, our potential must satisfy the

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† Supported in part by the U. S. Atomic Energy Commission.
[1] Ch. Zemach and A. Klein, Il Nuovo cimento **10**, 1078 (1958).
[2] A. J. Sommerfeld, *Partial Differential Equations in Physics* (Academic Press, Inc., New York, 1949), p. 232.

following conditions: At the origin, we require that

$$\begin{aligned} &\text{for} \quad p=-1, \quad |V(\mathbf{r})|<c/r^{1-\beta}, \quad \beta>0 \\ &\text{for} \quad p\geqslant 0, \quad |V(\mathbf{r})|<c/r^{2-\beta}, \quad \beta>0; \end{aligned} \tag{15}$$

At infinity we demand that

$$|V(\mathbf{r})|<c/(r)^{(p+3)/2+\beta}, \quad \beta>0. \tag{16}$$

II. SIMPLE POTENTIALS

All proofs are simplified in the case of an odd number of dimensions because of the well-known fact that the Hankel functions of half-integral order can be expressed in terms of trigonometric functions. For this reason we will specifically exhibit a proof for the case of five dimensions. However, in Appendix A it will be shown that our work can easily be extended to any number of dimensions. From Eq. (14) it can be seen that the one-dimensional problem ($p=-1$) is completely trivial, since each succeeding term in the Born series is multiplied by a higher inverse power of k. For the familiar three-dimensional case, where

$$G_0^{(3)}=-\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}, \tag{17}$$

a rather more elaborate analysis was necessary. We shall attempt to generalize the reasoning now to five dimensions where the fact that

$$G_0^{(5)}(\mathbf{r},\mathbf{r}')=-\frac{1}{8\pi|\mathbf{r}-\mathbf{r}'|^3}\times[e^{ik|\mathbf{r}-\mathbf{r}'|}-ik|\mathbf{r}-\mathbf{r}'|e^{ik|\mathbf{r}-\mathbf{r}'|}] \tag{18}$$

involves a positive power of k brings in additional complexities.

In this section we restrict ourselves to simple potentials defined precisely by Eqs. (19) and (20) below. The extension to potentials of actual interest will be given in Sec. III.

The first step in the proof involves the investigation of the behavior at large k of $g_1^{(5)}(\mathbf{r},\mathbf{r}')$ and $g_2^{(5)}(\mathbf{r},\mathbf{r}')$. Let a function $f_s(\mathbf{s})$ be defined by

$$\begin{aligned} f_s(\mathbf{s})&=1 \quad \text{if} \quad |\mathbf{s}|<S \\ &=0 \quad \text{if} \quad |\mathbf{s}|\geqslant S. \end{aligned} \tag{19}$$

When $V(\mathbf{s})$ is a simple potential, constants S, M_1, M_2, M_3, $\cdots$ can be found such that for all S

$$\begin{aligned} |V(\mathbf{s})|&\leqslant M_1 f_s(\mathbf{s}) \\ |\nabla_i V(\mathbf{s})|&\leqslant M_2 f_s(\mathbf{s}) \\ |\nabla_i\nabla_j V(\mathbf{s})|&\leqslant M_3 f_s(\mathbf{s}) \\ &\vdots \qquad\qquad \vdots \end{aligned} \tag{20}$$

In Appendix B it is proved that for the case of simple potentials, given $\epsilon>0$, there exists a k_0, such that if $k\geqslant k_0$, $|g_1^{(5)}(\mathbf{r},\mathbf{r}')|<\epsilon$ and $|g_2^{(5)}(\mathbf{r},\mathbf{r}')|<\epsilon/k$ independent of the values of $\mathbf{r}$ and $\mathbf{r}'$, i.e., $\|g_1^{(5)}\|<\epsilon$ and $\|g_2^{(5)}\|<\epsilon/k$. Let us now define

$$\|V\|=\max_{r,r'}\int |D_{r,r'}(\mathbf{s})|\,|V(\mathbf{s})|\,d\mathbf{s}. \tag{21}$$

According to Eqs. (10) and (18) $\|V\|$ is proportional to k. From Eqs. (11) and (12) we obtain

$$\begin{aligned} \|g_{3n}^{(5)}\|&\leqslant(\|g_2^{(5)}\|\|V\|)^n \\ \|g_{3n+1}^{(5)}\|&\leqslant(\|g_1^{(5)}\|)(\|g_2^{(5)}\|\|V\|)^n \\ \|g_{3n+2}^{(5)}\|&\leqslant(\|g_2^{(5)}\|)(\|g_2^{(5)}\|\|V\|)^n. \end{aligned} \tag{22}$$

We may now conclude that the Born series for *simple* potentials

$$g^{(5)}(\mathbf{r},\mathbf{r}')=\sum_{n=0}^{\infty} g_{3n}^{(5)}(\mathbf{r},\mathbf{r}')+\sum_{n=0}^{\infty} g_{3n+1}^{(5)}(\mathbf{r},\mathbf{r}')+\sum_{n=0}^{\infty} g_{3n+2}^{(5)}(\mathbf{r},\mathbf{r}') \tag{23}$$

converges uniformly and absolutely for sufficiently large k.

We remark that by examining the form of the Hankel functions we see that all previous arguments remain valid if k is allowed to represent a complex variable $k=\chi+i\eta$ with $n\geqslant 0$. Thus the Born series for the Green's function (for the case of simple potentials) converges uniformly and absolutely in the upper half k plane when $|k|$ is sufficiently large. We shall restrict ourselves in what follows, however, to real positive k.

By using the foregoing results, as in the previous paper,[3] one can now define a scattering amplitude and show that the Born series for the wave function converges at sufficiently high energy.

III. EXTENSION TO N DIMENSIONS AND NONSIMPLE POTENTIALS

For the simple potential we may write

$$g_1^{(n)}(\mathbf{r},\mathbf{r}')=\int G_0^{(n)}(k|\mathbf{r}-\mathbf{s}|)V(\mathbf{s})G_0^{(n)}(k|\mathbf{s}-\mathbf{r}'|)\,d\mathbf{s}, \tag{24}$$

where in $n=p+2$ dimensions $G_0^{(n)}$ is given by Eq. (14). In the appendix it is proved that for sufficiently large k one may replace the Hankel function in Eq. (14) by its asymptotic form

$$H_\nu^{(1)}(\rho)]_{\text{asymp}}=\left(\frac{2}{\pi\rho}\right)^{\frac{1}{2}} e^{[i\rho-\frac{1}{2}i\pi(\nu+\frac{1}{2})]}, \tag{25}$$

if at the same time one replaces the simple potential V by an effective potential V' which is still simple. In so doing, an error is introduced in $g_1^{(n)}$ of magnitude less than ϵ.

[3] Ch. Zemach and A. Klein, Il Nuovo Cimento **10**, 1078 (1958).

Upon the foregoing replacements one finds that in all dimensions the integral in Eq. (24) will have essentially the same form as the example calculated for the case of five dimensions in Appendix A. The basic proof given there will follow through with the following modifications: In $2n+1$ and $2n+2$ dimensions ($n=1,2,3\cdots$) we need n integrations by parts to bring down enough powers of k to prove the necessary theorems. If one examines the form of the volume element, the limits of integration and the form of the potential, one sees that the properties of the scale factors in n dimensions insures that the first $n-1$ integrations by parts yield no boundary terms, and that all integrals converge.

Real potentials can now be included within the framework of the previous arguments in the following manner:

In $n=p+2$ dimensions define

$$\begin{aligned} I_V{}^0(r)&=\int \frac{|V(\mathbf{s})|}{|\mathbf{r}-\mathbf{s}|^p}\mathbf{ds},\\ I_V{}^1(r)&=\int \frac{|\nabla V(\mathbf{s})|}{|\mathbf{r}-\mathbf{s}|^{p-1}}\mathbf{ds},\\ &\vdots\\ I_V{}^{p-1}(r)&=\int \frac{|\nabla_1\nabla_2\cdots\nabla_{p-1}V(\mathbf{s})|}{|\mathbf{r}-\mathbf{s}|}\mathbf{ds}. \end{aligned} \tag{26}$$

Suppose that for a given real potential $V(\mathbf{s})$, the function $I_V{}^j(r)$ as defined foregoing ($j=1,2\cdots p-1$) satisfies the three requirements

$$\begin{aligned} &I_V{}^j(r)<\infty \quad \text{for all } r\\ &I_V{}^j(r) \quad \text{is continuous in } r\\ &I_V{}^j(r)\sim 0(1/r) \quad \text{as} \quad r\to\infty. \end{aligned} \tag{27}$$

It then follows that $V(\mathbf{s})$ can be approximated by a simple potential in the sense that given $\epsilon>0$, a simple potential $U(\mathbf{s})$ can be constructed such that[4]

$$\int \frac{|\nabla_1\cdots\nabla_j V(\mathbf{s})-\nabla_1\cdots\nabla_j U(\mathbf{s})|}{|\mathbf{r}-\mathbf{s}|^{p-j}}\mathbf{ds}<\epsilon. \tag{28}$$

If $g_1{}^{(5)}(r,r')$, $g_2{}^{(5)}(r,r')$ and $\bar{g}_1{}^{(5)}(r,r')$, $\bar{g}_2{}^{(5)}(r,r')$ denote the first- and second-order g functions for V and U, respectively, it will be proven in Appendix C that given $\epsilon>0$ there exists a k_0 such that for $k\geqslant k_0$

$$|g_1{}^{(5)}-\bar{g}_1{}^{(5)}|<\epsilon$$

and

$$|g_2{}^{(5)}-\bar{g}_2{}^{(5)}|<\frac{\epsilon}{k}. \tag{29}$$

[4] See, for example, the methods of E. C. Titchmarch, *Theory of Functions* (Oxford University Press, New York, 1939), Chap. X and Sec. 12.2.

Now let

$$\begin{aligned} g_1&=\bar{g}_1+g_1-\bar{g}_1\\ g_2&=\bar{g}_2+g_2-\bar{g}_2. \end{aligned} \tag{30}$$

In Appendix B it is proved that

$$\begin{aligned} |g_1|&<\epsilon\\ |g_2|&<\epsilon/k. \end{aligned} \tag{31}$$

The convergence of the Born series for real potentials of the class specified in five dimensions now follows from Eqs. (22) and (23).

It is interesting to note that for the case of three dimensions it is necessary to prove only that $\|g_1\|<\epsilon$ to prove convergence of the Born series for the Green's function, whereas for the case of five dimensions we have found it necessary to show explicitly that both $\|g_1\|<\epsilon$ and $\|g_2\|<\epsilon/k$ before being able to show the convergence of the series. In fact, one sees in general that for the case of $2n+1$ and $2n+2$ dimensions ($n=1,2\cdots$) one must first show explicitly that

$$\|g_1\|<\epsilon, \quad \|g_2\|<\epsilon/k, \cdots, \quad \|g_n\|<\epsilon/k^{n-1}$$

before one can obtain an iteration formula to prove that the entire series converges. Our methods are then applicable to the general case.

APPENDIX A

We show here that, whereas the previous proofs seem manifestly simpler for the case of an odd number of dimensions, and seem to vary radically from dimension to dimension, all dimensions can be treated in approximately the same manner. Although the proof that we shall exhibit will be for the calculation of $g_1(r,r')$ in four dimensions only, it will be clear that the general principle can be applied to all quantities of interest in an arbitrary number of dimensions.

We recall that

$$\begin{aligned} &g_1{}^{(4)}(\mathbf{R},\mathbf{R}')\\ &=\frac{k}{3i\Omega}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int \frac{H_1{}^{(1)}(k|\mathbf{R}-\mathbf{S}|)H_1{}^{(1)}(k|\mathbf{S}-\mathbf{R}')}{H_1{}^{(1)}(k|\mathbf{R}-\mathbf{R}'|)}\\ &\qquad\times\frac{|\mathbf{R}-\mathbf{R}'|\,V(\mathbf{s})}{|\mathbf{R}-\mathbf{S}|\,|\mathbf{S}-\mathbf{R}'|}\mathbf{ds}, \end{aligned} \tag{A1}$$

where $V(\mathbf{s})$ is a simple potential. We will now prove that, given $\epsilon>0$, for $k>k_0$ we may replace $H_1{}^{(1)}(\rho)$ by $H_1{}^{(1)}(\rho)$ asymp. [see Eq. (25)], if at the same time we replace $V(s)$ by a suitable effective simple potential $V'(s)$. In so doing the error introduced in $g_1{}^{(4)}$ is of magnitude less than ϵ.

In order to smooth the way for the following proof let us first establish an upper bound for $|H_\nu{}^{(1)}(Z)|$ for $|Z|\leqslant A$. From the definition

$$H_\nu{}^{(1)}(Z)=J_\nu(Z)+iH_\nu(Z) \tag{A2}$$

since $|J_\nu(Z)| \leqslant C_\nu$ in the region under observation, we see first that

$$|H_\nu^{(1)}(Z)| \leqslant C_\nu + |N_\nu(Z)|. \tag{A3}$$

We next recall the expansion for the Neuman function

$$N_\nu(Z) = \frac{2}{\pi}\{\gamma + \log(\tfrac{1}{2}Z)\}J_\nu(Z) - \frac{1}{\pi}\sum_{r=0}^{\nu-1}\frac{(\nu-r-1)!}{r!}\left(\frac{2}{Z}\right)^{\nu-2r} + g_\nu(Z), \tag{A4}$$

where

$$g_\nu(Z) = -\frac{1}{\pi}\sum_{r=0}^{\infty}(-1)^r\frac{(Z/2)^{\nu+2r}}{r!\,(\nu+r)!} \times\left(1+\frac{1}{2}+\cdots+\frac{1}{r}+1+\frac{1}{2}+\cdots+\frac{1}{\nu+r}\right). \tag{A5}$$

One can readily establish that

$$|g_\nu(Z)| \leqslant \sum_{r=0}^{\infty}\left|\frac{Z^r}{r!}\frac{Z^{\nu+r}}{(\nu+r)!}\frac{\nu+2r}{2^{\nu+2r}}\right| \leqslant |e^{2Z}|. \tag{A6}$$

If we use the triangle inequality and combine the foregoing results, we obtain for $|Z| \leqslant A$

$$|H_\nu^{(1)}(Z)| \leqslant F_\nu(A) + \gamma C_\nu|\log(\tfrac{1}{2}Z)| + \sum_{r=0}^{\nu+1}\frac{(\nu-r-1)!}{r!}\left|\frac{2}{Z}\right|^{\nu-2r}, \tag{A7}$$

where

$$F_\nu(A) = \left|\left(1+\frac{2}{\pi}\gamma\right)C_\nu\right| + |e^{2A}|.$$

If we turn then to the integral (A1) we break up the region of integration into three subregions

$$\int = \int_{V_1} + \int_{V_2} + \int_{V-V_1-V_2}, \tag{A8}$$

where V_1 is a sphere of radius δ about the point R, and V_2 is a similar sphere about R'. We then consider two cases $|\mathbf{R}-\mathbf{R}'| \geqslant 2\delta$ and $|\mathbf{R}-\mathbf{R}'| < 2\delta$. For the first case let $k = A/\delta$, where

$$|H_1^{(1)}(A) - H_1^{(1)}\,\mathrm{asym}(A)| < k/A^{\frac{1}{2}}. \tag{A9}$$

We first examine the integral over V_1

$$g_1(V_1) = \frac{k}{3i\Omega}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int d\Omega\int_0^{\delta} u^2 du H_1(ku)f(\mathbf{u}), \tag{A10}$$

where we have made the transformation

$$\begin{aligned}\mathbf{u} &= \mathbf{S}-\mathbf{R}\\ \mathbf{du} &= \mathbf{ds}\end{aligned} \tag{A11}$$

and

$$f(\mathbf{u}) = \frac{H_1(k|\mathbf{R}'-\mathbf{S}|)}{H_1(k|\mathbf{R}-\mathbf{R}'|)}\frac{|\mathbf{R}-\mathbf{R}'|}{|\mathbf{R}'-\mathbf{S}|}V(\mathbf{u}+\mathbf{R}). \tag{A12}$$

In $V_1 f(u)$ is bounded, continuous, and differentiable to all orders, i.e., $|f(u)| < B_0$, $|f'(u)| < B_1$, $\cdots$. From Eq. (A7) it now follows that

$$|g_1(V_1)| \leqslant \frac{B_0 A}{3\Omega}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int d\Omega \times\int_0^{\delta} u\left[F_1(A) + C_1\gamma\log\tfrac{1}{2}ku + \frac{2}{ku}\right]du. \tag{A13}$$

After performing the integration in Eq. (A13), we see that

$$|g_1(V_1)| < D_1/k, \quad \text{where} \quad D_1 = D_1(A). \tag{A14}$$

Likewise, it can be shown that

$$|g_1(V_2)| < D_2(A)/k. \tag{A15}$$

Now let us consider $g_1(V-V_1-V_2)$. Because of Eq. (A9), $H_1(x)/H_1\,\mathrm{asym}(x)$ and $H_1\,\mathrm{asym}(x)/H_1(x)$ are bounded and differentiable to all orders for $|x| \geqslant A$. If we rewrite

$$g_1(V-V_1-V_2) = \frac{k}{3i\Omega}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_{V-V_1-V_2}\frac{H_1\,\mathrm{asym}(k|\mathbf{R}-\mathbf{S}|)H_1\,\mathrm{asym}(k|\mathbf{S}-\mathbf{R}'|)|\mathbf{R}-\mathbf{R}'|}{H_1\,\mathrm{asym}(k|\mathbf{R}-\mathbf{R}'|)|\mathbf{R}-\mathbf{S}||\mathbf{S}-\mathbf{R}'|} \times\left\{\frac{H_1(k|\mathbf{R}-\mathbf{S}|)H_1(k|\mathbf{S}-\mathbf{R}'|)H_1\,\mathrm{asym}(k|\mathbf{R}-\mathbf{R}'|)}{H_1\,\mathrm{asym}(k|\mathbf{R}-\mathbf{S}|)H_1\,\mathrm{asym}(k|\mathbf{S}-\mathbf{R}'|)H_1(k|\mathbf{R}-\mathbf{R}'|)}V(\mathbf{s})\right\}\mathbf{ds} \tag{A16}$$

and treat the function in curly brackets as the new effective simple potential $V'(\mathbf{s})$, since $V'(\mathbf{s})$ is still a simple potential we may show in the same way as for five dimensions that $|g_1(V-V_1-V_2)| < \text{constant}/k$. Thus, given $\epsilon > 0$ for $k \geqslant k_0$ we can make $|g_1| < \epsilon$ as seen from Eqs. (A14)–(A16).

For the case $|\mathbf{R}-\mathbf{R}'| < 2\delta$, the region of integration is broken up as follows:

$$\int_V = \int_{V_1} + \int_{V_2} + \int_{V-V_1-V_2}, \tag{A17}$$

where V_1 is sphere of radius η surrounding R', and V_2 is sphere of radius 3δ surrounding R, but excluding V_1.

We choose $\eta=\frac{1}{2}|\mathbf{R}-\mathbf{R}'|$. In exactly the same manner as in case I we can show that the integral over the sphere of radius η is proportional to $1/k$. For the large sphere of radius 3δ

$$g_1(\mathbf{R},\mathbf{R}')=\frac{k}{3i\Omega}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_0^{3\delta}u^2du H_1(ku)\times\int_{\Omega_1(u)}^{\Omega_2(u)}d\Omega f(\mathbf{u}), \quad \text{(A18)}$$

where

$$f(\mathbf{u})=\frac{H_1(k|\mathbf{R}'-\mathbf{S}|)|\mathbf{R}-\mathbf{R}'|}{H_1(k|\mathbf{R}'-\mathbf{R}|)|\mathbf{R}-\mathbf{S}|}V(\mathbf{u}+\mathbf{R}). \quad \text{(A19)}$$

The use of the geometrically obvious relation $|\mathbf{R}-\mathbf{R}'|/|\mathbf{R}'-\mathbf{S}|\leqslant 2$ shows that $f(\mathbf{u})$ has the same desirable properties as in case I, and we can again show that this integral is proportional to $1/k$. The remainder of the proof for this case follows through as before. Now choosing k_0 to be the larger of the two values required for the individual cases, we have the desired result.

APPENDIX B

We shall prove here for the case of a simple potential that given $\epsilon>0$, there exists k_0 such that if $k\geqslant k_0$, then $|g_1^{(5)}(r,r')|<\epsilon$ independent of r and r', i.e., $\|g_1^{(5)}\|<\epsilon$. Following that we show that $\|g_2^{(5)}\|<\epsilon/k$.

Because the integral for $g_1^{(5)}(r,r')$ is absolutely convergent, we may express it in hyper-spheroidal coordinates defined by

$$\begin{aligned}
x_1&=\Delta\xi\eta\\
x_2&=\Delta[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}}\cos\theta\\
x_3&=\Delta[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}}\sin\theta\cos\varphi_1\\
x_4&=\Delta[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}}\sin\theta\sin\varphi_1\cos\varphi_2\\
x_5&=\Delta[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}}\sin\theta\sin\varphi_1\sin\varphi_2, \text{ etc.,}
\end{aligned} \quad \text{(B1)}$$

where

$$\begin{aligned}
\Delta&=|r-r'|/2\\
\xi&=(|r-s|+|s-r'|)/2\Delta, \qquad 1\leqslant\xi<\infty\\
\eta&=(|r-s|-|s-r'|)/2\Delta, \quad -1\leqslant\eta\leqslant 1
\end{aligned} \quad \text{(B2)}$$

and θ, φ_1 and φ_2 are spherical coordinates such that

$$0\leqslant\theta\leqslant\pi, \quad 0\leqslant\varphi_1\leqslant\pi, \quad 0\leqslant\varphi_2\leqslant 2\pi, \quad \text{(B3)}$$

and

$$\mathbf{ds}=\Delta^5(\xi^2-\eta^2)(1-\eta^2)(\xi^2-1)\times\sin^2\theta\sin\varphi_1 d\xi d\eta d\theta d\varphi_1 d\varphi_2. \quad \text{(B4)}$$

We study the integral

$$g_1^{(5)}(r,\mathbf{r}')=-\frac{1}{8\pi}\int\mathbf{ds}V(\mathbf{s})e^{ik[|\mathbf{r}-\mathbf{s}|+|\mathbf{s}-\mathbf{r}'|-|\mathbf{r}-\mathbf{r}'|]}\times\frac{(1-ik|\mathbf{r}-\mathbf{s}|)(1-ik|\mathbf{r}'-\mathbf{s}|)|\mathbf{r}-\mathbf{r}'|^3}{(1-ik|\mathbf{r}-\mathbf{r}'|)|\mathbf{r}-\mathbf{s}|^3|\mathbf{r}'-\mathbf{s}|^3} \quad \text{(B5)}$$

or expanding Eq. (B5)

$$g_1^{(5)}=g_{1a}^{(6)}+g_{1b}^{(5)}+g_{1c}^{(5)}+g_{1d}^{(5)}, \quad \text{(B6)}$$

where

$$\begin{aligned}
g_{1a}^{(5)}&=-\frac{1}{8\pi}\int\mathbf{ds}\frac{V(\mathbf{s})e^{ik[|\mathbf{r}-\mathbf{s}|+|\mathbf{s}-\mathbf{r}'|-|\mathbf{r}-\mathbf{r}'|]}}{(1-ik|\mathbf{r}-\mathbf{r}'|)}\times\frac{|\mathbf{r}-\mathbf{r}'|^3}{|\mathbf{r}-\mathbf{s}|^3|\mathbf{r}'-\mathbf{s}|^3}\\
g_{1b}^{(5)}&=\frac{1}{8\pi}\int\mathbf{ds}\frac{V(\mathbf{s})e^{ik[|\mathbf{r}-\mathbf{s}|+|\mathbf{s}-\mathbf{r}'|-|\mathbf{r}-\mathbf{r}'|]}ik|\mathbf{r}-\mathbf{s}|\,|\mathbf{r}-\mathbf{r}'|^3}{(1-ik|\mathbf{r}-\mathbf{r}'|)|\mathbf{r}-\mathbf{s}|^3|\mathbf{r}'-\mathbf{s}|^3}\\
g_{1c}^{(5)}&=\frac{1}{8\pi}\int\mathbf{ds}\frac{V(\mathbf{s})e^{ik[|\mathbf{r}-\mathbf{s}|+|\mathbf{s}-\mathbf{r}'|-|\mathbf{r}-\mathbf{r}'|]}ik|\mathbf{r}'-\mathbf{s}|\,|\mathbf{r}-\mathbf{r}'|^3}{(1-ik|\mathbf{r}-\mathbf{r}'|)|\mathbf{r}-\mathbf{s}|^3|\mathbf{r}'-\mathbf{s}|^3}\\
g_{1d}^{(5)}&=\frac{1}{8\pi}\int\mathbf{ds}\frac{V(\mathbf{s})e^{ik[|\mathbf{r}-\mathbf{s}|+|\mathbf{r}'-\mathbf{s}|-|\mathbf{r}-\mathbf{r}'|]}k^2|\mathbf{r}-\mathbf{r}'|^2}{(1-ik|\mathbf{r}-\mathbf{r}'|)|\mathbf{r}-\mathbf{s}|^2|\mathbf{r}'-\mathbf{s}|^2}.
\end{aligned} \quad \text{(B7)}$$

Introducing the hyperspheroidal coordinates, for large k let us study, for example,

$$\begin{aligned}
|g_{1d}|&\leqslant k\Delta^3\left|\int_\Omega d\Omega\int_{-1}^{1}d\eta(1-\eta^2)\times\int_1^\infty d\xi\frac{(\xi^2-1)}{(\xi^2-\eta^2)}V(\xi,\eta,\Omega)e^{2ik\Delta\xi}\right|\\
&\equiv k\Delta^3|I|.
\end{aligned} \quad \text{(B8)}$$

After integrating I by parts with respect to ξ, we obtain

$$I=\int d\Omega\int d\eta(1-\eta^2)\left[\frac{1}{2ik\Delta}V(\xi,\eta,\Omega)\frac{(\xi^2-1)e^{2ik\Delta\xi}}{(\xi^2-\eta^2)}\right]_1^\infty+\frac{1}{(2ik\Delta)}\int_1^\infty d\xi\frac{\partial}{\partial\xi}\left[(V(\xi,\eta,\Omega))\left(\frac{\xi^2-1}{\xi^2-\eta^2}\right)\right]e^{2ik\Delta\xi}. \quad \text{(B9)}$$

When Eq. (16) is used, the integrated term vanishes at both limits, and we may now integrate by parts once more to increase the power of k in the denominator. We finally obtain

$$|g_{1d}^{(5)}|\leqslant\alpha_k(r,r')+\beta_k(r,r')+\gamma_k(r,r')+\delta_k(r,r')+\lambda_k(r,r'). \quad \text{(B10)}$$

Let us now treat each term of Eq. (B10) in detail. We have

$$\alpha_k=\frac{\Delta}{k}\int d\Omega\int_{-1}^{1}d\eta V(1,\eta,\Omega)e^{2ik\Delta}. \quad \text{(B11)}$$

$\xi=1$ corresponds to a line integral along the vector $\mathbf{r}=\mathbf{r}'$. We will obtain contributions only from that part of the integration region which is inside the potential sphere $|\mathbf{s}|\leqslant S$. We select a number R so large that if both $r\geqslant R$ and $r'\geqslant R$, then $g_1(\mathbf{r},\mathbf{r}')$ as given by Eq. (B5) is less than ϵ in magnitude for all k. (That such a

choice is possible can be seen by examining Eq. (B5) *after* integrating by parts once.) We consider therefore only the interesting case where at least one of the variables, say r', is less than R. From the inequality

$$2(\Delta-\Delta\eta)=|r-r'|+|r'-s|-|r-s| \leqslant 2|r'-s| \leqslant 2R'+2S, \quad \text{(B12)}$$

we infer

$$\Delta\eta \geqslant \Delta-(R'+S). \quad \text{(B13)}$$

Hence, in Eq. (B11) the range of η is effectively limited by the inequality

$$1 \geqslant \eta \geqslant 1-\Delta^{-1}(R+S). \quad \text{(B14)}$$

Thus

$$|\alpha_k| \leqslant \frac{M_1}{k}\Omega(R+S). \quad \text{(B15)}$$

We next consider

$$\beta_k=\frac{2\Delta}{k}\int d\Omega\int d\eta(1-\eta^2) \times\int_1^\infty d\xi 2\xi\frac{(1-\eta^2)}{(\xi^2-\eta^2)}\frac{\partial V}{\partial\xi}e^{2ik\Delta(\xi-1)}. \quad \text{(B16)}$$

Since

$$\frac{\xi(1-\eta^2)}{(\xi^2-\eta^2)} \leqslant 1, \quad \text{(B17)}$$

$$|\beta_k| \leqslant \frac{4\Delta}{k}\int d\Omega\int_{-1}^1 d\eta\int_1^\infty |\nabla V_\xi|\,\mathbf{ds}_\xi. \quad \text{(B18)}$$

With the definition $f_s(\mathbf{s})=f_s(\xi,\eta)f_s(\Omega)$, we find upon substitution of Eqs. (20) and (B18)

$$|\beta_k| \leqslant \frac{4\Delta M_2\Omega}{k}\int_{-1}^1 d\eta\int_{-1}^\infty f_s(\xi,\eta)\mathbf{ds}_\xi. \quad \text{(B19)}$$

As ξ varies from 1 to ∞ for fixed η and Ω, the vector $\mathbf{s}_\xi$ traces out a hyperbolic path beginning somewhere on the straight line segment running from $\mathbf{r}$ to $\mathbf{r}'$. The total length of this arc, which is intercepted by the sphere $|\mathbf{s}| \leqslant S$ depends on the position of $\mathbf{r}$ and $\mathbf{r}'$, but in any case never exceeds a circumference $2\pi S$. Hence, in view of Eq. (B19) we obtain

$$|\beta_k| \leqslant \frac{4\Omega M_2}{k}(R+S)(2\pi S). \quad \text{(B20)}$$

We now treat γ_k, where

$$\gamma_k=\frac{\Delta^2}{k}\int d\Omega\int_{-1}^1 d\eta \times\int_1^\infty \frac{(\xi^2-1)(1-\eta^2)}{(\xi^2-\eta^2)}(\nabla_\xi{}^2V)e^{2ik\Delta(\xi-1)}\mathbf{ds}_\xi. \quad \text{(B21)}$$

in the same way as β_k, except that $(\xi^2-1)^{\frac{1}{2}}(1-\eta^2)^{\frac{1}{2}}\Delta$ is included with the θ integration to give an additional line integral to be considered. Since θ is a spherical coordinate, we are interested in an arc of a circle cutting the potential sphere. This will be less than the circumference of a great circle of the potential sphere. Thus

$$|\gamma_k| \leqslant \frac{\Omega M_3}{k}(R+S)(2\pi S)^2. \quad \text{(B22)}$$

Again

$$\delta_k=\frac{2\Delta}{k}\int d\Omega\int_{-1}^1 d\eta\int_1^\infty d\xi V(\xi,\eta,\Omega) \times\frac{(1-\eta^2)^2}{(\xi^2-\eta^2)^2}e^{2ik\Delta(\xi-1)}. \quad \text{(B23)}$$

If we define

$$f_s(\mathbf{s})\equiv f_s(\Omega)f_s(\xi,\eta)\equiv f_s(\Omega)f_s(\xi)f_s(\eta), \quad \text{(B24)}$$

we have

$$|\delta_k| \leqslant \frac{4M_1\Omega}{k}\Delta\int_1^\infty d\xi f_s(\xi)=\frac{4M_1\Omega\Delta\xi}{k}\Big]_{\xi_1}^{\xi_2}, \quad \text{(B25)}$$

where ξ_2 and ξ_1 are the curves of constant ξ which bound the potential sphere. We thus have

$$\Delta(\xi_2-\xi_1)=\tfrac{1}{2}(|\mathbf{r}-\mathbf{s}_2|+\mathbf{r}'-\mathbf{s}_2| -|\mathbf{r}-\mathbf{s}_1|-|\mathbf{r}'-\mathbf{s}_1|) \leqslant |\mathbf{s}_2-\mathbf{s}_1| \leqslant 2S \quad \text{(B26)}$$

since S_1 and S_2 are points on the surface of the sphere. Finally, we obtain

$$|\delta_k| \leqslant 8M_1\Omega S/k. \quad \text{(B27)}$$

To conclude the proof we must study the integral

$$\lambda_k=\frac{8\Delta}{k}\int d\Omega\int_{-1}^1 d\eta(1-\eta^2)^2\int_1^\infty d\xi V(\xi,\eta,\Omega) \times\frac{\xi^2}{(\xi^2-\eta^2)^3}e^{2ik\Delta(\xi-1)}. \quad \text{(B28)}$$

Now

$$|\lambda_k| \leqslant \int d\Omega f_s(\Omega)\Big[\frac{8M_1\Delta}{k}\int_{-1}^1 d\eta(1-\eta^2)^2\int_{\sqrt{2}}^\infty d\xi\frac{\xi^2}{(\xi^2-1)^3} +\frac{8M_1\Delta}{k}\int_{-1}^1 d\eta(1-\eta^2)\int_1^{\sqrt{2}}\frac{d\xi}{(\xi^2-\eta^2)^3}\Big]. \quad \text{(B29)}$$

After noting that

$$\int_{-1}^1 d\eta(1-\eta^2)^2\int_{\sqrt{2}}^\infty d\xi\frac{\xi^2}{(\xi^2-1)^3} \leqslant A, \quad \text{(B30)}$$

$$\int_{-1}^1 d\eta\int_1^{\sqrt{2}}\frac{d\xi}{(\xi^2-\eta^2)} \leqslant \int_{-1}^1\frac{d\eta}{(1-\eta^2)^{\frac{1}{2}}}, \quad \text{(B31)}$$

and

$$\Delta d\theta = dS_\theta(\eta=0,\ \xi=\sqrt{2}), \tag{B32}$$

and applying the previous reasoning, we find that

$$|\lambda_k| \leqslant \frac{8M_1}{k}(4\pi)(2\pi S)[A+B]. \tag{B33}$$

The remaining contributions to $g_1^{(5)}$ can be treated similarly.

In order now to prove that $\|g_2^{(5)}\| < (\epsilon/k)$ for $k \geqslant k_0$ we follow again essentially the same argument as that just given. We have

$$g_2^{(5)}(r,r') = \frac{k\Delta^3 k\Delta}{\pi(1-2ik\Delta)} \int d\Omega \int_{-1}^{1} d\eta \times \int_1^\infty d\xi F(\xi,\eta,\Omega) e^{2ik\Delta(\xi-1)} g(\xi,\eta,\Omega) k \int d\Omega' \times \int_{-1}^{1} d\eta' \int_1^\infty d\xi' F(\xi',\eta',\Omega') e^{2ik\Delta'(\xi'-1)}, \tag{B34}$$

where

$$F(\xi,\eta,\Omega) = (1-\eta^2)(\xi^2-1)/(\xi^2-\eta^2)V(\xi,\eta,\Omega) \tag{B35}$$

$$g(\xi,\eta,\Omega) = k(\Delta')^4/\pi(1-2ik\Delta'). \tag{B36}$$

Integrating by parts twice with respect to ξ and bounding the result, we find

$$|g_2^{(5)}(\mathbf{r},\mathbf{r}')| \leqslant \frac{\Delta}{k} \int d\Omega \Big[\int_{-1}^{1} d\eta \Big| V(1,\eta,\Omega) g(1,\eta) - \int_{-1}^{1} d\eta \int_1^\infty d\xi \frac{(F''g + 2g'F' + Fg'')}{\Delta^2} \Big| \times \Big| k\Delta'^2 \int d\Omega' \int_{-1}^{1} d\eta' \int_1^\infty d\xi' \times \frac{(\xi'^2-1)(1-\eta'^2)}{(\xi'^2-\eta'^2)} \frac{V(\xi',\eta',\Omega')}{\xi'^2} \Big| \Big], \tag{B37}$$

where a prime represents differentiation with respect to ξ. Note that $V(\xi',\eta',\Omega')/\xi'^2$ is a simple potential. The second factor enclosed by absolute value signs is then of the form already treated in the study of $g_1^{(5)}$ and is therefore known to be less than ϵ for k sufficiently large. The first factor can be shown to be bounded by similar arguments. Together it is possible to conclude the result $\|g_2\| < \epsilon/k$.

APPENDIX C

We now wish to prove the following statement. Given $\epsilon > 0$, there exists a k_0 such that for $k \geqslant k_0$

$$|g_1 - \bar{g}_1| < \epsilon \tag{C1a}$$

$$|g_2 - \bar{g}_2| < \epsilon/k \tag{C1b}$$

under the conditions on the potential stated in (1.16) and (3.4). The proof is given for the now familiar case of five dimensions, the generalization to higher and lower dimensions being obvious. First consider $|g_{1d}^{(5)} - \bar{g}_{1d}^{(5)}|$ after having integrated by parts once

$$|g_{1d}^{(5)} - \bar{g}_1 d^{(5)}| = |g_{1A}^{(5)} + g_{1B}^{(5)}| \leqslant |g_{1A}^{(5)}| + |g_{1B}^{(5)}|, \tag{C2}$$

where

$$g_{1A}^{(5)} = \frac{1}{2i} \frac{k\Delta}{1-2ik\Delta} \Delta^2 \int d\Omega \int_1^1 d\eta \int \mathbf{ds}_\xi \frac{(1-\eta^2)(\xi^2-1)}{(\xi^2-\eta^2)} \times \nabla_\xi [V(\xi,\eta,\Omega) - U(\xi,\eta,\Omega)] e^{2ik\Delta(\xi-1)} \tag{C3}$$

$$g_{1B}^{(5)} = \frac{1}{2i} \frac{k\Delta}{1-2ik\Delta} \Delta^2 \int d\Omega \int_{-1}^{1} d\eta \int_1^\infty d\xi 2\xi \frac{(1-\eta^2)^2}{(\xi^2-\eta^2)^2} \times [V(\xi,\eta,\Omega) - U(\xi,\eta,\Omega)] e^{2ik\Delta(\xi-1)}. \tag{C4}$$

One now introduces five-dimensional spherical coordinates as follows:

$$\begin{aligned} x_1 &= s' \cos\alpha, \quad 0 \leqslant s' < \infty \\ x_2 &= s' \sin\alpha \cos\theta, \quad 0 \leqslant \alpha \leqslant \pi \\ x_3 &= s' \sin\alpha \sin\theta \cos\varphi_1, \quad 0 \leqslant \theta \leqslant \pi \\ x_4 &= s' \sin\alpha \sin\theta \sin\varphi_1 \cos\varphi_2, \quad 0 \leqslant \varphi_1 \leqslant \pi \\ x_5 &= s' \sin\alpha \sin\theta \sin\varphi_1 \sin\varphi_2, \quad 0 \leqslant \varphi_2 \leqslant 2\pi. \end{aligned} \tag{C5}$$

In five dimensions one easily can show the following relations to be valid:

$$d\mathbf{s} = s'^4 ds' \sin^3\alpha d\alpha \sin^2\theta d\theta \sin\varphi_1 d\varphi_1 d\varphi_2 \tag{C6}$$

$$d\mathbf{s} = \Delta^4 (\xi^2-\eta^2)[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}} d\Omega d\eta \mathbf{ds}_\xi \tag{C7}$$

$$s' \sin\alpha = \Delta[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}} \tag{C8}$$

$$(\xi^2-\eta^2) = |\mathbf{r}-\mathbf{s}|\,|\mathbf{r}'-\mathbf{s}|\Delta^2, \tag{C9}$$

where

$$\mathbf{s} = \frac{\mathbf{r}+\mathbf{r}'}{2} + \mathbf{s}'. \tag{C10}$$

After some algebraic manipulation and the use of simple inequalities, one obtains

$$|g_{1A}| \leqslant \tfrac{1}{2} \int \mathbf{ds} \left(\frac{1}{|\mathbf{r}-\mathbf{s}|^2} + \frac{1}{|\mathbf{r}'-\mathbf{s}|^2} \right) \left| \frac{\mathbf{r}+\mathbf{r}'}{2} - \mathbf{s} \right| \times \sin\alpha\, |\nabla_\xi [V(\mathbf{s}) - U(\mathbf{s})]|. \tag{C11}$$

Likewise one sees that

$$|g_{1B}| \leqslant \int \mathbf{ds} \frac{\Delta^3}{(|\mathbf{r}-\mathbf{s}|\,|\mathbf{r}'-\mathbf{s}|)^3} \frac{\Delta^2(1-\eta^2)^2}{|s'|^2 \sin^2\alpha} \times |V(\mathbf{s})-U(\mathbf{s})|. \quad \text{(C12)}$$

Note that in the neighborhood of a singularity of either the type $1/|\mathbf{r}-\mathbf{s}|$ or $1/|\mathbf{r}'-\mathbf{s}|$, as $\mathbf{s}\to\mathbf{r}$ for example, from Eqs. (B12) and (C10) that

$$\Delta(1-\eta^2) \leqslant 4|\mathbf{r}'-\mathbf{s}| \quad \text{(C13)}$$

and

$$|s'| \sim \Delta/2. \quad \text{(C14)}$$

Now applying conditions expressed in Eqs. (26)–(28) to Eqs. (C11) and (C12), it is easy to see that

$$|g_1^{(5)}-\bar{g}_1^{(5)}| < \epsilon.$$

Finally, let us very briefly outline the method for proving that $|g_2^{(5)}-\bar{g}_2^{(5)}| < \epsilon/k$. First we write

$$g_2(\mathbf{r},\mathbf{r}')-\bar{g}_2(\mathbf{r},\mathbf{r}') = \frac{k\Delta^4}{\pi} \frac{k\Delta}{1-2ik\Delta} \int d\Omega \int d\eta \int_1^\infty d\xi \frac{(1-\eta^2)(\xi^2-1)}{(\xi^2-\eta^2)} \times [V-U] e^{2ik\Delta(\xi-1)} \times \frac{k\Delta'^4}{\pi} \frac{k\Delta'}{1-2ik\Delta'} \times \int d\Omega' \int_{-1}^1 d\eta' \int_1^\infty d\xi' \frac{(1-\eta'^2)(\xi'^2-1)}{(\xi'^2-\eta'^2)} \times [V'-U'] e^{2ik\Delta'(\xi'-1)}, \quad \text{(C16)}$$

where

$$\Delta' = (\xi+\eta)\Delta. \quad \text{(C17)}$$

We now integrate by parts twice with respect to ξ' and once with respect to ξ. By using methods previously demonstrated, after much laborious calculation, one can indeed show that (C1b) is valid.

Rigorous Derivation of the Phase Shift Formula for the Hilbert Space Scattering Operator of a Single Particle

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For a single nonrelativistic particle moving in a spherically symmetric potential, the existence of the Hilbert space wave operators and S operator is proved and phase shift formulas for these operators are deduced. The probability, $P(\Omega)$, for scattering into the solid angle Ω is obtained from the time dependent theory. The relation between $P(\Omega)$ and the R matrix of the standard plane wave formulation of scattering theory is established. For collimated incoming packets, it is shown that $P(\Omega)$ can be expressed as an energy average of the differential cross section.

I. INTRODUCTION

THE importance of the asymptotic behavior of the field operators in quantum field theories has recently motivated mathematically rigorous studies of the asymptotic behavior of the solutions of the nonrelativistic Schroedinger equation.[1–5] In these studies the Hamiltonian operators of the free and interacting particle are defined as Hilbert space operators following Von Neumann[6] and Kato,[7] so that the kind of convergence involved in the asymptotic limits can be precisely specified. Suitable restrictions are placed on the scattering potential $V(\mathbf{x})$; for example, that $V(\mathbf{x})$ be square integrable over any finite region of three-dimensional space, and that as $r \to \infty$ $V(\mathbf{x})$ be $0(r^{-1-\epsilon})$, where r is the radial variable in spherical coordinates and $\epsilon > 0$. It is then possible to prove that for every Hilbert space element u (i.e., for every normalizable wave function, $u(\mathbf{x})$), there are elements $u_\pm$ belonging to the continuum subspace of the total Hamiltonian H such that as the time t approaches $\mp\infty$,

$$\exp(-iH_0t)u \to \exp(-iHt)u_\pm \tag{1.1}$$

in the sense of strong convergence in Hilbert Space. In Eq. (1.1) H_0 is the kinetic energy operator and $H=H_0+V(\mathbf{x})$. Wave operators $\Omega_\pm$ are defined by the relations $u_\pm=\Omega_\pm u$, and it is shown that they and their adjoints $\Omega_\pm{}^*$ obey the relations

$$\Omega_\pm{}^*\Omega_\pm = 1 \tag{1.2a}$$

and

$$\Omega_\pm\Omega_\pm{}^* = P_c, \tag{1.2b}$$

where 1 is the unit operator and P_c is the projection operator onto the continuum subspace of H. The S operator is defined as the operator, which connects the incoming and outgoing states associated through Eq. (1.1) with a given time-dependent continuum state. It follows that

$$S=\Omega_-{}^*\Omega_+ \tag{1.3}$$

and that S is unitary. Equations (1.1) to (1.3) thus provide a mathematically rigorous time-dependent basis for scattering theory.

The present paper adds to the foregoing considerations in three respects. First, Eq. (1.1) is proved for potentials which are effectively $0(r^{-2+\epsilon})$ rather than $0(r^{-\frac{1}{2}+\epsilon})$ as $r \to 0$. Second, explicit phase shift formulas for $\Omega_\pm$ and S are obtained. Third, the experimentally important formula for the scattering probability as an energy average over the usual differential cross section is deduced from the time-dependent Hilbert space formalism.

The material is presented as follows. In Sec. II a well-known eigenfunction expansion for the Schroedinger equation is stated so that it can be used to define the Hamiltonian operators. In Sec. III, the Hamiltonians are defined. In Sec. IV, Eq. (1.1) is proved and the formulas for $\Omega_\pm$ and S are obtained. In Sec. V the formula for the scattering probability is derived.

This section will be concluded with a statement of the precise conditions imposed on $V(r)$. It is assumed that $V(r)$ is Lebesgue integrable over any finite interval not including the origin, that for $0<R<\infty$

$$\int_0^R rV(r)dr < \infty, \tag{1.4a}$$

$$\int_R^\infty V(r)dr < \infty, \tag{1.4b}$$

and that either

$$\int_r^\infty V(s)ds \text{ belongs to } L^2(R,\infty), \tag{1.5a}$$

or as $r \to \infty$,

$$V(r)=0(r^{-1-\epsilon}). \tag{1.5b}$$

The notation $L^2(a,b)$ designates the class of functions, which are Lebesgue measurable and square integrable

[1] J. M. Cook, J. Math. Phys. **36**, 82 (1957).
[2] J. M. Jauch, Helv. Phys. Acta **31**, 127 and 661 (1958).
[3] J. M. Jauch and I. I. Zinnes, Nuovo cimento **11**, 553 (1959).
[4] M. N. Hack, Nuovo cimento **9**, 731 (1958).
[5] S. T. Kuroda, Nuovo cimento **12**, 431 (1959).
[6] J. Von Neumann, *Mathematical Foundations of Quantum mechanics*, translated by R. T. Beyer (Princeton University Press, Princeton, New Jersey, 1955).
[7] Tosio Kato, Trans. Am. Math. Soc. **70**, 195 (1951).

on the interval (a,b). Equations (1.4) are used to establish the eigenfunction expansion; one or the other of Eqs. (1.5) is joined to Eqs. (1.4) in the proof of Eq. (1.1).

II. EIGENFUNCTION EXPANSION

In this section, the bound state and continuum solutions, $Y_{ml}(\theta,\phi)r^{-1}\psi_l(r)$, of the Schroedinger equation are used to generate a mean-square eigenfunction expansion of the Hilbert space elements, u, which is used in Sec. III for the definition of H and H_0. The expansion theorem could be obtained as a special case of a general theorem of Titchmarsh[8] by adapting his proof to the conditions of Eq. (1.4). However, for the simple problem under discussion, the elementary approach used here serves its purpose in a direct way in terms of formulas which the physicist will find familiar. For ease in reference in later sections, the angular and radial parts of the expansion theorem are treated separately.

Let L^2 designate the Hilbert space of complex-valued Lebesgue measurable functions, $u(x_1,x_2,x_3)$, which are square integrable on $-\infty<x_i<\infty$, $i=1, 2, 3$. Let $u(r,\theta,\phi)$ be an abbreviation for $u(r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$. Then $r(\sin\theta)^{\frac{1}{2}}u(r,\theta,\phi)$ is measurable and square integrable on $(0\leqslant r<\infty, 0\leqslant\theta\leqslant\pi, 0\leqslant\phi<2\pi)$. Let $Y_{ml}(\theta,\phi)$ designate the normalized spherical harmonics. As is well known, it can be shown that[9]

$$r(\sin\theta)^{\frac{1}{2}}u(r,\theta,\phi)=\underset{L\to\infty}{\text{l.i.m.}}\,\Sigma_L(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\alpha_{ml}(r), \quad (2.1)$$

where

$$\alpha_{ml}(r)=\int_{4\pi}\bar{Y}_{ml}(\theta,\phi)ru(r,\theta,\phi)d\Omega. \quad (2.2)$$

In Eq. (2.1) the notation Σ_L stands for

$$\sum_{l=0}^{L}\sum_{m=-l}^{l}.$$

The notation l.i.m. means the limit in mean square on the interval $(0\leqslant r<\infty,\ 0\leqslant\theta\leqslant\pi,\ 0\leqslant\phi<2\pi)$. In Eq. (2.2), $d\Omega$ stands for $\sin\theta d\theta d\phi$ and $\int_{4\pi}$ indicates integration over $(0\leqslant\theta\leqslant\pi, 0\leqslant\phi<2\pi)$. The functions $\alpha_{ml}(r)$ belong to $L^2(0,\infty)$ and have the property that

$$\|u\|^2\equiv\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dx_3|u(x_1,x_2,x_3)|^2$$
$$=\Sigma_\infty\int_0^\infty|\alpha_{ml}(r)|^2dr. \quad (2.3)$$

Conversely, given any set $\{\beta_{ml}(r)\}$ of functions belonging to $L^2(0,\infty)$ and such that the right-hand side of Eq. (2.3) is finite, the right-hand side of Eq. (2.1) exists and defines a function $g(x_1,x_2,x_3)$ belonging to L^2. Moreover, if $\gamma_{ml}(r)$ is the function calculated for $g(x_1,x_2,x_3)$ from Eq. (2.2), $\gamma_{ml}(r)$ equals $\beta_{ml}(r)$ almost everywhere. Equations (2.1) and (2.2) thus establish a one to one correspondence between the elements of L^2 and the sets, $\{\alpha_{ml}(r)\}$, of functions for which the right-hand side of Eq. (2.3) is finite.

Since each $\alpha_{ml}(r)$ belongs to $L^2(0,\infty)$, it can itself be expanded in mean square on $(0,\infty)$ according to

$$\alpha_{ml}(r)=\underset{N\to\infty}{\text{l.i.m.}}\sum_{n=0}^{N}\alpha_{mln}\psi_{ln}(r)$$
$$+\underset{\omega\to\infty}{\text{l.i.m.}}\int_0^\omega\phi_{ml}(k)\psi_l(r,k)dk, \quad (2.4)$$

where

$$\alpha_{mln}=\int_0^\infty\alpha_{ml}(r)\psi_{ln}(r)dr, \quad (2.5a)$$

and

$$\phi_{ml}(k)=\underset{\omega\to\infty}{\text{l.i.m.}}\int_0^\omega\alpha_{ml}(r)\psi_l(r,k)dr. \quad (2.5b)$$

Furthermore, for each (ml),

$$\int_0^\infty|\alpha_{ml}(r)|^2dr=\sum_{n=0}^{\infty}|\alpha_{mln}|^2+\int_0^\infty|\phi_{ml}(k)|^2dk. \quad (2.6)$$

The $\psi_{ln}(r)$, $n=0, 1, \cdots$, are the normalized eigensolutions of the radial equation

$$-u''+(l(l+1)r^{-2}+2\mu V(r))u(r)=k^2u(r), \quad (2.7)$$

for $k^2\leqslant 0$. The function $\psi_l(r,k)$ is the solution for $k>0$, which is normalized so that

$$\psi_l(r,k)\longrightarrow(2/\pi)(\sin(kr-l\pi/2+\delta_l(k))$$

as $r\to\infty$; $\delta_l(k)$ is the phase shift. For all k the solutions are $0(r^{l+1})$ as $r\to 0$. The scattered particle's mass is μ; its total energy is $k^2/2\mu$.

With each $\alpha_{ml}(r)$ belonging to $L^2(0,\infty)$, Eqs. (2.4) and (2.5) associate a function $\phi_{ml}(k)$ belonging to $L^2(0,\infty)$ and a set of constants α_{mln} such that the right-hand side of Eq. (2.6) is finite. Conversely, given a function $x_{ml}(k)$ and a set of constants β_{mln} with the above properties, Eq. (2.4) defines a function $\beta_{ml}(r)$ belonging to $L^2(0,\infty)$. If $\xi_{ml}(k)$ and γ_{mln} are calculated for $\beta_{ml}(r)$ from Eqs. (2.5), $\beta_{mln}=\gamma_{mln}$ for all n and $\xi_{ml}(k)=x_{ml}(k)$, almost everywhere. Thus Eqs. (2.4) and (2.5) establish a one to one correspondence between the $\alpha_{ml}(r)$ belonging to $L^2(0,\infty)$ and the sets $\{\phi_{ml}(k),\alpha_{mln}\}$ for which the right hand side of Eq. (2.6) is finite.

A proof of the radial expansion theorem stated above has been given by Kodaira.[10] In this proof it was assumed that $V(r)$ is continuous on $(0,\infty)$, that $V(r)=0(r^{-2+\epsilon})$ as $r\to 0$, and that $V(r)=0(r^{-1-\epsilon})$ as $r\to\infty$. These conditions are equivalent to those of Eq. (1.4) for physical applications, except that Eq. (1.4) allows discontinuous potential wells of the kind which are

[8] E. C. Titchmarsh, *Eigenfunction Expansions, Part II* (Oxford University Press, New York, 1958), Chaps. 12 and 15.

[9] A proof is given in O. E. Lanford III, Thesis, Wesleyan University, 1959, Chap. II. This paper henceforth will be referred to as I.

[10] K. Kodaira, Am. J. Math. **71**, 921 (1949).

frequently convenient in practice. One of the authors (T.A.G.) has proved the expansion theorem using Eq. (1.4). The proof will be omitted.

Equations (2.1)–(2.6) jointly establish a one to one correspondence between functions $u(x_1,x_2,x_3)$ belonging to L^2 and the sets of functions and constants $\{\phi_{ml}(k),\alpha_{mln}\}$ such that

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int_0^{\infty}|\phi_{ml}(k)|^2dk+\sum_{n=0}^{\infty}|\alpha_{mln}|^2\right\}<\infty. \quad (2.8)$$

Moreover, by Eqs. (2.3) and (2.6)

$$\|u\|^2=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int_0^{\infty}|\phi_{ml}(k)|^2dk+\sum_{n=0}^{\infty}|\alpha_{mln}|^2\right\}. \quad (2.9)$$

The set $\{\phi_{ml}(k),\alpha_{mln}\}$ will be referred to as the transform, Fu, of the Hilbert space element, u. This element is then the inverse transform, $F^{-1}\{\phi_{ml}(k),\alpha_{mln}\}$, of $\{\phi_{ml}(k),\alpha_{mln}\}$. It is easy to verify that the elements $\{\phi_{ml}(k),\alpha_{mln}\}$ such that the right-hand side of Eq. (2.9) is finite constitute a Hilbert space with a norm given by the right-hand side of Eq. (2.9) and self-evident rules for addition, etc. The transform depends on the potential. It will be convenient to denote by F_0u the transform calculated with $V(r)\equiv 0$. In this case, there are no bound states so no coefficients α_{mln} appear.

III. OPERATORS H AND H_0

The transforms introduced in Sec. II are defined in terms of the solutions of the Schroedinger equation. Hence, it is physically clear that H must be the operator multiplication by $(k^2/2\mu)$ in the space of the transforms $\{\phi_{ml}(k),\alpha_{mln}\}$ and that H_0 must be the corresponding operator for $V(r)=0$, provided that the operators thus defined are unique and self-adjoint.

For a given $V(r)$ and $l=0$, however, it is well known that Eq. (2.7) belongs to the limit circle case at $r=0$. This implies that $\psi_0(r,k)$ (and, thus, the transform) is not unique; it also implies that $\psi_0(r,k)$ is not necessarily $0(r)$ as $r\to 0$. Hence, a boundary condition must be imposed to fix $\psi_0(r,k)$ uniquely. That the boundary condition $\psi_0(r,k)=0(r)$ as $r\to 0$ is the correct one is suggested by physical considerations. It is required by the physical interpretation of the quantum theory that the free particle Hamiltonian H_0 be the self-adjoint operator multiplication by $|\mathbf{k}|^2/2\mu$ in the space of Fourier-Plancherel transforms $\hat{u}(k_1,k_2,k_3)$ of the functions $u(x_1,x_2,x_3)$ belonging to L^2. This follows from the interpretation of $|\hat{u}(k_1,k_2,k_3)|^2$ as the probability density for momentum. It may be shown[11] that the operator multiplication by $k^2/2\mu$ in the space of transforms with $V(r)=0$ is identical with H_0 if and only if $\psi_0(r,k)=0(r)$ as $r\to 0$.

The boundary condition being thus determined, the operator H is defined as follows: The element, u, whose transform is $\{\phi_{ml}(k),\alpha_{mln}\}$ is in the domain $D(H)$ of H if and only if

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left\{\int_0^{\infty}|k^2\phi_{ml}(k)|^2dk+\sum_{n=0}^{\infty}|k_{ln}^2\alpha_{mln}|^2\right\}<\infty. \quad (3.1)$$

Then, by definition,

$$Hu=F^{-1}\{(k^2/2\mu)\phi_{ml}(k),(k_{ln}^2/2\mu)\alpha_{mln}\}, \quad (3.2)$$

where k_{ln}^2 is the eigenvalue of the eigenfunction $\psi_{ln}(r)$ of Eq. (2.7). H_0 is defined analogously for $V(r)=0$. It is readily verified that H and H_0 are self-adjoint operators.[12]

Having defined H and H_0, it is a straightforward matter to define the unitary operators $\exp(-iHt)$ and $\exp(-iH_0t)$, which determine the time dependence of the scattered wave packet. This is done in Chap. III of I with the expected result that if $Fu=\{\phi_{ml}(k),\alpha_{mln}\}$,

$$\exp(-iHt)f=F^{-1}\{\phi_{ml}(k)\exp(-ik^2t/2\mu),\ \alpha_{mln}\exp(-ik_{ln}^2t/2\mu)\} \quad (3.3)$$

A corresponding formula is valid for H_0. Equation (3.3) is the starting point in the derivation of Eq. (1.1), which is carried out in the next section.

This section will be concluded with a few remarks about the use of the eigenfunction transform as a means of defining H. The method just presented can be generalized to non spherically symmetrical potentials and to an arbitrary number of particles. The essential steps in such a program have been carried out in Chapters XII and XIII of reference 8 where the existence of a unique[13] eigenfunction transform is established on the basis of physically reasonable assumptions. The transform established by Titchmarsh can be reduced in the problem under consideration to the one established directly in Sec. II.

The eigenfunction transform method of defining H differs from that used by Kato[7] although the two methods must of course lead to the same final result. In order to point up the difference, Kato's method will be briefly described.

The kinetic energy operator is defined as the closure of the differential operator T_1, which is defined to be $-\nabla^2/2\mu$ on a suitably chosen linear manifold D_1. It is then proved that H_0 is equal to the operator, multiplication by $|\mathbf{k}|^2/2\mu$, in the space of Fourier-Plancherel transforms. With H_0 thus defined, the potential $V(x_1,x_2,x_3)$ is restricted sufficiently that Vu is defined everywhere on the domain of H_0. The total Hamiltonian, H, is defined as the closure of an operator H_1, which itself is taken to be $-\nabla^2/2\mu+V$ for elements of D_1. It is proved that $H=H_0+V$, the domain of H being

[11] See Appendix A.

[12] See Chap. III of I.

[13] In footnote 8, the requirement that for $V(r)=0$ the Green's function $G_0(\mathbf{x},\mathbf{y},E)$ be singular only at $\mathbf{x}=\mathbf{y}$ accomplishes the same result as regards uniqueness as the kinetic energy argument used above.

the same as that of H_0. Kato's simple and elegant method, which he has formulated for the many particle problem, has the merit of guaranteeing a self-adjoint Hamiltonian without requiring the introduction of eigenfunction transforms.

Because in the problem under consideration $V(r)$ is more singular than the potentials envisaged in Kato's proof, and because for a partial wave analysis the existence of the eigenfunction transform is essential to begin with, the authors found it simplest to employ the definition of H given in Eqs. (3.1) and (3.2). When Kato's conditions on $V(r)$ are joined to those in Eq. (1.4), the two definitions of H yield the same operator.

IV. ASYMPTOTIC LIMITS

The purpose of this section is to prove Eq. (1.1). Let u belong to L^2 and be such that $Fu=\{\phi_{ml}(k),0\}$ so that u is orthogonal to the subspace spanned by the bound states.[14] Let $u_t=\exp(-iHt)u$. By the expansion theorems of Sec. II and Eq. (3.3),

$$r(\sin\theta)^{\frac{1}{2}}u_t(r,\theta,\phi)=\text{l.i.m.}_{L\to\infty}\sum_L(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)u_{ml}(r,t), \quad (4.1)$$

where

$$u_{ml}(r,t)=\text{l.i.m.}_{\omega\to\infty}\int_0^\omega \exp(-ik^2t/2\mu)\phi_{ml}(k)\psi_l(r,k)dk. \quad (4.2)$$

The asymptotic behavior of $\psi_l(r,k)$ [see below Eq. (2.7)] now motivates the consideration of the function $\tilde{u}_t(r,\theta,\phi)$ defined by

$$r(\sin\theta)^{\frac{1}{2}}\tilde{u}_t(r,\theta,\phi)=\text{l.i.m.}_{L\to\infty}\sum_L(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\tilde{u}_{ml}(r,t), \quad (4.3)$$

where

$$\tilde{u}_{ml}(r,t)=\text{l.i.m.}_{\omega\to\infty}\int_0^\omega \exp(-ik^2t/2\mu)\phi_{ml}(k)x_l(r,k)dk, \quad (4.4)$$

and in Eq. (4.4), $x_l(r,k)=(2/\pi)^{\frac{1}{2}}\sin(kr-l\pi/2+\delta_l(k))$. It is easy to show using the theory of Fourier transforms in $L^2(-\infty,\infty)$ that $\tilde{u}_{ml}(r,t)$ belongs to $L^2(0,\infty)$ for all t and that

$$\int_0^\infty|\tilde{u}_{ml}(r,t)|^2dr\leqslant 2\int_0^\infty|\phi_{ml}(k)|^2dk. \quad (4.5)$$

As the first main step in the derivation of Eq. (1.1), it will now be shown that

$$\lim_{|t|\to\infty}\|u_t-\tilde{u}_t\|=0. \quad (4.6)$$

By Eq. (2.3)

$$\|u_t-\tilde{u}_t\|^2=\sum_{l=0}^\infty\sum_{m=-l}^{l}\int_0^\infty|u_{ml}(r,t)-\tilde{u}_{ml}(r,t)|^2dr. \quad (4.7)$$

Minkowski's inequality applies to the integrals of Eq. (4.7). Therefore, by using Eq. (4.5) and the corresponding equation for $\int_0^\infty|u_{ml}(r,t)|^2dr$, which follows from Eq. (2.6), it is seen that the convergence of the series on the right-hand side of Eq. (4.7) is uniform with respect to t for $-\infty<t<\infty$. Therefore, if

$$\lim_{|t|\to\infty}\int_0^\infty|u_{ml}(r,t)-\tilde{u}_{ml}(r,t)|^2dr=0 \quad (4.8)$$

for all (l,m), Eq. (4.6) is valid.

The rest of the discussion requires $k>0$. For this reason, functions $u_{mlN}(r,t)$ and $\tilde{u}_{mlN}(r,t)$ are defined by restricting the k integration in Eqs. (4.2) and (4.4) to the interval $[N^{-1},N]$, $(1<N<\infty)$. It is not hard to prove (see p. 55 of I) that

$$\int_0^\infty|u_{ml}(r,t)-\tilde{u}_{ml}(r,t)|^2dr\to 0 \quad \text{as} \quad |t|\to\infty$$

if

$$\lim_{|t|\to\infty}\int_0^\infty|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=0 \quad (4.9)$$

for all N. Now

$$u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)=\int_{1/N}^N\exp(-ik^2t/2\mu)\phi_{ml}(k)\times[\psi_l(r,k)-x_l(r,k)]dk. \quad (4.10)$$

Also, for all r and N, $\phi_{ml}(k)(\psi_l(r,k)-x_l(r,k))$ is summable on $[1/N,N]$. Hence, the Riemann-Lebesgue lemma shows that

$$\lim_{|t|\to\infty}[u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)]=0 \quad (4.11)$$

for all $0\leqslant r<\infty$. Consequently, if in Eq. (4.9) the limit can be carried under the integral sign, the proof that $\|u_t-\tilde{u}_t\|\to 0$ will be accomplished. Consider first

$$\int_0^R|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr.$$

For $0\leqslant r\leqslant R$ and $1/N\leqslant k\leqslant N$, $\psi_l(r,k)-x_l(r,k)$ is bounded. Hence, by Eq. (4.10) $|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t|\leqslant K$ for all t and consequently, for all $1<N<\infty$ and all $0<R<\infty$

$$\lim_{|t|\to\infty}\int_0^R|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=\int_0^R\lim_{|t|\to\infty}|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=0. \quad (4.12)$$

It is therefore sufficient to show that

$$\lim_{R\to\infty}\int_R^\infty|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2dr=0, \quad (4.13)$$

uniformly with respect to t for $-\infty<t<\infty$.

[14] The elements, u, constitute what has been referred to as the continuum subspace of H in earlier sections.

One sufficient condition is readily obtained from the asymptotic formula

$$\psi_l(r,k)-x_l(r,k)=0\left[\int_r^\infty V(y)dy\right]+0(1/r), \quad (4.14)$$

for $k>0$ and $r\to\infty$. [Equation (4.14) is readily deduced from Eq. (4.16).] Suppose $\int_r^\infty |V(y)|dy$ belongs to $L^2(R,\infty)$ for sufficiently large R. Then the Schwarz inequality applied to Eq. (4.10) shows that for all t and sufficiently large r,

$$|u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2\leqslant g(r), \quad (4.15)$$

where $g(r)$ belongs to $L(R,\infty)$. Thus the condition expressed by Eq. (4.13) is satisfied. Consequently, Eq. (4.6) is valid.

The above condition on $V(r)$ can be replaced by the condition, $V(r)=0(r^{-1-\epsilon})$ as $r\to\infty$, for some $\epsilon>0$. This proved as follows. For $k>N^{-1}$ and $r>R(N,\epsilon)$, $\psi_l(r,k)$ satisfies the integral equation,

$$\psi_l(r,k)=x_l(r,k)-1/k\int_r^\infty \sin k(r-s)\times q(s)\psi_l(s,k)ds, \quad (4.16)$$

where $q(s)=l(l+1)/s^2+2\mu V(s)$. It follows from the iteration of Eq. (4.16) that as $r\to\infty$,

$$\psi_l(r,k)=x_{nl}(r,k)+0(r^{-(n+1)\epsilon}), \quad (4.17)$$

where $x_{nl}(r,k)$ is the function obtained by iterating Eq. (4.16) n times. Given ϵ, n can be chosen so that $n\epsilon>1$. This suffices to make $\psi_l(r,k)-x_{nl}(r,k)$ belong to $L^2(R,\infty)$ so that the argument below Eq. (4.13) can be applied to $\psi_l(r,k)-x_{nl}(r,k)$. Furthermore,

$$x_{nl}(r,k)-x_l(r,k)=\int_r^\infty dr_1G_k(r,r_1)x_l(r_1)+\cdots+\int_r^\infty dr_1\int_{r_1}^\infty dr_2\cdots\int_{r_{n-1}}^\infty dr_nG_k(r,r_1)G_k(r_1,r_2)\cdots\times G_k(r_{n-1},r_n)x_l(r_n), \quad (4.18)$$

where $G_k(x,y)=-k^{-1}q(y)\sin k(x-y)$.

With reference to Eq. (4.10), now consider

$$\xi(r,t)\equiv\int_{1/N}^N \exp(-ik^2t/2\mu)\phi_{ml}(k)\times[x_{nl}(r,k)-x_l(r,k)]dk. \quad (4.19)$$

For all r and t, Eq. (4.18) can be substituted into Eq. (4.19) and the k integral carried out first in each of the terms of the resulting sum. Moreover, the products

$$k^{-p}\sin k(r-r_1)\cdots\sin k(r_{p-1}-r_p)\sin(kr_p-l\pi/2+\delta_l(k))$$

can be decomposed into a sum of 2^p terms of the form $\sin(kZ-l\pi/2+\delta_l(k))$, or $\cos(kZ-l\pi/2+\delta_l(k))$ where Z is of the form $2r_i-2r_j+-+\cdots\pm r$.[15] In the definition of Z, r_i, r_j, etc., are selected from r_1, r_2, r_3, $\cdots$, r_p, and each distinct combination of 0, 1, 2, $\cdots$, p of them appears exactly once. Let

$$g_p(Z,t)=\int_{1/N}^N \exp(-ik^2t/2\mu)\phi_{ml}(k)k^{-p}\times\sin[kZ-l\pi/2+\delta_l(k)]dk. \quad (4.20)$$

By the theory of Fourier transforms

$$\int_0^\infty dZ|g_p(Z,t)|^2\leqslant\pi\int_{1/N}^N k^{-2p}|\phi_{ml}(k)|^2dk. \quad (4.21)$$

If $h_p(Z,t)$ is defined by Eq. (4.20) with $\cos(kZ-l\pi/2+\delta_l(k))$ in place of $\sin(kZ-l\pi/2+\delta_l(k))$, Eq. (4.21) applies with $h_p(Z,t)$ in place of $g_p(Z,t)$. With the k integrations done, $\xi(r,t)$ is given in part by a sum of terms of the form

$$\int_r^\infty dr_1q(r_1)\int_{r_1}^\infty dr_2q(r_2)\cdots\int_{r_{i-1}}^\infty dr_iq(r_i)g_p(Z,t)\times\int_{r_i}^\infty dr_{i+1}q(r_{i+1})\cdots\int_{r_{p-1}}^\infty dr_pq(r_p), \quad (4.22)$$

where Z contains r_i but none of the r_l for $l>i$. In addition, there are analogous terms with $h_p(Z,t)$ in place of $g_p(Z,t)$. Finally, there are terms with $g_p(r,t)$ and $h_p(r,t)$ which factor out of the integrals over the r_i. By applying the Schwarz inequality and Eq. (4.21) to the integrals containing $g_p(Z,t)$ and $h_p(Z,t)$, and by noting that as $r\to\infty$ $q(r)=0(r^{-1-\epsilon})$, it is readily verified that for all t as $r\to\infty$,

$$\xi(r,t)=g_p(r,t)0(r^{-\epsilon})+h_p(r,t)0(r^{-\epsilon})+0(r^{-\frac{1}{2}(1+\epsilon)}), \quad (4.23)$$

for all fixed l, m, and N. In Eq. (4.10), $(\psi_l(r,k)-x_l(r,k))$ is now written as $(\psi_l(r,k)-x_{nl}(r,k))+(x_{nl}(r,k)-x_l(r,k))$. It then follows from Eq. (4.17) (with $n\epsilon>1$) and Eq. (4.19) that as $r\to\infty$,

$$u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)=\xi(r,t)+0(r^{-1-\epsilon}) \quad (4.24)$$

Finally, Eqs. (4.24), (4.23), and (4.21) show that as $R\to\infty$,

$$\int_R^\infty |u_{mlN}(r,t)-\tilde{u}_{mlN}(r,t)|^2=0(R^{-\epsilon}) \quad (4.25)$$

for all ϵ, l, m, N, and t. Therefore, Eq. (4.13) is satisfied and the validity of Eq. (4.6) is established.

The last step in the discussion is the proof that as $t\to\pm\infty$, $\tilde{u}(r,t)$ approaches its outgoing and incoming parts, respectively. Let $\phi_{ml}(k)$ be the function in Eq.

[15] If p is even, sine functions are obtained; if p is odd, cosine functions occur. If the number of factors r_i, r_j is even, r enters with a plus sign.

(4.2) and by definition let

$$r(\sin\theta)^{\frac{1}{2}}u_l^{\pm}(r,\theta,\phi) = \underset{L\to\infty}{\text{l.i.m.}} \sum_L (\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)u_{ml}^{\pm}(r,t), \quad (4.26)$$

where

$$u_{ml}^{\pm}(r,t) = \underset{\omega\to\infty}{\text{l.i.m.}} \int_0^{\omega} \exp(-ik^2t/2\mu)\phi_{ml}(k) \times (2\pi)^{-\frac{1}{2}} \exp[\pm i(kr-(l+1)\pi/2+\delta_l(k))]dk. \quad (4.27)$$

The $u_{ml}^{\pm}(r,t)$ belong to $L^2(0,\infty)$ for all t and their norms satisfy Eq. (4.5) without the factor of two. Moreover, by comparing Eqs. (4.3) and (4.4) with Eqs. (4.26) and (4.27) it is seen that

$$\tilde{u}_l = u_l^+ + u_l^-. \quad (4.28)$$

It will be shown at the end of this section that

$$\lim_{t\to\mp\infty} \|u_l^{\pm}\| = 0 \quad (4.29)$$

Therefore, by Eqs. (4.28), (4.6), and the definition of u_l above Eq. (4.1), if $Fu=\{\phi_{ml}(k),0\}$,

$$\lim_{t\to\pm\infty} \|[\exp(-iHt)]u-u_l^{\pm}\| = 0, \quad (4.30)$$

where $u_l^{\pm}$ are defined by Eqs. (4.26) and (4.27).

The desired asymptotic limits follow directly from Eq. (4.30). Let g belong to L^2 and let $F_0g=\{\chi_{ml}(k)\}$. Equation (4.30) applies to g in the form in which H is replaced by H_0 and the $u^{\pm}{}_l$ are replaced by functions $g_l^{\pm}$, which are defined by replacing $\phi_{ml}(k)$ by $\chi_{ml}(k)$ and setting $\delta_l(k)$ equal to zero in Eqs. (4.26) and (4.27). Now let $g_{\pm}=F^{-1}\{\chi_{ml}(k)\exp(\pm i\delta_l(k)),0\}$. The application of Eqs. (4.30), (4.26), and (4.27) to each of these functions shows that

$$\lim_{t\to\mp\infty} \|e^{-iHt}g_{\pm}-e^{-iH_0t}g\| = 0. \quad (4.31)$$

Thus Eq. (1.1) is established.

The phase shift formulas for the wave operators can be given concisely in terms of F and F_0. In order to do this, the element $\{\theta_{ml}(k)\}=F_0u$ is identified with the element $\{\theta_{ml}(k),0\}$ of the Hilbert space Γ consisting of all $\{\phi_{ml}(k),\alpha_{mln}\}$ such that the right-hand side of Eq. (2.9) is finite. With this convention, F and F^{-1} establish a one to one correspondence between L^2, and Γ while F_0 and F_0^{-1} establish a one to one correspondence between L^2 and the continuum subspace of Γ. The formulas for $\Omega_{\pm}$ are now very simple. By the definition of $\Omega_{\pm}$ below Eq. (1.1) and the definition of $g_{\pm}$ below Eq. (4.30),

$$\Omega_{\pm} = F^{-1}\exp(\pm i\delta_l(k))F_0. \quad (4.32)$$

By using (4.32) and the norm-preserving properties of F and F_0, it is easy to show that

$$\Omega_{\pm}{}^* = F_0^{-1}[\exp(\mp i\delta_l)]\tilde{P}_cF, \quad (4.33)$$

where $\tilde{P}_c$ is the projection operator for the continuum subspace of Γ, $(\tilde{P}_c\{\phi_{ml}(k),\alpha_{mln}\}=\{\phi_{ml}(k),0\})$. Equations (1.2) follow directly from Eqs. (4.32) and (4.33). Finally, from Eqs. (1.3), (4.32) and (4.33) it is seen that

$$S = F_0^{-1}[\exp(2i\delta_l(k))]F_0. \quad (4.34)$$

The relation of the Hilbert space operator, S, to the R matrix of the plane wave formulation of scattering theory will be taken up in the next section. This section will be concluded with an outline of the proof of Eq. (4.29), the complete details of which are given in Chapter IV of I.

By Eqs. (4.26) and (2.3), Eq. (4.29) will hold as $t\to\infty$ if

$$\lim_{t\to\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} |u_{ml}^-(r,t)|^2 dr = 0. \quad (4.35)$$

The series in Eq. (4.35) converges uniformly with respect to t, so it remains to be shown that the integrals tend toward zero. This is done by approximating $\phi_{ml}(k)\exp(-i\delta_l(k))$ (Eq. (4.27)) in mean square by a step function zero near the origin and zero for large k. This reduces the problem to the consideration of integrals of the type

$$\int_0^{\infty} \left| \int_a^b dk \exp(-ik^2t/(2\mu)-ikr) \right|^2 dr, \quad (4.36)$$

where $0<a<b<\infty$. For sufficiently large t, and all r, it can be shown that

$$\left| \int_a^b dk \exp(-ik^2t/(2\mu)-ikr) \right|^2 < A(r^2+B)^{-1}, \quad (4.37)$$

where A and B are positive constants, Moreover, the integral over k tends toward zero by the Riemann-Lebesgue lemma. Thus the $\lim(t\to\infty)$ can be taken inside the integrals over r in Eq. (4.36) and the limit is zero. Therefore Eq. (4.29) is valid insofar as u_l^- is concerned. The proof for $t\to-\infty$ is obtained by an identical argument.

V. RELATION OF S TO THE R MATRIX OF THE PLANE WAVE THEORY AND TO THE SCATTERING CROSS SECTION

In this section, the probability $P(\Omega)$ for scattering into a given solid angle, Ω, is computed from the time dependent formalism. The conditions under which $P(\Omega)$ can be described in terms of the R matrix are then discussed. Finally, a mathematically nonrigorous, but physically convincing argument is given, which shows that for wave packets of the type used in conventional scattering experiments,

$$P(\Omega) = \sigma(\Omega)P(\mathbf{a}), \quad (5.1)$$

where $\sigma(\Omega)$ is the usual scattering cross section averaged over energy, and $P(\mathbf{a})$ is the two dimensional proba-

bility density for the incident particle to strike the point, **a**, where the scatterer is located in a plane perpendicular to the motion of the incident particle. This is the result which one would desire for it guarantees that when multiple scattering and interference effects can be neglected the average number of particles scattered into Ω for N incident particles is equal to $Nt\rho\sigma(\Omega)$, where t is the target thickness and ρ the number of scatterers per unit volume.

The formula for $P(\Omega)$ is obtained as follows. Let $V(\Omega;a,b)$ designate the region $(0\leqslant a\leqslant r\leqslant b\leqslant\infty$, $\theta_0\leqslant\theta\leqslant\theta_1$, $\phi_0\leqslant\phi\leqslant\phi_1)$. Let $u_t=\exp(-iHt)u$, where $Fu=\{\phi_{ml}(k),0\}$ as in Sec. IV and consider the probability

$$P_t(\Omega;a,b)=\int_{V(\Omega;a,b)}|u_t|^2d\mathbf{x} \tag{5.2}$$

that the scattered particle be in $V(\Omega;a,b)$ at time t. From Eqs. (4.26), (4.27) and (4.30) it is easy to see that

$$\lim_{t\to\pm\infty}\left(P_t(\Omega;a,b)-\int_{V(\Omega;a,b)}|u_t^{\pm}(r,\theta,\phi)|^2d\mathbf{x}\right)=0, \tag{5.3}$$

and that for all t

$$\int_{V(\Omega;a,b)}|u_t^{\pm}(r,\theta,\phi)|^2d\mathbf{x}=\lim_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}\sum_{l'=0}^{L}\sum_{m'=-l'}^{l'}\times\int_{\Omega}Y_{ml}(\theta,\phi)\bar{Y}_{m'l'}(\theta,\phi)d\Omega\int_a^b u_{ml}^{\pm}(r,t)\bar{u}_{m'l'}^{\pm}(r,t)dr, \tag{5.4}$$

the convergence of the series being uniform with respect to t. From Eq. (4.27) and the theory of Fourier transforms

$$\int_{-\infty}^{\infty}u_{ml}^{\pm}(r,t)\bar{u}_{m'l'}^{\pm}(r,t)dr=\int_0^{\infty}\exp[\pm i(\delta_l(k)-\delta_{l'}(k)-(l-l')\pi/2)]\times\phi_{ml}(k)\bar{\phi}_{m'l'}(k)dk. \tag{5.5}$$

Furthermore, for any finite c

$$\int_{-\infty}^{c}u_{ml}^{+}(r,t)\bar{u}_{m'l'}^{+}(r,t)dr=\int_0^{\infty}u_{ml}^{+}(c-s,t)\bar{u}_{m'l'}^{+}(c-s,t)ds, \tag{5.6}$$

where, by Eq. (4.27),

$$u_{ml}^{+}(c-s,t)=\text{l.i.m.}_{\omega\to\infty}\int_0^{\omega}\exp(-ik^2t/2\mu)\phi_{ml}(k)(2\pi)^{-\frac{3}{2}}\exp(ikc)\times\exp[i(-ks-(l+1)\pi/2+\delta_l(k))]dk. \tag{5.7}$$

Now, to within a factor $\exp[i(kc-(l+1)\pi+2\delta_l(k))]$, $u_{ml}^{+}(c-s,t)$ has the same form as $u_{ml}^{-}(s,t)$. Hence, it is easily seen from the arguments below Eq. (4.35) and the Schwarz inequality that, for all finite c,

$$\lim_{t\to\infty}\int_{-\infty}^{c}u_{ml}^{+}(r,t)\bar{u}_{m'l'}^{+}(r,t)dr=0. \tag{5.8}$$

The same kind of argument applies to $u_{ml}^{-}(r,t)$ for $t\to-\infty$. Therefore, by Eqs. (5.2), (5.3), (5.4), and (5.8), for all $0\leqslant a<\infty$,

$$\begin{aligned}\lim_{t\to\pm\infty}P_t(\Omega;a,\infty)&=\lim_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}\sum_{l'=0}^{L}\sum_{m'=-l'}^{l'}\int_{\Omega}Y_{ml}(\theta,\phi)\bar{Y}_{m'l'}(\theta,\phi)d\Omega\\&\quad\times\int_0^{\infty}\exp[\pm i(\delta_l(k)-\delta_{l'}(k)-(l-l')\pi/2)]\times\phi_{ml}(k)\bar{\phi}_{m'l'}(k)dk\\&=\lim_{L\to\infty}\int_0^{\infty}dk\int_{\Omega}d\Omega\Big|\sum_{l=0}^{L}\sum_{m=-l}^{l}Y_{ml}(\theta,\phi)\phi_{ml}(k)\times\exp[\pm i(\delta_l-l\pi/2)]\Big|^2.\end{aligned} \tag{5.9}$$

For finite a and b the limit is zero. Thus, the scattered particle is asymptotically outside of any sphere of finite radius a.

The probability, $P(\Omega)$, for scattering into the solid angle Ω should clearly be defined by the relation

$$P(\Omega)=\lim_{t\to\infty}P_t(\Omega,a,\infty). \tag{5.10}$$

Equation (5.9) then provides a formula for $P(\Omega)$ in terms of the phase shifts and the properties of the incident wave packet. The formula can be rendered more concise in terms of the Fourier transforms of the incoming and outgoing wave packets. As was shown in Sec. IV, as $t\to\infty$, $u_t\to\exp(-iH_0t)u^{\pm}$, where $F_0u^{\pm}=\{\phi_{ml}(k)\exp(\pm i\delta_l(k))\}$. Furthermore, as is proved in Appendix A, the Fourier-Plancherel transforms $\hat{u}^{\pm}(k,\theta,\phi)$ of $u^{\pm}$ satisfy the relation

$$k(\sin\theta)^{\frac{1}{2}}\hat{u}^{\pm}(k,\theta,\phi)=\lim_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\times(-i)^l\phi_{ml}(k)\exp(\pm i\delta_l(k)). \tag{5.11}$$

Consequently, by Eqs. (5.10), (5.9), and (5.11)

$$P(\Omega)=\int_0^{\infty}\int_{\Omega}|\hat{u}^{+}(k,\theta,\phi)|^2k^2dkd\Omega. \tag{5.12}$$

The physical interpretation of Eq. (5.12) is straightforward. The probability that the particle be scattered into Ω is equal to the probability that the momentum vector of the outgoing packet lie in Ω. This well-known

result, which has just been shown to be a rigorous consequence of the time-dependent formalism, is the basis for the physical interpretation of calculations in which $\hat{u}^+(k,\theta,\phi)$ is obtained from a time-independent formalism.

The connection of the Hilbert space formulas with the R matrix can now be readily deduced. Let $P_-(\Omega)$ designate the probability that the incident particle be scattered into Ω in the absence of the scatterer. [Use $\hat{u}^-(k,\theta,\phi)$ in place of $\hat{u}^+(k,\theta,\phi)$ in Eq. (5.12).] Let

$$P'(\Omega)=\int_0^\infty\int_\Omega|\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)|^2k^2dkd\Omega. \quad (5.13)$$

It is easy to prove that

$$|P'(\Omega)-P(\Omega)|\leqslant P_-(\Omega)+2(P_-(\Omega)P(\Omega))^{\frac{1}{2}}. \quad (5.14)$$

Therefore, if the incident beam is appropriately collimated, the scattering probability can be calculated accurately from $P'(\Omega)$ except near the forward direction. Now, by Eq. (5.11),

$$\begin{aligned}&k(\sin\theta)^{\frac{1}{2}}(\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi))\\&=\text{l.i.m.}_{L\to\infty}\sum_{l=0}^{L}\sum_{m=-l}^{l}(\sin\theta)^{\frac{1}{2}}Y_{ml}(\theta,\phi)\\&\quad\times[\exp(2i\delta_l(k))-1](-i)^l\phi_{ml}(k)\exp(-i\delta_l(k))\\&=\text{l.i.m.}_{L\to\infty}\int_{4\pi}k(\sin\theta)^{\frac{1}{2}}R_L(\theta,\phi;\theta',\phi';k)\\&\qquad\times\hat{u}^-(k,\theta',\phi')d\Omega', \quad (5.15)\end{aligned}$$

where

$$\begin{aligned}&R_L(\theta,\phi;\theta',\phi';k)\\&=\sum_{l=0}^{L}\sum_{m=-l}^{l}Y_{ml}(\theta,\phi)\bar{Y}_{ml}(\theta',\phi')[\exp(2i\delta_l(k))-1],\\&=\sum_{l=0}^{L}(4\pi)^{-1}(2l+1)P_l(\cos\Theta)\\&\qquad\times[\exp(2i\delta_l(k))-1]. \quad (5.16)\end{aligned}$$

In obtaining Eq. (5.16), the addition theorem for spherical harmonics was used. The angle Θ is the angle between the vectors $\mathbf{k}'(k,\theta',\phi')$ and $\mathbf{k}(k,\theta,\phi)$. Aside from a multiplicative factor, $R_L(\theta,\phi;\theta',\phi';k)$ is just the sum of the first L terms of the series for the scattering amplitude which appears in the stationary-state formulation of scattering theory for monochromatic incident plane waves. Suppose that the series (5.16) converges to a function $R(\theta,\phi;\theta',\phi';k)$ in such a way that

$$\begin{aligned}&\lim_{L\to\infty}\int_{4\pi}k(\sin\theta)^{\frac{1}{2}}R_L(\theta,\phi;\theta',\phi';k)\hat{u}^-(k,\theta',\phi')d\Omega'\\&\quad=\int_{4\pi}k(\sin\theta)^{\frac{1}{2}}R(\theta,\phi;\theta',\phi';k)\hat{u}^-(k,\theta'\phi')d\Omega' \quad (5.17)\end{aligned}$$

for almost all (k,θ,ϕ). Then, the limit functions in Eqs. (5.15) and (5.17) are equal almost everywhere, and

$$\begin{aligned}&\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)\\&\quad=\int_{4\pi}R(\theta,\phi;\theta',\phi';k)\hat{u}^-(k,\theta',\phi')d\Omega'. \quad (5.18)\end{aligned}$$

In this case, the scattering probability can be calculated from the incoming wave packet through Eqs. (5.18) and (5.13). The relation of $R(\theta,\phi;\theta',\phi';k)$ to the R matrix is the following. The R matrix, $R(\mathbf{k},\mathbf{k}')$, is defined by the formal relation[16]

$$\begin{aligned}&\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)\\&=\int\int\int(-2\pi i)R(\mathbf{k},\mathbf{k}')\delta(E-E')\hat{u}^-(\mathbf{k}')d\mathbf{k}', \quad (5.19)\end{aligned}$$

where $E=k^2/2\mu$ and $\delta(E-E')$ is the Dirac delta function. Equation (5.19) means

$$\begin{aligned}&\hat{u}^+(k,\theta,\phi)-\hat{u}^-(k,\theta,\phi)\\&\quad=-2\pi ik\mu\int_{4\pi}R(\mathbf{k},\mathbf{k}')\hat{u}^-(\mathbf{k}')d\Omega', \quad (5.20)\end{aligned}$$

where $|\mathbf{k}|=|\mathbf{k}'|$. By comparing Eqs. (5.20) and (5.18), it is seen that the R matrix is defined on the energy shell whenever the limit $R(\theta,\phi;\theta',\phi';k)$ of $R_L(\theta,\phi;\theta',\phi';k)$ exists and Eq. (5.17) is valid.

From the physical point of view, there is no point in discussing potentials for which Eq. (5.18) does not hold, because if the series in Eq. (5.16) does not converge fairly rapidly, the phase shift approach will be useless for computation anyway. It is possible, of course, to contemplate potentials for which the series (5.16) diverges for $\Theta=0$ since in practice the calculation of nonforward scattering using Eqs. (5.13) and (5.18) need not require integration over $\Theta=0$. The convergence of the series (5.16) and the validity of Eq. (5.17) can be tested by using the Born approximation for the phase shifts.[17] As is well known, it is sufficient for convergence for $\Theta\neq0$ that as $r\to\infty$ $V(r)=0(r^{-2-\epsilon})$, $\epsilon>0$.[18] The stronger condition $V(r)=0(r^{-3-\epsilon})$ is sufficient to guarantee absolute and uniform convergence for $0\leqslant\theta\leqslant\pi$.

The usual formula for $P'(\Omega)$ in terms of the differential scattering cross section is obtained by specializing $\hat{u}^-(k,\theta,\phi)$ so that it conforms to experimental conditions. This has been done by Ekstein,[16] Eisenbud,[19]

[16] See, for example, H. Eckstein, Phys. Rev. **101**, 880 (1956).
[17] D. S. Carter, Thesis, Princeton University, 1952 (unpublished).
[18] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), 1st ed., p. 187, problem 5.
[19] L. Eisenbud, Thesis, Princeton University, 1948 (unpublished).

and Jauch.[20] An alternative formulation, based on the same physical arguments, is presented below.

Suppose that the scatterer is located at the point whose cartesian coordinates are $(a_1,a_2,0)$ in the reference frame in which the scattered beam is directed along the positive x_3 axis. If the change of location of the scatterer from the origin to $(a_1,a_2,0)$ is taken into account in the usual way, it follows from Eqs. (5.13) and (5.18) that

$$P'(\Omega)=\int_\Omega d\Omega\int_0^\infty dk\left|\int_{4\pi}R(\theta,\phi;\theta',\phi';k)\times\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k,\theta',\phi')d\Omega'\right|^2. \quad (5.21)$$

Now, with a typical beam (beam diam ~ 1 cm, momentum $\sim 10^8$ cm^{-1}), $\hat{u}^-(k,\theta',\phi')$ goes to zero strongly outside a forward cone of apex angle $\sim 10^{-8}$ rad centered on the x_3 axis. Thus, in cases of physical interest $R(\theta,\phi;\theta',\phi';k)$ can certainly be replaced by $R(\theta,\phi;0,0;k)$. This leads to

$$P'(\Omega)\approx\int_\Omega d\Omega\int_0^\infty dk\sigma_k(\theta,\phi)\times\left|(2\pi)^{-1}\int_0^\pi\int_0^{2\pi}\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k,\theta',\phi')\times k^2\sin\theta'd\theta'd\phi'\right|^2, \quad (5.22)$$

where

$$\sigma_k(\theta,\phi)=|k^{-1}\sum_{l=0}^\infty(2l+1)P_l(\cos\theta)\exp(i\delta_l(k))\sin\delta_l(k)|^2. \quad (5.23)$$

It will be recognized that $\sigma_k(\theta,\phi)$ is the differential cross section as usually defined. Equation (5.22) can be further transformed by noting that with $k\sim 10^8$ and $\theta'\sim 10^{-8}$, it will be a very good approximation to write[21]

$$(2\pi)^{-1}\int_0^\pi\int_0^{2\pi}\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k,\theta',\phi')k^2\sin\theta'd\theta'd\phi'$$
$$\approx(2\pi)^{-1}\int_{-\infty}^\infty\int_{-\infty}^\infty\exp(i\mathbf{k}'\cdot\mathbf{a})\hat{u}^-(k_1,k_2,k)dk_1dk_2$$
$$\approx(2\pi)^{-\frac{1}{2}}\int_{-\infty}^\infty\exp(-ikx_3)u^-(a_1,a_2,x_3)dx_3. \quad (5.24)$$

Finally, with conventional collimation, it should be possible to describe the beam in terms of packets of the form

$$u^-(x_1,x_2,x_3)=g(x_1,x_2)e(x_3). \quad (5.25)$$

In this event, Eq. (5.22) becomes

$$P'(\Omega)\approx P(\mathbf{a})\int_\Omega d\Omega\int_0^\infty dk\sigma_k(\theta,\phi)|\hat{e}(k)|^2, \quad (5.26)$$

where $\hat{e}(k)$ is the Fourier transform of $e(x_3)$[$\hat{e}(k)=0$ for $k<0$] and $P(\mathbf{a})=|g(a_1,a_2)|^2$. Since $u^-(x_1,x_2,x_3)$ is normalized, $\int_{-\infty}^\infty\int_{-\infty}^\infty P(\mathbf{a})da_1da_2=1$ and $\int_0^\infty|\hat{e}(k)|^2=1$. Equation (5.26), which because of Eq. (5.14) is practically equivalent to Eq. (5.1), is the final result. It shows how the cross section is to be averaged over the energy spectrum of the incoming beam, and shows explicity through $P(\mathbf{a})$ how the scattering decreases when the target is not in the center of the beam.

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APPENDIX A

In this appendix, the relation between the Fourier-Plancherel transform, $\hat{u}(k_1,k_2,k_3)$, of $u(x_1,x_2,x_3)$ and the transform, $\{\phi_{ml}(k)\}$, for $V=0$ is established. Let $u_n(r,\theta,\phi)$ be equal to $u(r,\theta,\phi)$ for $0\leqslant r\leqslant n$ and zero otherwise. Because of the norm-preserving properties of both transforms and because $u_n\to u$ in mean square, $\hat{u}_n\to\hat{u}$, and $\phi_{mln}(k)\to\phi_{ml}(k)$ in mean square. ($\{\phi_{mln}(k)\}\equiv F_0u_n$.) Since $\hat{u}_n$ and $\hat{u}$ belong to L^2, they possess expansions of the form given in Eqs. (2.1)–(2.3). Let $\gamma_{mln}(k)$ and $\gamma_{ml}(k)$ correspond, respectively, to the quantity called $\alpha_{ml}(r)$ in these equations. Clearly, $\gamma_{mln}(k)\to\gamma_{ml}(k)$ in mean square. Furthermore,

$$\gamma_{mln}(k)=k\int_0^\pi\int_0^{2\pi}\bar{Y}_m(\theta,\phi)d\Omega(2\pi)^{-\frac{1}{2}}\times\int_0^n r'^2dr'\int_0^\pi\int_0^{2\pi}\exp(-i\mathbf{k}\cdot\mathbf{r}')u(r',\theta',\phi')d\Omega', \quad (A1)$$

where $\mathbf{k}$ is the radius vector to the point (k,θ,ϕ). In Eq. (A1), the order of integration can be reversed and the exponential can be expanded in terms of spherical harmonics and Bessel functions. In this way, there results

$$\gamma_{mln}(k)=(-i)^l\int_0^n\int_0^\pi\int_0^{2\pi}(kr)^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)\times\bar{Y}_{ml}(\theta,\phi)ru(r,\theta,\phi)drd\Omega$$
$$=(-i)^l\phi_{mln}(k). \quad (A2)$$

The last equality in Eq. (A2) follows from Eqs. (2.2) and (2.5) and the fact that for $V=0$ $\psi_l(r,k)$ is equal to $(kr)^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)$. It follows from Eq. (A2) and the con-

[20] See the first article of footnote 2. In this discussion the energy spread of the incoming packet is not considered.

[21] The final result in Eq. (5.24) is obtained from the theory of Fourier transforms and implies physically harmless mathematical restrictions on $u^-(x_1,x_2,x_3)$.

vergence of $\gamma_{mln}(k)$ and $\phi_{mln}(k)$ that

$$\gamma_{ml}(k)=(-i)^l\phi_{ml}(k) \tag{A3}$$

almost everywhere. Furthermore, from the definition of $\gamma_{ml}(k)$ it is easy to see that for any finite K and $p>0$

$$\int_0^K\int_0^\pi\int_0^{2\pi} k^p|\hat{u}(k,\theta,\phi)|^2k^2dkd\Omega = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^K k^p|\phi_{ml}(k)|^2dk. \tag{A4}$$

By taking $p=4$, it follows that $\|k^2\hat{u}\|<\infty$ if and only if Eq. (3.1) is satisfied. (Note that $V(r)=0$.) Furthermore, from Eq. (A3) and the bi-uniqueness of the transforms in question, it follows that when $\|k^2\hat{u}\|<\infty$, the function whose Fourier-Plancherel transform is $(k^2/2\mu)\hat{u}$ is identical with $F_0^{-1}\{(k^2/2\mu)\phi_{ml}(k)\}$. Hence, H_0, as defined by Eqs. (3.1) and (3.2), is equal to the operator multiplication by $k^2/2\mu$ in the space of Fourier-Plancherel transforms.

To see that the foregoing is true only with the boundary condition $\psi_0(x,k)=0(x)$ for $x\to 0$, consider the radial part of the transform for $l=0$ without this condition.[22] For any function $u(r)$ belonging to $L^2(0,\infty)$

$$u(r)=\lim_{\omega\to\infty}\int_0^\omega \psi^\alpha(r,k)\phi^\alpha(k)dk, \tag{A5}$$

where

$$\phi^\alpha(k)=\lim_{\omega\to\infty}\int_0^\omega \psi^\alpha(x,k)u(x)dx. \tag{A6}$$

[22] E. C. Titchmarsh, *Eigenfunction Expansions Associated with Second Order Differential Equations* (Oxford University Press, London, England, 1946), p. 59.

The function $\psi^\alpha(r,k)$ is given by

$$\psi^\alpha(x,k)=\frac{2^{\frac{1}{2}}}{\pi^{\frac{1}{2}}}\left\{\frac{\cos\alpha}{(\cos^2\alpha+k^2\sin^2\alpha)^{\frac{1}{4}}}\sin kx - \frac{k\sin\alpha}{(\cos^2\alpha+k^2\sin^2\alpha)^{\frac{1}{4}}}\cos kx\right\}. \tag{A7}$$

For $\alpha=0$, $\psi^\alpha(x,k)$ reduces to the function $\psi_0(x,k)$ which figures in Eqs. (2.4)–(2.6). Now consider the function $g(x_1,x_2,x_3)=\exp(-pr)$. It belongs to L^2 and it is readily verified that $\int\int\int|k^2\hat{g}(k_1,k_2,k_3)|^2d\mathbf{k}<\infty$. Therefore, g belongs to the domain of the operator, multiplication by $k^2/2\mu$ in the space of Fourier-Plancherel transforms.

Let $x^\alpha(k)$ be the transform of g defined by Eqs. (2.1)–(2.6) for $V=0$ using the $\psi^\alpha(x,k)$. (Only the term with $l=0$ contributes.) In this case the function $u(r)$ in Eqs. (A5) and (A6) is $2\pi^{\frac{1}{2}}r\exp(-pr)$. Direct calculation now shows that as $k\to\infty$,

$$\begin{aligned} x^\alpha(k)&=(2\sqrt{2}/k^2)(1+0(k^{-2})); && \sin\alpha\neq 0,\\ &=0(k^{-3}), && \sin\alpha=0. \end{aligned} \tag{A8}$$

From Eq. (A8) it is clear that $k^2x^\alpha(k)$ belongs to $L^2(0,\infty)$ if and only if $\sin\alpha=0$. Therefore, $g(x_1,x_2,x_3)$ is in the domain of the operator, multiplication by $k^2/2\mu$ in the space of the transform defined by Eqs. (2.1)–(2.6) if and only if $\sin\alpha=0$. Thus, the domains of the operators, multiplication by $k^2/2\mu$ in the space of Fourier-Plancherel transforms, $\hat{u}$, and multiplication by $k^2/2\mu$ in the space of the transforms F_0u are identical if and only if $\sin\alpha=0$.

Analyticity of the Fourth Order Scattering Amplitude with Two Complex Invariants*

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The partial Feynman amplitude corresponding to a particular fourth order diagram is examined as a function of energy and momentum transfer with both of these variables complex. The region of regularity of this function is found, and the types of singularities at the remaining points are determined. An approach which requires only elementary calculations is indicated. The condition for the validity of Mandelstam's representation in the fourth order is obtained. Spectral representations for exchange scattering processes at fixed momentum transfer are discussed as another application of the principal results.

1. INTRODUCTION

IT is the purpose of this paper to give a systematic discussion of the analytic properties of the partial scattering amplitude associated with a particular fourth order Feynman diagram. We allow two invariants, the total four-momentum squared and the square of the four-momentum transfer, to be complex. We also show how the analytic properties of an integral as a function of several complex variables can be studied.

Perturbation-theoretic problems involving one complex variable have been studied by a number of authors. Karplus, Sommerfield, and Wichmann[1] made a systematic study of the third- and of the fourth-order amplitudes. The two papers of reference 1 are referred to in the sequel as I and II. Our results constitute an extension of the results of II.

Perturbation-theoretic problems involving more than one complex variable have been studied by Källén and Wightman,[2] by Mandelstam,[3–5] by Oehme,[6,7] and by Taylor.[8] In each of these works an essential part of the argument involves an explicit evaluation of certain functions. Our analysis, on the other hand, is based on Feynman's integral representation[9] of perturbation theory amplitudes, and we relate the singularities of an amplitude to the singularities of the integrand without carrying out the integration explicitly.[10]

We obtain a new derivation of the condition for the validity of Mandelstam's double integral representation in the fourth order. Our derivation, however, avoids the intricate calculations by which Mandelstam[4] originally obtained the same condition. Another application of our analysis of singularities deals with spectral representations for exchange scattering processes at fixed momentum transfer. Our method can be applied directly to the study of analyticity of certain higher order amplitudes (i.e., those amplitudes considered in Appendix B and corresponding to diagrams illustrated in Fig. 10) for which direct calculations would not be feasible.

As in II, we restrict our discussion to the partial amplitude associated with the diagram of Fig. 1. The other diagrams of the fourth order either are topologically equivalent to that of Fig. 1, or else are reducible, in which case the analytic properties of the corresponding partial amplitudes can be studied without difficulty see also footnote 4). The partial amplitude associated with the diagram of Fig. 1 will be called *the four-point function.*

In Sec. 2 we determine the geometric configuration of the surfaces to which the singularities of the four-point function are restricted. In Sec. 3 we determine which points of these surfaces are regular and which are singular for the four-point function. In Sec. 4 we consider the applications to Mandelstam's representation and to exchange scattering. In Appendix A we describe the method used for the determination of singularities. In Appendix B we prove two theorems regarding the singularities of Feynman amplitudes corresponding to a certain class of diagrams to which the diagram of Fig. 1 belongs. In Appendix C we discuss briefly the dependence of the four-point function on the external masses. In Appendix D we determine the types of

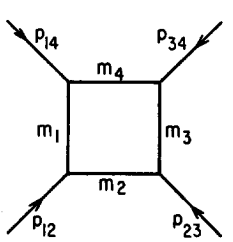

FIG. 1. Fourth-order Feynman diagram for a scattering process.

* This work was supported in part by a U. S. Air Force contract, monitored by the Air Force Office of Scientific Research of the Air Research and Development Command.

[1] R. Karplus, C. M. Sommerfield, and E. H. Wichmann, I, Phys. Rev. **111**, 1187 (1958); II, Phys. Rev. **114**, 376 (1959). Further references are given in paper I.

[2] G. Källén and A. S. Wightman, Mat. Fys. Skr. Dan. Vid. Selsk. **1**, No. 6 (1958). The vertex function in perturbation theory is discussed in Appendix III.

[3] S. Mandelstam, Phys. Rev. **112**, 1344 (1958).

[4] S. Mandelstam, Phys. Rev. **115**, 1741 (1959).

[5] S. Mandelstam, Phys. Rev. **115**, 1752 (1959).

[6] R. Oehme, Phys. Rev. **111**, 1430 (1958).

[7] R. Oehme, Nuovo cimento **13**, 778 (1959).

[8] J. G. Taylor (preprint).

[9] Perturbation methods and Feynman integral representations are described in M. J. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1955), Chap. 8 and Appendix V.

[10] Our method is an extension of the discussion by R. J. Eden, Proc. Roy. Soc. (London) **A210**, 388 (1952); cf. also M. Grisaru, Phys. Rev. **111**, 1719 (1958), footnote 8.

singularities of the four-point function at its singular points, and prove in this way the existence of singularities of the function at the points in question.

We now review certain definitions and facts from footnote 2. We consider the four-point function F corresponding to the diagram of Fig. 1, and we consider the masses and the momenta there indicated.[11] We define

$$p_{13}=p_{12}+p_{23}, \quad p_{24}=p_{23}+p_{34}, \tag{1.1}$$

and

$$y_{kl}=-(p_{kl}^2-m_k^2-m_l^2)/2m_km_l. \tag{1.2}$$

We ignore a constant factor, and we have

$$F=\int_0^1 dx_1\int_0^1 dx_2\int_0^1 dx_3\int_0^1 dx_4 \times\frac{\delta(1-x_1-x_2-x_3-x_4)}{m_1m_2m_3m_4D^2}, \tag{1.3}$$

with

$$D=\sum_{k=1}^{4} x_k^2+2\sum_{k<l} x_kx_ly_{kl}. \tag{1.4}$$

We impose stability conditions on the external masses

$$y_{12}>-1, \quad y_{23}>-1, \quad y_{34}>-1, \quad y_{14}>-1. \tag{1.5}$$

For convenience we also impose stability conditions on the internal masses

$$y_{12}<1, \quad y_{23}<1, \quad y_{34}<1, \quad y_{14}<1. \tag{1.6}$$

The restrictions (1.6) will be removed in Appendix C. If $-1\leq y_{kl}\leq 1$, we define θ_{kl} as in II by

$$\cos\theta_{kl}=y_{kl}, \quad 0\leq\theta_{kl}\leq\pi. \tag{1.7}$$

Our primary interest will be with $F=F(y_{13},y_{24})$ on its physical sheet, which we define by

$$-\pi<\arg(y_{13}-1),\arg(y_{24}-1)<\pi, \tag{1.8}$$

with the condition that F be real and positive for y_{13}, y_{24} real and greater than one. We shall, however, consider also the analytic continuation of F to the boundary of the physical sheet, i.e., to the two hyperplanes

$$-\infty<y_{13}<1 \quad \text{and} \quad -\infty<y_{24}<1. \tag{1.9}$$

2. SURFACES OF SINGULARITIES

According to Appendices A and B, we may have a singularity of F if the determinant of some principal minor of the matrix

$$\begin{bmatrix} 1 & y_{12} & y_{13} & y_{14} \\ y_{12} & 1 & y_{23} & y_{24} \\ y_{13} & y_{23} & 1 & y_{34} \\ y_{14} & y_{24} & y_{34} & 1 \end{bmatrix} \tag{2.1}$$

[11] In order to avoid complications with infrared divergences, we assume that all of the internal masses m_j are nonzero. We also assume that all particles have spin zero; it is pointed out in I that there is no loss of generality in such an assumption.

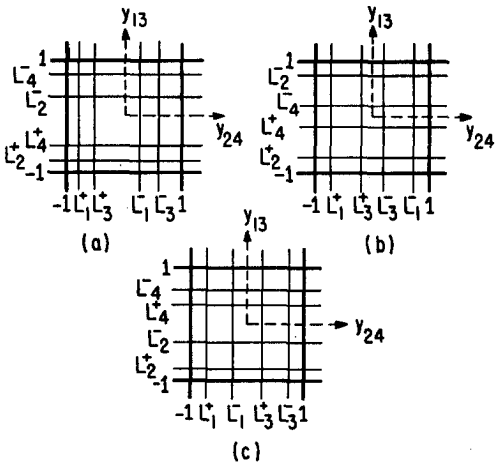

FIG. 2. The possible arrangements of the lines $y_{13}=L_{13}^{(j)}$ and $y_{24}=L_{24}^{(k)}$.

vanishes. The two 2×2 minors which are relevant for us give the values

$$y_{13}=\pm1, \tag{2.2a}$$

$$y_{24}=\pm1. \tag{2.2b}$$

The 3×3 minor defined by indices 1, 2, 3 has the determinant

$$K_4=1-y_{12}^2-y_{13}^2-y_{23}^2+2y_{12}y_{13}y_{23} \tag{2.3}$$

[cf. Eq. (II, B2)]. The solutions of the equation $K_4=0$ may be written

$$y_{13}=\cos(\theta_{12}\pm\theta_{23})\equiv L_4^{\pm}. \tag{2.4a}$$

The remaining 3×3 minors give analogous equations $K_2=0$, $K_1=0$, $K_3=0$, which yield

$$y_{13}=\cos(\theta_{34}\pm\theta_{14})\equiv L_2^{\pm}, \tag{2.4b}$$

$$y_{24}=\cos(\theta_{23}\pm\theta_{34})\equiv L_1^{\pm}, \tag{2.4c}$$

$$y_{24}=\cos(\theta_{14}\pm\theta_{12})\equiv L_3^{\pm}, \tag{2.4d}$$

respectively. Note that each of the Eqs. (2.2a,b) and (2.4a-d) places a restriction on only one of the variables y_{13}, y_{24}, while the other remains arbitrary. Of the quantities $L_j^{\pm}$ only the L_j^{+} were used in II.

Let us assume that the six quantities ±1, $L_2^{\pm}$, $L_4^{\pm}$ are all distinct, and that ±1, $L_1^{\pm}$, $L_3^{\pm}$ are likewise all distinct. (Degenerate cases in which some of these quantities coincide are discussed in Appendix C.) From Eqs. (2.4a-d) it follows that $-1<L_j^{\pm}<1$. Let us label the quantities $L_2^{\pm}$, $L_4^{\pm}$ as $L_{13}^{(1)}, \cdots, L_{13}^{(4)}$, where $L_{13}^{(j)}<L_{13}^{(j+1)}$, and let us label $L_1^{\pm}$, $L_3^{\pm}$ as $L_{24}^{(1)}, \cdots, L_{24}^{(4)}$, where $L_{24}^{(j)}<L_{24}^{(j+1)}$. We see that $L_j^{+}<L_j^{-}$, and that we can always label the lines in Fig. 1 in such a way that

$$L_2^{+}=L_{13}^{(1)}, \quad L_1^{+}=L_{24}^{(1)}. \tag{2.5}$$

One may verify that the same superscript j occurs in both $L_2^{-}=L_{13}^{(j)}$ and in $L_1^{-}=L_{24}^{(j)}$; moreover, $L_4^{+}=L_{13}^{(k)}$ implies $L_3^{+}=L_{24}^{(k)}$ and $L_4^{-}=L_{13}^{(l)}$ implies

$L_3^- = L_{24}^{(1)}$. The three possible arrangements of lines given by Eqs. (2.2a,b) and (2.4a-d) are shown in Fig. 2.

We now consider the surface defined by setting the determinant of the matrix (2.1) equal to zero; we write, with the notation $y_{ij}=y_{ji}$, $y_{ii}=1$,

$$\Delta \equiv \Delta(y_{13},y_{24}) \equiv \det(y_{ij}) = 0. \tag{2.6}$$

Expansion of the determinant gives

$$\begin{aligned}\Delta(y_{13},y_{24}) = 1 - \sum_{i<j} y_{ij}^2 + 2 \sum_{i<j<k} y_{ij}y_{jk}y_{ik} \\ + y_{12}^2y_{34}^2 + y_{13}^2y_{24}^2 + y_{14}^2y_{23}^2 - 2y_{12}y_{13}y_{24}y_{34} \\ - 2y_{12}y_{14}y_{23}y_{34} - 2y_{13}y_{14}y_{23}y_{24}.\end{aligned} \tag{2.7}$$

We first restrict ourselves to real y_{13}, y_{24}; in this case Eq. (2.6) defines a curve in the real y_{13},y_{24}-plane. This curve, which consists of several branches, will be denoted by Γ. To learn more about Γ we first compute the discriminants of Eq. (2.6). Theorem 3 of Appendix B states that if

$$\Delta = Ay_{13}^2 + By_{13} + C = ay_{24}^2 + by_{24} + c, \tag{2.8}$$

then

$$B^2 - 4AC = 4K_1K_3, \quad b^2 - 4ac = 4K_2K_4 \tag{2.9}$$

[cf. Eq. (II, 29)]. Equations (2.9) imply that each of the lines $y_{13}=L_{13}^{(i)}$ and $y_{24}=L_{24}^{(k)}$ is tangent to Γ, and at only one point. Moreover, there are no other vertical or horizontal lines tangent to Γ. Next, we observe that in the expansion (2.7) y_{13}^2 and y_{24}^2 occur only as $(y_{13}^2-1)(y_{24}^2-1)$. It follows that the lines $y_{13}=\pm 1$, $y_{24}=\pm 1$ are asymptotes to Γ, and that these are the only vertical and horizontal asymptotes. We now examine the signs of the discriminants (2.9), and conclude that there is one branch of Γ in each of the following five regions:

$$\begin{aligned}&(1)\quad y_{13} \le L_{13}^{(1)}, \quad y_{24} \le L_{24}^{(1)} \\ &(2)\quad y_{13} \ge L_{13}^{(4)}, \quad y_{24} \le L_{24}^{(1)} \\ &(3)\quad y_{13} \ge L_{13}^{(4)}, \quad y_{24} \ge L_{24}^{(4)} \\ &(4)\quad y_{13} \le L_{13}^{(1)}, \quad y_{24} \ge L_{24}^{(4)} \\ &(5)\quad L_{13}^{(2)} \le y_{13} \le L_{13}^{(3)}, \quad L_{24}^{(2)} \le y_{24} \le L_{24}^{(3)}.\end{aligned} \tag{2.10}$$

Each of these branches will be labeled by a corresponding subscript: $\Gamma_1, \cdots, \Gamma_5$. For convenience, we shall also refer to Γ_4 as Γ_0. A typical graph of Γ is shown in Fig. 3.

It will be useful for us to know which of the branches $\Gamma_1, \Gamma_2, \Gamma_4$ is tangent to each of the lines $y_{13}=L_{13}^{(1)}=L_2^+$, $y_{24}=L_{24}^{(1)}=L_1^+$. Expressions for the points of tangency to the lines defined by L_j^+ are given in Eqs. (II, 27-28); e.g., Γ is tangent to $y_{13}=L_2^+$ at y_{24} given by

$$y_{24} = (\cos\theta_{12}\sin\theta_{34} + \cos\theta_{23}\sin\theta_{14})/\sin(\theta_{34}+\theta_{14}). \tag{2.11}$$

The equations for the remaining points of tangency may be obtained from Eq. (2.11) by an appropriate permutation of indices. Now to determine when Γ_1 and when

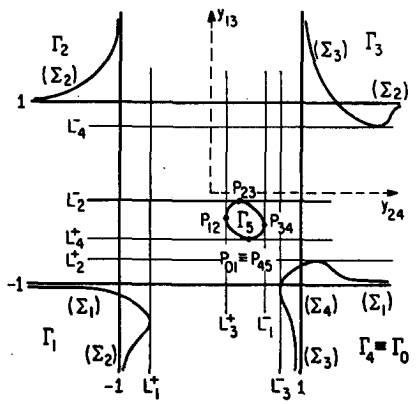

FIG. 3. The curve Γ. A symbol (Σ_j) indicates that the given part of Γ is joined to the surface Σ_j defined in the text.

Γ_4 is tangent to $y_{13}=L_2^+$, we use Eq. (2.11) in special cases and observe that as long as the lines of tangency are displaced continuously, but do not come into coincidence with one another or with the asymptotes, the points of tengency will not move from one branch Γ_j to another. We summarize the locations of the points of tangency to $y_{13}=L_2^+$. Let us write

$$\Theta = \theta_{12}+\theta_{23}+\theta_{34}+\theta_{14}. \tag{2.12}$$

Then, Γ_4 is tangent to $y_{13}=L_2^+$ if

$$\Theta < 2\pi \quad \text{and} \quad \theta_{14}+\theta_{34} < \pi, \tag{2.13a}$$

or if

$$\Theta > 2\pi \quad \text{and} \quad \theta_{14}+\theta_{34} > \pi. \tag{2.13b}$$

On the other hand, Γ_1 is tangent to $y_{13}=L_2^+$ if

$$\Theta < 2\pi \quad \text{and} \quad \theta_{14}+\theta_{34} > \pi, \tag{2.13c}$$

or if

$$\Theta > 2\pi \quad \text{and} \quad \theta_{14}+\theta_{34} < \pi. \tag{2.13d}$$

Obvious modifications will give the locations of the points of tangency to $y_{24}=L_1^+$. The locations of the points of tangency to lines $y_{13}=L_{13}^{(4)}$ and $y_{24}=L_{24}^{(4)}$, however, will not be of any further interest to us, and will not be described here.

Let us now describe the surface defined by Eq. (2.6) with y_{13}, y_{24} complex; this surface will be denoted by Σ. First, consider the fourth degree system of equations (α and β real, $\alpha \neq 0$):

$$\Delta(y_{13},y_{24}) = 0, \tag{2.14a}$$

$$y_{13} = \alpha y_{24} + \beta. \tag{2.14b}$$

The real solutions of Eqs. (2.14a, b) are the intersections of Γ with the real line (2.14b). We see from Fig. 3 that for a fixed α and for β varying from $-\infty$ to ∞ there are ordinarily three intervals on the β axis for which the equations have four real sets of solutions, separated by two intervals

$$\beta_1(\alpha) < \beta < \beta_2(\alpha) \quad \text{and} \quad \beta_3(\alpha) < \beta < \beta_4(\alpha), \tag{2.15}$$

for which the equations have two sets of real solutions and two complex conjugate sets. For some values of α the real line (2.14b) intersects one branch Γ_j at three points near a point of inflection. Then, there are one or two additional intervals in which Eqs. (2.14a, b) have four real sets of solutions.

Now, let us select an $\alpha \neq 0$ such that the above complication does not occur, and let us select one of the intervals (2.15), say $\beta_1(\alpha) < \beta < \beta_2(\alpha)$. As β varies over this interval, the complex solutions of Eqs. (2.14a, b) vary over a curve C_α lying on the surface Σ. This curve joins one branch Γ_j with the arc $(P_{j-1,j}P_{j,j+1})$ of Γ_5 (see Fig. 3). As α varies over the positive or over the negative real axis (depending on whether the original choice was $\alpha > 0$ or $\alpha < 0$, respectively), the curves C_α sweep out a surface, which we shall denote by Σ_j. (We also set $\Sigma_0 \equiv \Sigma_4$.) If for a given α and β the line (2.14b) intersects a single branch $\Gamma_{j\pm1}$ at three points, then the corresponding curve C_α breaks into two parts, one of which joins Γ_j to $\Gamma_{j\pm1}$, while the other joins $\Gamma_{j\pm1}$ to the arc $(P_{j-1,j}P_{j,j+1})$ of Γ_5. We see that the complex surface Σ_j joins all or a part of Γ_j to the arc $(P_{j-1,j}P_{j,j+1})$, and it may also join these curves to a part of Γ_{j+1} and to a part of Γ_{j-1}. These facts are illustrated in Fig. 3.

Each surface Σ_j consists of two disconnected pieces, having Im $y_{13} > 0$ and Im $y_{13} < 0$, respectively. We note that for $\alpha > 0$ in Eq. (2.14b) we obtain Σ_2 and Σ_4, which have on each piece Im y_{13} and Im y_{24} of the same sign. For $\alpha < 0$, we obtain Σ_1 and Σ_3, which have on each piece Im y_{13} and Im y_{24} of opposite signs.

Let us observe that every point (y_{13}, y_{24}) of Σ with Im y_{13}, Im $y_{24} \neq 0$ lies on some Σ_j; this follows from the fact that for such a point we may always find real α and β with $\alpha \neq 0$ such that $y_{13} = \alpha y_{24} + \beta$. Finally, the points of Σ with one member of the pair (y_{13}, y_{24}) real and the other complex are those points of Σ which join Σ_j to $\Sigma_{j\pm1}$. These points correspond to $\alpha = 0$ or to $1/\alpha = 0$ (α/β finite) in Eq. (2.14b). It is clear from Fig. 3 that they all lie on the boundary of the physical sheet of F, i.e., on the hyperplanes (1.9). Our description of the geometric configuration of Σ is now complete.

3. REGULAR AND SINGULAR POINTS OF THE SURFACES

In this section we determine which points of the surfaces described in Sec. 2 are regular and which are singular for the four-point function F. The method which we use in this section are largely, but not entirely, those described in Appendix A.

As long as we restrict our discussion to the singularities of the successive integrals in the definition (1.3) of F, we can use the discussion of Appendix D to strengthen some of the conclusions of Appendix A. Lemma 1*A* then gives two conditions, and the fulfillment of one of these is both necessary and sufficient for the existence of a singularity of an integral. Lemma 2*A* can likewise now be stated in a stronger form.

It is convenient to introduce symbols which signify, with reference to a particular singularity of a given n fold integral, how many times each of the conditions (1) and (2) of Lemma 1A is fulfilled in the successive integrations [the condition (1) requires the integrand to have an end-point singularity, and (2), to have coincident singularities]. We shall say that a given singularity is of type (E^kC^{n-k}) if condition (1) is fulfilled k times, and condition (2), $n-k$ times. For the function F we have singularities of types (E^2C^1), (E^1C^2), and (C^3).

We have emphasized in Appendix A that in continuing an integral analytically, it may be necessary to deform the contour. In general, an analytic continuation of the expression (1.3) gives the result

$$F = \int_{A_1} dx_i \int_{A_2(x_i)} dx_j \int_{A_3(x_i,x_j)} dx_k \times \frac{1}{(\prod m_l) D^2(x_i, x_j, x_k; y_{pq})}, \tag{3.1}$$

where A_1, $A_2(x_i)$, and $A_3(x_i, x_j)$ are appropriately chosen arcs between 0 and 1, between 0 and $1-x_i$, and between 0 and $1-x_i-x_j$, respectively. We indicated explicitly the dependence of the arcs on the variables of integration.

We recall from II that $D \neq 0$ if $y_{13}, y_{24} > 1$, and in this case we take the contours along the positive real axes. The following lemma is evident.

Lemma 1. Let F be continued analytically from the region where $y_{13}, y_{24} > 1$. Let $x_i = x_i^0$ be a fixed number, $0 \leq x_i^0 \leq 1$, and let us assume that along the path of continuation

$$D(x_i^0, x_j, x_k; y_{pq}) \neq 0 \tag{3.2a}$$

for

$$0 \leq x_j,\ x_k,\ x_j + x_k \leq 1 - x_i^0. \tag{3.2b}$$

Then the contours $A_2(x_i^0)$, $A_3(x_i^0, x_j)$ of Eq. (3.1) may be taken along the real axes. If along the path of continuation $D(x_i^0, x_j^0, x_k; y_{pq}) \neq 0$ for $0 \leq x_k \leq 1 - x_i^0 - x_j^0$, then the contour $A_3(x_i^0, x_j^0)$ may be taken along the real axis.

In particular, we see that in continuing to the region where Im y_{13} and Im y_{24} are both nonzero and of the same sign, we may retain the contours along the real axes. Then $D \neq 0$ in the region of integration, and F is analytic.

Let us consider now the singularities of the type (E^2C^1); these are restricted to the planes defined by Eqs. (2.2a-b). For Eq. (2.2a), $y_{13} = \pm 1$, the singularities of F are associated with zeros of D at the endpoints of integration $x_2 = x_4 = 0$. From Eqs. (1.3) and (1.4)

we obtain

$$F=\int_0^1 dx_2\int_0^{1-x_2} dx_4\int_0^{1-x_2-x_4} dx_1 \times\frac{1}{(\prod m_l)[1+2x_1(1-x_1)(y_{13}-1)+X]^2}, \quad (3.3)$$

where $X=0$ for $x_2=x_4=0$. We see that for $x_2=x_4=0$, the integrand is regular if $y_{13}=1$; while if $y_{13}\to -1$ then the integrand has poles in the x_1-plane which approach $x_1=\frac{1}{2}$ from opposite half-planes. Lemma 1 states that the contour in question may be taken along positive real axis. We conclude that F is singular at $y_{13}=-1$, y_{24} arbitrary. The case of Eq. (2.2b) is analogous.

Next we consider singularities of type (E^1C^2); these are restricted to planes defined by Eqs. (2.4a-d). For Eq. (2.4a), $y_{13}=L_4^{\pm}$, the singularities of F are associated with zeros of D at the endpoint $x_4=0$. As pointed out in II, our problem reduces to that of the vertex function. Note the Lemma 1 allows us to use real contours for $x_4=0$, as in the foregoing. An analysis of the vertex function (I and Appendix A of II) shows that we do not have singularity at $y_{13}=L_4^-$, and we have a singularity at $y_{13}=L_4^+$ of type (E^1C^2) if and only if

$$\theta_{12}+\theta_{23}>\pi \quad (3.4)$$

(we assume that $L_4^+\neq -1$). Hence F is singular at $y_{13}=L_4^+$, y_{24} arbitrary, if the inequality (3.4) holds; F has no singularities of type (E^1C^2) (and associated with the endpoint $x_4=0$) at $y_{13}=L_4^-$, nor at $y_{13}=L_4^+$ if the inequality (3.4) does not hold. The treatment of Eqs. (2.4b-d) is analogous.

It should be pointed out that the conclusions of the last two paragraphs, even if expected on the basis of the results of I and II, actually constitute an extension of these results. In I and II only the thresholds of spectral representations are determined. Our conclusions make some assertions about the singularities of F in the region where it is complex, and in particular, about the singularities of the spectral function Im F [see Eq. (II,8)]. We also note that our discussion can be applied directly to determine the singularities of the vertex function $F_v(y_{13})$, or of the associated spectral function Im F_v.

The remaining singularities of F are of the type (C^3), and they lie on the surface Σ (which includes the curve Γ). There are two properties of these singularities which we should mention. First, it is pointed out in Appendix A, and illustrated in Fig. 9, how analytic continuation around a singularity of type (E^1) can alter the nature of a singularity of type (C^1) in a particular integral. Thus, if we approach a point (y_{13},y_{24}) of Γ with Im $y_{13}\to 0\pm$, Im $y_{24}\to 0\pm$ and with Im $y_{13}\to 0\pm$, Im $y_{24}\to 0\mp$, F may be singular at (y_{13},y_{24}) in one case and not in the other, and these two limits have to be investigated separately. We shall speak of these two cases as limits from *corresponding* and from *opposite* half-planes, respectively.

The second property is the following: Remark 1 of Appendix A, properly generalized, states that analytic continuation around a singularity of type (C^3) does not alter the nature of another singularity of a particular integral. We see that although the definition (1.8) of the physical sheet of F is ambiguous in case F has branch points within the physical sheet, nevertheless one can unambiguously determine the points of singularity of F in the physical sheet.[12] We do not consider the continuation of F around singularities of types other than (C^3) since these all lie on the boundary of the physical sheet; see (1.9).

We proceed to determine the singularities of F on Σ. We recall from II that F is analytic in a certain region R of the real y_{13}, y_{24}-plane; R is bounded by lines

$$y_{13}=L_{13},\quad y_{24}=L_{24}. \quad (3.5)$$

($L_{13}=-1$ or L_2^+ or L_4^+, $L_{24}=-1$ or L_1^+ or L_3^+) and sometimes also by arc $(P_{01}P_{12})$ of Γ_5. We see that F has no singularities on Γ_3, and, by Lemma 2A, it has none on Σ_3. Moreover, for $y_{13}>L_{13}^{(3)}$ the limits Im $y_{13}\to 0+$ and Im $y_{13}\to 0-$ are always equal, and at any point of Γ_2 either both limits described above give singularities, or neither limit gives singularities. A similar conclusion holds for Γ_4. Next, F is regular at (y_{13},y_{24}) on the physical sheet if Im y_{13}, Im y_{24} are both different from zero and of the same sign, as we pointed out in connection with Lemma 1. It follows that F has no singularities on Σ_2 and on Σ_4, and on those points of Γ_2 and Γ_4 which are joined to Σ_2, Σ_3, or Σ_4.

We still have to discuss singularities on Γ_1, Γ_5, Σ_1, and on those points of Γ_2 and Γ_4, which are joined to Σ_1. We shall make use of the following lemma.[13]

Lemma 2. Every point of Γ_1 other than a point of tangency to a line of singularities is a singular point of F when one of the two limits described above is taken, and is a regular point when the other limit is taken. The same conclusion holds for Γ_5 if the thresholds are $L_{13}=L_{13}^{(3)}$, $L_{24}=L_{24}^{(3)}$ [case (iv) below].

Proof. We first give a proof for the case in which the curve in question is tangent to one of the (singular) lines $y_{13}=L_{13}$, $y_{24}=L_{24}$. Let us assume for definiteness that we are dealing with Γ_1 which is tangent to the line $y_{13}=L_{13}=L_k^+$. [We note that Γ_1 is tangent to a line of singularities if and only if we have case (ii) described below.] Let us write

$$F(y_{13},y_{24})=\int_0^1 dx_k f(x_k,y_{13},y_{24}). \quad (3.6)$$

[12] Oehme (footnote 7) has given a detailed discussion of the physical sheet in the case of the vertex function.

[13] This lemma is analogous to a conclusion of Källén and Wightman (footnote 2) who show how the singular nature of the points of their hypersurface $\Phi=0$ changes when the hypersurface crosses a branch cut which delimits the physical sheet.

At the point of tangency of Γ_1 to $y_{13}=L_{13}$, f has coincident singularities of type (C^2) at $x_k=0$. (The presence of one singularity follows from our assumption that the line $y_{13}=L_k^+$ is singular. Moreover, Lemma 2A implies that upon a small change of parameters the singularity splits into two singularities of type (C^2); we note that there are no (E^1C^1) or (E^2) singularities with (y_{13},y_{24}) near the point of tangency and x_1 near zero.) If a point, say $(y_{13}^0+i\epsilon, y_{24}^0+i\epsilon)$, in the limit $\epsilon\to 0+$ is singular for F, and lies on Γ_1 near the point of tangency, then f has coincident singularities which are on opposite sides of the contour. As we displace y_{13} from $y_{13}^0+i\epsilon$ around the branch point $y_{13}=L_{13}$ to $y_{13}^0-i\epsilon$, as in Fig. 9(a), then the singularities of f are displaced as shown in Fig. 9(b), and we do not have a singularity at $(y_{13}^0-i\epsilon, y_{24}^0+i\epsilon)$ in the limit $\epsilon\to 0+$. If the point $(y_{13}^0+i\epsilon, y_{24}^0+i\epsilon)$ is regular for F in the limit $\epsilon\to 0+$, then f also has two coincident singularities, but now these lie on one side of the contour, or miss the contour. We may now apply the same argument as previously. Lemma 2A allows us to extend our conclusion to the remaining points of Γ_1. (If Γ_1 is also tangent to the line $y_{24}=L_{24}$, then it is necessary to repeat the above argument with reference to the new point of tangency.)

The above argument also applies to Γ_5 if we have case (iv). To prove the lemma for Γ_1 if Γ_1 is not tangent to one of the lines $y_{13}=L_{13}$, $y_{24}=L_{24}$, we proceed as follows. We choose a suitable point (y_{13},y_{24}) of Γ_1 and such external masses that the specified tangency conditions hold, and then we vary the external masses to their desired values and use Lemma 2A. We then use again Lemma 2A to extend our results to all of Γ_1 with the desired mass values. The validity of this procedure can be checked in detail for each of the cases listed below. [See the transitions between the cases described in Appendix C; see also the Remark following the description of case (iv).] The lemma follows.

We now discuss various cases separately. The cases listed below correspond to the various cases of II, except that we made two separate cases, (ii) and (iv), of case (ii) of II. A description of the real region R of analyticity for the various cases is given in detail in II. We recall Eq. (2.12): $\Theta=\theta_{12}+\theta_{23}+\theta_{34}+\theta_{14}$, and we shall call two angles θ_{ij} and θ_{kl} adjacent if they have one subscript in common.

Cases (i) and (ii): $\Theta<2\pi$. In these cases the region R is bounded by the lines $y_{13}=L_{13}=L_{13}^{(1)}$ or -1, and $y_{24}=L_{24}=L_{24}^{(1)}$ or -1. We have case (i) if the sum of any two adjacent angles is less then π, and then $L_{13}=L_{24}=-1$. We have case (ii) if the sum of angles in a pair of adjacent angles is greater than π, and then at least one of the two equations $L_{13}=L_{13}^{(1)}$, $L_{24}=L_{24}^{(1)}$ holds.

In these cases there are no singularities on Γ_5, and therefore there are none on Γ_1 (Lemma 2A). If we make the extension from Γ_5 to Γ_1 via Σ_1, then there will be no singularities on Γ_1 either. We now recall that the construction of Σ_1 depended on the use of $\alpha<0$ in Eq. (2.14b). We conclude that for those points of Γ_1 which are joined to Σ_1, F is regular if we take the limit from opposite half-planes, and singular if we take the limit from corresponding half-planes (Lemma 2). Moreover, one sees, by following a similar argument, that the situation is reversed for those points of Γ_1 which are joined to Σ_2 or to Σ_4. We also observe that F is always regular on Γ_2 and Γ_4.

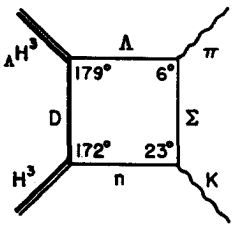

FIG. 4. A Feynman diagram with $\Theta>2\pi+2\min(\theta_{ij})$. The binding energy of Λ in ${}_\Lambda H^3$ was taken as 0.2 Mev [B. W. Downs and R. H. Dalitz, Phys. Rev. 114, 593 (1959)].

Case (iii): $2\pi<\Theta<2\pi+2\min(\theta_{12},\theta_{23},\theta_{34},\theta_{14})$. In this case the lines $y_{13}=L_{13}^{(j)}$, $y_{24}=L_{24}^{(k)}$ are ordered as in Fig. 2, case (a) or (b), and R is bounded by lines $y_{13}=L_{13}^{(2)}$, $y_{24}=L_{24}^{(2)}$, and by arc $(P_{01}P_{12})$ of Γ_5 (Fig. 3). Thus, there are singularities on arc $(P_{01}P_{12})$, on Σ_1, and on those points of Γ_2 and Γ_4 which are joined to Σ_1 [see the relations (2.13a-d) and Fig. 3]. Moreover, at every point of Γ_1, F is singular if we take the limit from opposite half-planes, and regular for the limit from corresponding half-planes. [We note that Γ_1 is tangent to $y_{13}=L_{13}^{(1)}$ or to $L_{24}=L_{24}^{(1)}$ if and only if F is regular on the line in question. This statement is also valid for case (iv). For cases (i) and (ii) the situation is reversed.]

Case (iv): $\Theta>2\pi+2\min(\theta_{12},\theta_{23},\theta_{34},\theta_{14})$. In this case the lines $y_{13}=L_{13}^{(j)}$, $y_{24}=L_{24}^{(k)}$ are ordered as in Fig. 2(c), and R is bounded by lines $y_{13}=L_{13}^{(3)}$, $y_{24}=L_{24}^{(3)}$. Arguments analogous to those used above lead to the following conclusion: F is singular on arc $(P_{23}P_{34})$ for limits from corresponding half-planes, on arcs $(P_{12}P_{23})$ and $(P_{34}P_{45})$ and (Lemma 2A) on arc $(P_{01}P_{12})$ for limits from opposite half-planes, on Σ_1, on Γ_1 for limits from opposite half-planes, and on Γ_2 and Γ_4 at those points which are joined to Σ_1. F is regular on Γ_1 and on Γ_5 if the other limits than specified above are taken.

A Feynman diagram which falls into case (iv) and which represents a physical process is shown in Fig. 4.

Remark. The above conclusions seem to lead, but do not, to certain inconsistencies. One of these confusing points is as follows. Let us suppose that Γ_1 is tangent to a line, say $y_{24}=L_1^+$, which is not singular. If (y_{13},y_{24}) is at the point of tangency, then there are coincident singularities at $x_1=0$, and it may appear that there should be endpoint singularities if (y_{13},y_{24}) is displaced from the point of tangency along the line $y_{24}=L_1^+$. However, we would like to point out that the singularities at $x_1=0$ need not be at the endpoint of integration, since other singularities in the x_1-plane may impose a deformation of the contour, and the coincident singularities at $x_1=0$ may be separated from the endpoint

$x_1=0$ by a branch cut. Thus there is no inconsistency. The case of singularities of Γ_5 in case (iv) is analogous. It is obvious that in such cases it is allowable to use Lemma 2A to determine the continuation of singularities past the point of tangency.

In Sec. 2 we pointed out that the points (y_{13},y_{24}) of Σ with one member of the pair real and the other complex join two different parts Σ_j and $\Sigma_{j\pm1}$ of Σ. In passing from Σ_j to $\Sigma_{j\pm1}$ through these points we cross the boundary of the physical sheet [see (1.9)]. Thus the fact that we may have singularities on Σ_1 but not on Σ_2 or Σ_4 does not contradict Lemma 2A.

We make two general observations concerning the singularities of F, in addition to the observation expressed in Lemma 2. For the first, we note that all of the curves and surfaces with singularities other than Σ_1 lie on the boundary of the physical sheet. We see that F has no singularities in the physical sheet if and only if $\Theta\leq 2\pi$; see Appendix C for the case $\Theta=2\pi$.

The second observation is the following: If a given branch of Γ is tangent to a line of singularities $y_{ik}=L_j^+$, then we have singularities on Γ (for either of the two limits) on one side of the point of tangency, and not on the other side. This observation can be easily understood if we realize that for the point of tangency one of the sets of coincident singularities occurs at the endpoint of the contour.

4. APPLICATIONS

Mandelstam's Representation

On the basis of Sec. 3 we see that if $\Theta\leq 2\pi$, then a double application of Cauchy's theorem establishes the validity of Mandelstam's double integral representation,

$$F(y_{13},y_{24})=\frac{1}{\pi^2}\int_{-\infty}^{L_{13}}dv\int_{-\infty}^{L_{24}}dw\frac{\rho(v,w)}{(v-y_{13})(w-y_{24})}, \quad (4.1)$$

where

$$\rho(y_{13},y_{24})=-\tfrac{1}{4}\lim_{\epsilon,\epsilon'\to 0+}[F(y_{13}+i\epsilon,\, y_{24}+i\epsilon')-F(y_{13}+i\epsilon,\, y_{24}-i\epsilon')-F(y_{13}-i\epsilon,\, y_{24}+i\epsilon')+F(y_{13}-i\epsilon,\, y_{24}-i\epsilon')]. \quad (4.2)$$

On the other hand, if $\Theta>2\pi$ then the existence of singularities of F for complex y_{13}, y_{24} precludes the validity of a representation such as in Eq. (4.1). Our conclusions are in agreement with those obtained by Mandelstam.[4]

Our techniques may also be used for a further study of representations such as in Eq. (4.1). To give an illustration, we give a new proof of the fact[4] that in case (i) the function ρ is nonzero in the region bounded by Γ_1 rather than in the entire region $-\infty<y_{13},y_{24}<-1$. We write, for $y_{13},y_{24}>-1$,

$$F(y_{13},y_{24})=\frac{1}{\pi}\int_{-\infty}^{-1}\frac{dv}{v-y_{13}}g(v,y_{24}), \quad (4.3)$$

where for $y_{13}<-1$; $-1<y_{24}$,

$$g(y_{13},y_{24})=(2i)^{-1}\lim_{\epsilon\to 0+}\times[F(y_{13}+i\epsilon,\, y_{24})-F(y_{13}-i\epsilon,\, y_{24})]. \quad (4.4)$$

For the specified values of y_{13} and y_{24}, g is the imaginary (absorptive) part of F. The next step is to construct a spectral representation for $g(y_{13},y_{24})$, where y_{13} is a parameter less than -1. For this purpose we define g for other values of y_{24} by analytic continuation from the values $y_{24}>-1$.

Equation (4.4) shows that all singularities of g lie on the surfaces described in Sec. 2. We are primarily interested in the dependence of g on y_{24}, and the only points which we need to investigate are $y_{24}=-1$ and the intersection of the line $y_{13}=$ const. with Γ_1. Let us show that g is regular for $y_{24}=-1$. We use the relation

$$\lim_{\epsilon\to 0+}(-1)^n n![(1/(x+i\epsilon)^{n+1}-1/(x-i\epsilon)^{n+1}]=-2\pi i\delta^{(n)}(x), \quad (4.5)$$

which follows by differentiation from the case $n=0$. We obtain

$$g(y_{13},y_{24})=\pi\int_0^1 dx_1\int_0^1 dx_2\int_0^1 dx_3\int_0^1 dx_4\times\delta(1-\textstyle\sum x_k)\delta'(D)/\prod m_i. \quad (4.6)$$

Let us look more closely at the region where D vanishes. We rearrange the terms of Eq. (1.4) as follows:

$$D=(x_1-x_3)^2+2x_1x_3(y_{13}+1)+(x_2-x_4)^2+2x_2x_4(y_{24}+1)+2x_1(x_2y_{12}+x_4y_{14})+2x_3(x_2y_{23}+x_4y_{34}). \quad (4.7)$$

Since we are dealing with case (i), we have

$$y_{12}+y_{14}>0, \quad y_{23}+y_{34}>0. \quad (4.8)$$

An examination of Eq. (4.7) and of the inequalities (4.8) shows that there exists $\eta>0$ which depends on y_{13} but which does not depend on y_{24} (for $y_{24}>-1$) and is such that $D>0$ when $0\leq x_1,x_3\leq\eta$ and $0\leq x_2$, $x_4\leq 1$ (with $\sum x_i=1$). Lemma 1 (of Sec. 3) now allows us to take the contour along the real axis for the integral over x_2 and x_4 when $0\leq x_1,x_3\leq\eta$, and we see that $D>0$ when x_2 and x_4 vary over this contour. Furthermore, the boundaries of the region with $D=0$ (or, expressions defining these boundaries) depend analytically on y_{24} for $y_{24}>-1$, but at $y_{24}=-1$ they are enlarged in a discontinuous way. We now wish to continue g analytically from $y_{24}>-1$ to $y_{24}=-1-\epsilon_0$ (ϵ_0 greater than zero and sufficiently small). To do so, we must continue analytically the boundaries of the region of integration, and we see that in this continuation the boundaries do not reach the endpoints $x_1=x_3=0$. Since the singularities of F at $y_{24}=-1$ are associated with these endpoints of integration, we conclude that g is regular at $y_{24}=-1$.

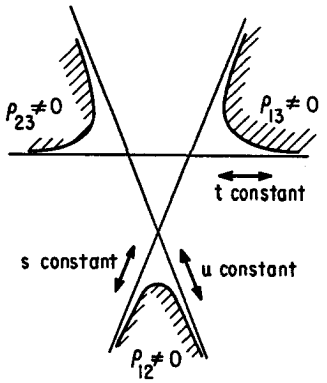

FIG. 5. The regions with nonzero spectral functions ρ_{ij}. We assume case (i) in each region.

We also conclude that g is singular at the point $y_{24}=y_{24}^0$ where (y_{13},y_{24}^0) lies on Γ_1,[14] and that we have the following spectral representation for g (for $y_{13}<-1$ and $y_{24}^0<y_{24}$; $y_{24}^0<-1$):

$$g(y_{13},y_{24})=\frac{1}{2\pi i}\int_{-\infty}^{y_{24}^0}\frac{dw}{w-y_{24}}\lim_{\epsilon'\to 0+}\times[g(y_{13},w+i\epsilon')-g(y_{13},w-i\epsilon')]. \quad (4.9)$$

Our assertion about the function ρ now follows.

Spectral Representations for Exchange Scattering

In II the spectral representations were considered in which the energy (s) of the process or the square of the four-momentum transfer ($-t$) is held constant. Mandelstam, however, has pointed out a basic symmetry among the three invariants s, t, and u, ($-u$) being the square of the four-momentum transfer for exchange scattering. From this symmetry arises the interest in spectral representations with u constant.

The interest in such spectral representations arises more directly in connection with momentum transfer limitations of dispersion relations. Consider a process for which the complete scattering amplitude admits a double integral representation of the form (4.1). Then, following Mandelstam,[3-5] there are three associated spectral functions ρ_{ij} which are nonzero in the regions shown in Fig. 5. Some of the Feynman diagrams which contribute to the three functions ρ_{ij} in the $N-N$ case are shown in Fig. 6. A single fourth-order diagram as in Fig. 1 has a nonzero spectral function in only one of these regions, as we see from Eq. (4.1).

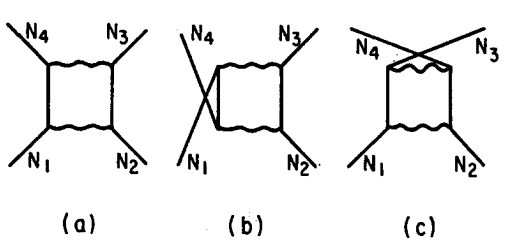

FIG. 6. N-N diagrams with specified nonzero spectral functions ρ_{ij} for (a) $\rho_{13}\neq 0$, for (b) $\rho_{23}\neq 0$, and for (c) $\rho_{12}\neq 0$.

[14] An entire function which vanishes at infinity is identically zero; see E. C. Titchmarsh, *The Theory of Functions* (Oxford University Press, New York, 1939), 2nd edition, p. 165. We also note that the existence of a singularity of g at $y_{24}=y_{24}^0$ implies a part of Lemma 2 (Sec. 3), and is implied by that lemma.

Consider now the process of Fig. 1, with p_{12} and p_{23} incoming (positive timelike) and p_{34} and p_{14} outgoing (negative timelike). Then

$$s=(p_{12}+p_{23})^2,\quad t=(p_{12}+p_{14})^2,\quad u=(p_{12}+p_{34})^2. \quad (4.10)$$

These invariants are linearly related as follows:

$$s+t+u=p_{12}^2+p_{23}^2+p_{34}^2+p_{14}^2. \quad (4.11)$$

Let F_{12} and F_{13} be two partial Feynman amplitudes which give nonzero contributions to ρ_{12} and ρ_{13}, respectively (we can take $F_{13}=F$). We see from Fig. 5 that a spectral representation for F_{12} with t constant is analogous to a spectral representation for F_{13} with u constant. (This is also suggested by Fig. 6.) Thus it appears that the study of spectral representations in the fourth order with u constant is a first step toward understanding spectral representations (or dispersion relations) for large space-like momentum transfer.

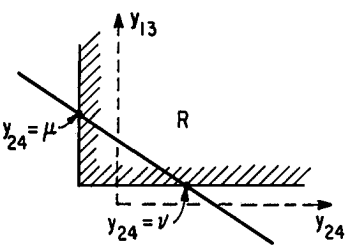

FIG. 7. The limits of integration in Eq. (4.13).

Equation (4.11) with u constant is equivalent to

$$y_{13}+\gamma y_{24}=\lambda, \quad (4.12)$$

for some real constants γ and λ, with $\gamma>0$. Now we conclude from Sec. 3 that in cases (i) and (ii) we have for any real λ

$$F(\lambda-\gamma y_{24},y_{24})=\frac{1}{\pi}\left(\int_{-\infty}^{\mu}+\int_{\nu}^{\infty}\right)\frac{dx}{x-y_{24}}\lim_{\epsilon\to 0+}\times\operatorname{Im}F(\lambda-\gamma x-i\epsilon,x+i\epsilon). \quad (4.13)$$

The limits of integration μ, ν depend on the boundaries of the real region R of analyticity of F (Fig. 7). If λ is sufficiently small then the integral extends over the entire real axis.

We see from Eq. (4.13) that the points (y_{13},y_{24}) which are arguments of F approach the curve Γ from opposite half-planes, and thus, in case (i) the function Im F of Eq. (4.13) is regular on Γ_1 when $\epsilon=0$. Thus we may indefinitely continue the functions of Eq. (4.13) analytically in λ. It is interesting to speculate whether this conclusion is a special feature of perturbation theory or whether it has a more general validity. At

present all attempts to establish dispersion relations without recourse to perturbation theory are applicable only to limited values of momentum transfer,[15] because the singularities of the absorptive part of the scattering amplitude for larger values of momentum transfer are not yet understood.[16]

In case (ii), the function Im F [of Eq. (4.13)] has singularities on that part of Γ_1 which is joined to the surface Σ_2 or to Σ_4 (see Fig. 3). In cases (iii) and (iv), the representation (4.13) is not valid for those values of λ for which the system of Eqs. (4.12) and $\Delta(y_{13},y_{24})=0$ has solutions lying on Σ_1, but this representation is valid for all other values of λ.

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APPENDIX

A. Determination of Singularities of Integrals

Necessary Condition for Singularities

The following lemma is implied by the discussion of Eden:[10]

Lemma 1A. Let an arc A be given in the complex z plane as a contour of integration, let N denote a neighborhood of the contour A, and let D be a domain in the complex c plane. Let $f(z,c)$ be regular in either variable, except for a finite number of isolated singularities or branch points, for any value of the other variable, when $z\epsilon N$, $c\epsilon D$. (We have to include the possibility that the domains D and N extend over more than one Riemann sheet of f.) Then

$$\omega(c)=\int_A f(z,c)dz \qquad (A.1)$$

can be singular at $c=c_0\epsilon D$ only if one of the following two conditions holds:

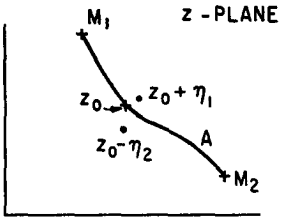

FIG. 8. Illustration of the condition (2) for singularities of $\omega(c)$.

(1) $f(z,c_0)$ as a function of z has a singularity at an endpoint of the contour, or
(2) for c_1 in a neighborhood of c_0, $f(z,c_1)$ is singular at $z=z_0+\eta_1$ and at $z=z_0-\eta_2$,

where $z_0+\eta_1$ and $z_0-\eta_2$ lie on opposite sides of the contour A, z_0 is a point of the contour, and $\eta_1, \eta_2 \to 0$ as $c_1 \to c_0$. (See Fig. 8.)

In general, if $f(z,c)$ has singularities at $z_1=z_0+\eta_1$ and at $z_2=z_0-\eta_2$, and $\eta_1, \eta_2 \to 0$ as $c \to c_0$, we shall say that f has coincident singularities (as a function of z) at $c=c_0$. We note that if the point $z=z_0$ is not an endpoint of A, then in general z_1 and z_2 will lie on opposite sides or on the same side of the contour depending on the chosen Riemann surface of $\omega(c)$. A typical situation is shown in Fig. 9; here $\omega(c)$ may have a singularity at the point P, where $c=c_0$, but not at the point Q, where $c=c_0$ likewise.

Let us suppose now that $f(z,c,\xi)$ depends on the parameter ξ in the same way as on the other two variables, i.e., in analogy with the specifications of Lemma 1A. Then $\omega=\omega(c,\xi)$ also depends on ξ analytically. The condition that f have coincident singularities will in general be equivalent to an equation $g(c,\xi)=0$. Let us suppose that we have coincident singularities at (c_0,ξ_0): $g(c_0,\xi_0)=0$, and let us suppose that these singularities approach the contour from opposite sides. Then, if we vary (c,ξ) and the contour in such a way that

(1) the variation is continuous,
(2) no singularity crosses the contour,
(3) $g(c,\xi)=0$, i.e., the singularities in the z plane stay coincident,
(4) the singularities do not reach an endpoint of the contour,

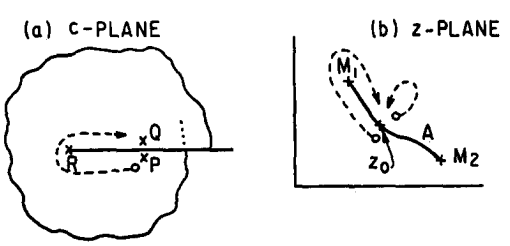

FIG. 9. (a) Riemann surfaces for $\omega(c)$; $c=c_0$ at P and at Q, and R is the branch point associated with the endpoint M_1 of integration. (b) The displacement of singularities in the z plane when c is displaced from a neighborhood of P to a neighborhood of Q as shown in Fig. 9(a).

[15] H. Lehmann, Nuovo cimento **10**, 579 (1958).

[16] One can show that the function Im A corresponding to an arbitrary amplitude A can be continued to indefinitely large space-like momentum transfers if one assumes that (i) A satisfies Mandelstam's representation, and (ii) those spectral functions of A which are located in the region of ρ_{12}, see Fig. 5, have no tangents which are parallel to their asymptotes. Then the singularities on the curves which bound the spectral functions cannot occur for limits from opposite half-planes, as otherwise these singularities would extend into the complex region. Our assertion now follows as in the text.

we still shall have coincident singularities approaching the contour from opposite sides. (Note that we must keep the endpoints of the contour fixed in order to retain the same function ω.) If we start with coincident singularities which approach the contour from one side, or do not approach it at all, and if we vary (c,ξ) and the contour as described, then an analogous conclusion holds.

Furthermore, we can effect the analytic continuation of $\omega(c,\xi)$ [or of $\omega(c)$] by satisfying conditions (1) and (2). These considerations lead to the following lemma:

Lemma 2A. Let $g(c_0,\xi_0)=0$, and let us continue $\omega(c,\xi)$ analytically from (c_0,ξ_0) to (c_1,ξ_1) in such a way that the conditions (3) and (4) are satisfied. If the coincident singularities do not approach the contour from opposite sides for (c_0,ξ_0), then ω is regular at (c_1,ξ_1). If the coincident singularities approach the contour from opposite sides for (c_0,ξ_0), they also approach the contour from opposite sides for (c_1,ξ_1), and hence ω may be singular at (c_1,ξ_1).

The above lemmas, as well as the considerations that follow, can be readily generalized to functions involving a larger number of complex variables and to multiple integrals.

Remark 1. Let us consider a surface S of singularities with points satisfying $g(c,\xi)=0$, as described in Lemma 2A, and let $(c',\xi')\epsilon S$. Let us continue $\omega(c,\xi)$ around the point (c',ξ'). Then the new branch of the function ω, which is obtained by such a continuation, also has singularities on the surface S. Moreover, the singularities associated with endpoints of integration are the same for the two branches of ω. (This fact was implied in the statement of Lemma 2A: if ω is singular on S, then the variation of (c,ξ) subject to the condition $g(c,\xi)=0$ is to be understood as a limiting process, which may involve several branches of ω.) The above fact can be understood from Fig. 8; a continuation of ω as described above implies a displacement of the singularities which are near coincidence, and of the contour, but the essential aspects of the figure would remain unchanged.

Remark 2. We see from Lemma 1A that the entire singular part of the function ω at the singularity $c=c_0$ is obtained by integrating $f(z,c)$ in the neighborhood of one, or possibly a few, points.

Remark 3. We make here one observation regarding the singularities of multiple integrals. The first integration, say over α, has singularities which are associated with neighborhoods of points $\alpha_1, \cdots, \alpha_k$. In the next integration we may expect to find coincident singularities where one singularity is associated with $\alpha=\alpha_i$, and the other, with $\alpha=\alpha_j\neq\alpha_i$. However, such coincident singularities do not lead to a singularity of the integral: We may write the multiple integral as a sum of two terms, where the first includes integration in a neighborhood of α_i, and the other, in a neighborhood of α_j. Neither of the two terms can have a singularity arising from the coincidence mentioned in the foregoing, and so the sum cannot be singular.

A Sufficient Condition for Singularities

We do not consider in this paper the general question whether the fulfillment of one of the two conditions of Lemma 1A is sufficient for the existence of a singularity, or else what additional conditions must be imposed. However, we give for reference the theorem which was used in I and II for the determination of singularities. This theorem has also been used by a number of other authors, but no published proof is known to us. This theorem as stated is applicable to all the Feynman amplitudes discussed in Appendix B, but a more general formulation can be given.

Theorem 1. Let a bounded region V of integration in the Euclidean n space be given. Let $g(u_1,\cdots,u_n)\equiv g(\mathbf{u})$, $h(\mathbf{u})$, and $k(\mathbf{u})$ be three real continuous functions in V such that

$$g(\mathbf{u})+zh(\mathbf{u})>0 \quad \text{and} \quad k(\mathbf{u})>0, \tag{A.2}$$

whenever $\mathbf{u}\epsilon V$ and $0<z<\delta$, and such that $g(\mathbf{u})=0$ for some $\mathbf{u}\epsilon V$. Let $p>0$ and let $[g(\mathbf{u})+zh(\mathbf{u})]^p>0$ for $\mathbf{u}\epsilon V$, $0<z<\delta$. Then the function

$$G(z)=\int_V \frac{k(\mathbf{u})d\tau_u}{[g(\mathbf{u})+zh(\mathbf{u})]^p} \tag{A.3}$$

is singular at $z=0$.

Proof. Let us first observe that $g(\mathbf{u})\geqq 0$ for $\mathbf{u}\epsilon V$, and that the sets

$$V_0=\{\mathbf{u}\epsilon V: g(\mathbf{u})=0\}, \quad W_0=\{\mathbf{u}\epsilon V: h(\mathbf{u})\leq 0\} \tag{A.4}$$

are closed and disjoint. These facts imply that $G(z)$ is regular for $0<z<\delta$ and for z with $\operatorname{Im} z\neq 0$.[17] Let $\epsilon>0$, and let

$$V_{1\epsilon}=\{\mathbf{u}\epsilon V: g(\mathbf{u})<\epsilon\}, \quad V_{2\epsilon}=\{\mathbf{u}\epsilon V: g(\mathbf{u})\geq\epsilon\}. \tag{A.5}$$

The set V_0 is nonempty, and it follows that $V_{1\epsilon}$ has a positive measure. We may write $G=G_{1\epsilon}+G_{2\epsilon}$, where

$$G_{j\epsilon}(z)=\int_{Vj\epsilon} \frac{k(\mathbf{u})d\tau_u}{[g(\mathbf{u})+zh(\mathbf{u})]^p}, \quad j=1,2. \tag{A.6}$$

The function $G_{2\epsilon}$ is regular at $z=0$, and we shall examine the function $G_{1\epsilon}$ more closely. The fact that the sets V_0 and W_0 are closed and disjoint implies that for sufficiently small ϵ there exists $m>0$ such that

$$h(\mathbf{u})\geq m \quad \text{for} \quad \mathbf{u}\epsilon V_{1\epsilon}. \tag{A.7}$$

Let λ satisfy $0<\lambda<\frac{1}{2}\delta$; $G_{1\epsilon}(z)$ has a power series

[17] A detailed proof of this fact has been given by Taylor (see work cited in footnote 8, Appendix). An intuitive argument depends on the observation that for such z the denominator in the integral of Eq. (A.3) does not vanish.

expansion around λ,[18]

$$G_{1\epsilon}(z)=\sum_{n=0}^{\infty}(-1)^n\beta_n(z-\lambda)^n, \tag{A.8}$$

where

$$\beta_n=(-1)^nG_{1\epsilon}{}^{(n)}(\lambda)/n! \tag{A.9a}$$

$$=\frac{p\Gamma(n+p)}{n(n-1)!\Gamma(p+1)}$$

$$\times\int_{V_{1\epsilon}}\frac{k(\mathbf{u})d\tau_u}{[g(\mathbf{u})+\lambda h(\mathbf{u})]^p\{[g(\mathbf{u})/h(\mathbf{u})]+\lambda\}^n}. \tag{A.9b}$$

We construct numbers α_n such that $\alpha_n\leq\beta_n$ by taking the maximum values of $[g(\mathbf{u})/h(\mathbf{u})]+\lambda$ and by omitting the factor $\Gamma(n+p)/(n-1)!\Gamma(p+1)\geq 1$

$$\alpha_n=\frac{p}{n[(\epsilon/m)+\lambda]^n}\int_{V_{1\epsilon}}\frac{k(\mathbf{u})d\tau_u}{[g(\mathbf{u})+\lambda h(\mathbf{u})]^p}. \tag{A.10}$$

The power series

$$\sum_{n=0}^{\infty}(-1)^n\alpha_n(z-\lambda)^n \tag{A.11}$$

has the radius of convergence $(\epsilon/m)+\lambda$ (note that $\lim_{n\to\infty}n^{1/n}=1$), and our argument is valid for any $\epsilon>0$. It follows that a power series for $G(z)$ around the point λ must have a radius of convergence r not greater than λ. On the other hand, our previous remark about the regularity of $G(z)$ implies that $r\geq\lambda$. Thus $r=\lambda$, and this conclusion is valid whenever $0<\lambda<\frac{1}{2}\delta$. The existence of a singularity of $G(z)$ at $z=0$ now follows.

B. On the Singularities of Certain Feynman Amplitudes

We consider now the nth order Feynman amplitude associated with the diagram consisting of n external momenta joined by a single closed loop and with no other internal lines, as in Fig. 10. We show in this appendix that all the singularities of such an amplitude, considered as a function of the invariants, lie on hypersurfaces which can be found by setting appropriate determinants of invariants equal to zero. This result for the vertex function, and for certain singularities of the four-point function, was obtained in reference 2 and in II, respectively. [The hypersurface $\Phi=0$ of work cited in footnote 2, Appendix III, is precisely the hypersurface $K_4=0$, see Eq. (2.3), if the variables are properly identified.] We also give in this appendix one important property of such determinants.

Let us define for $1\leq i<j\leq n$

$$p_{ij}=p_{i,i+1}+p_{i+1,i+2}+\cdots+p_{j-1,j}. \tag{B.1}$$

[18] For needed facts from the theory of functions see, e.g., Titchmarsh, work cited in footnote 13, especially Chapters I and VII.

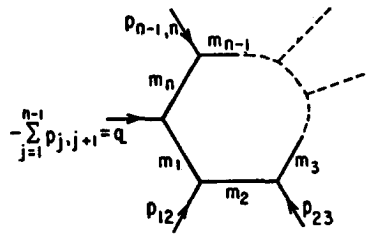

FIG. 10. Feynman diagram with a single closed loop.

The amplitude M_n associated with the diagram of Fig. 10 can be written as follows[11]:

$$M_n=(\text{const.})\int_0^1 d\alpha_1\cdots\int_0^1 d\alpha_n\frac{\delta(1-\alpha_1-\cdots-\alpha_n)}{D_0{}^{n-2}}, \tag{B.2}$$

where

$$D_0=\sum_{i=1}^{n}\alpha_im_i{}^2-\sum_{i<j}\alpha_i\alpha_jp_{ij}{}^2. \tag{B.3}$$

We introduce quantities y_{ij} as in II

$$p_{ij}{}^2=m_i{}^2+m_j{}^2-2m_im_jy_{ij}\quad\text{for}\quad i<j, \tag{B.4a}$$

$$y_{ji}=y_{ij},\quad y_{ii}=1. \tag{B.4b}$$

We further define x_k by

$$x_k=\alpha_km_k\Big/\sum_{j=1}^{n}\alpha_jm_j. \tag{B.5}$$

If we require that $\sum\alpha_i=1$, then we can find the inverse transformation

$$\alpha_k=\frac{x_k}{m_k}\Big/\sum_{j=1}^{n}\frac{x_j}{m_j}. \tag{B.6}$$

In terms of the new variables, D_0 takes the following form (we again use the condition $\sum\alpha_i=1$):

$$D_0=D/\{\textstyle\sum(x_j/m_j)\}^2, \tag{B.7}$$

where

$$D=\sum_{i=1}^{n}x_i{}^2+2\sum_{i<j}x_ix_jy_{ij}=\sum_{i,j=1}^{n}y_{ij}x_ix_j. \tag{B.8}$$

The existence of the inverse transformation (B.6) implies that the transformation has a Jacobian $J\neq 0$.[19] We now obtain

$$M_n=(\text{const.})\int_0^1 dx_1\cdots\int_0^1 dx_n$$

$$\times\frac{\{\sum(x_k/m_k)\}^{2(n-2)}}{J}\frac{\delta(1-\sum x_k)}{D^{n-2}}. \tag{B.9}$$

According to Appendix A, we may have a singularity if in the integration over each variable x_i the integrand

[19] The denominators in Eqs. (B.5) and (B.6) need not be real and positive since it may be necessary to deform the contours. However, unless the zeros of D result in a singularity of M_n, we may always choose such contours that the denominators are different from zero, and then $J\neq 0$.

has coincident singularities, or if the integrand is singular at one endpoint (only $x_i=0$ is relevant, as we see by continuation from the region where each $y_{ij}>1$). We say, as in Sec. 3, that a given singularity is of type (E^kC^{n-k-1}) if in the $(n-1)$ fold integral endpoint singularities occur k times, and coincident singularities, $n-k-1$ times.

Theorem 2. The singularities of M_n which are of type (C^{n-1}) lie on the hypersurface $\det(y_{ij})=0$. The singularities of M_n which are of type (E^kC^{n-k-1}) and are associated with the boundary $x_{i_1}=\cdots=x_{i_k}=0$ lie on the hypersurface $\det(v_{ij})=0$, where (v_{ij}) is the $(n-k)\times(n-k)$ principal minor of (y_{ij}) obtained from (y_{ij}) by deleting rows and columns with indices $i_1, \cdots, i_k$.

For the proof of the theorem we need the following fact regarding quadratic polynomials. Let

$$q(\beta_0,\cdots,\beta_n)=\sum_{i,j=0}^{n}\alpha_{ij}\beta_i\beta_j, \tag{B.10}$$

where $\alpha_{ij}=\alpha_{ji}$. For inhomogeneous polynomials we set $\beta_0=1$. Let us define

$$R(\beta_j)q=B_j^2-4A_jC_j, \tag{B.11}$$

where $q=A_j\beta_j^2+B_j\beta_j+C_j$, and where A_j, B_j, and C_j are independent of β_j.

Lemma 1B. Let q be given by Eq. (B.10) with $\beta_0=1$. Let us write

$$R(\beta_{i+1})R(\beta_{i+2})\cdots R(\beta_n)q=A_i\beta_i^2+B_i\beta_i+C_i. \tag{B.12}$$

Then

$$R(\beta_1)R(\beta_2)\cdots R(\beta_n)q=(-1)^{n(n+1)/2}2^{n(n+1)}\times A_n{}^{n-1}A_{n-1}{}^{n-2}\cdots A_2\det(\alpha_{ij}). \tag{B.13}$$

A proof by induction is straightforward.

Now let us prove the first part of the theorem. Elimination of the δ function in Eq. (B.9) by integration over x_n gives

$$D=\sum_{i,j=0}^{n-1}u_{ij}x_ix_j, \tag{B.14}$$

where $x_0=1$ and (u_{ij}) is a matrix such that $\det(u_{ij})=\det(y_{ij})$. The integral over x_{n-1} can have a (C^1) singularity only if $R(x_{n-1})D=0$. Similarly, the integral over x_{n-2} can have a (C^1) singularity only if the (C^1) singularities of the integrand are coincident (see Remark 3 of Appendix A), or if $R(x_{n-2})R(x_{n-1})D=0$. We continue this process; if the coefficient of x_i^2 vanishes at a certain point, then the singularity of M_n is not of type (C^{n-1}) and our hypothesis is contradicted. The first part of the theorem follows now from the lemma. The second part follows from the first if we observe that the problem for the second part is formally the same as the problem for the first part, aside from the number of variables. This completes the proof.

A determinant of a symmetric matrix, such as described in Theorem 2, is a quadratic in each of the invariants. It may be useful to know the discriminant of this quadratic (e.g., to find the tangents which are parallel to the coordinate axes, as was done in Sec. 2.) We now determine these discriminants.

We start with the Jacobi ratio theorem for determinants.[20]

Theorem. Let (a_{ij}) be a nonsingular $n\times n$ matrix. Then the determinant of any minor of (a_{ij}) divided by the determinant of the complementary minor of the inverse matrix (b_{ij}) equals $\det(a_{ij})$.

In particular, let us assume (without loss of generality) that the minor of (a_{ij}) is defined by the last $n-r$ rows and columns. We know that $b_{pq}=A_{pq}/\det(a_{ij})$, where A_{pq} is the cofactor of the p,q entry of (a_{ij}). Then the foregoing theorem asserts that

$$\det[(a_{kl})^{k,l>r}]\Big/\det\left[\left(\frac{A_{pq}}{\det(a_{ij})}\right)^{p,q\le r}\right]=\det(a_{ij}), \tag{B.15}$$

or

$$\{\det[(a_{kl})^{k,l>r}]\}\{\det(a_{ij})\}^{r-1}=\det[(A_{pq})^{p,q\le r}]. \tag{B.16}$$

We now consider a symmetric matrix (y_{ij}). (The condition $y_{ii}=1$ is not necessary for us. Neither is the condition that (y_{ij}) be nonsingular, since Eq. (B.16) is valid, by continuity, for singular matrices as well.) Let Y_{pq} be the cofactor of the p,q entry of (y_{ij}). The symmetry of (y_{ij}) implies that $Y_{pq}=Y_{qp}$. We also write $K_p{}^{(n)}=Y_{pp}$, to conform to the previous notation. Equation (B.16) with $r=2$ now states

$$\det[(y_{kl})^{k,l>2}]\det(y_{ij})=K_1{}^{(n)}K_2{}^{(n)}-Y_{12}{}^2. \tag{B.17}$$

We assume that the quantity y_{12} is a variable, distinct from all other y_{ij} (except y_{21}). Then the determinant (y_{ij}) is a quadratic in y_{12}, and upon writing

$$\det(y_{ij})=ay_{12}{}^2+by_{12}+c, \tag{B.18}$$

we easily see that

$$a=-\det[(y_{kl})^{k,l>2}],\quad Y_{12}=-(ay_{12}+\tfrac{1}{2}b). \tag{B.19}$$

Equations (B.17)–(B.19) now give at once $b^2-4ac=4K_1{}^{(n)}K_2{}^{(n)}$. These considerations of course apply to arbitrary y_{pq}, and we obtain the following theorem:

Theorem 3. Let (y_{ij}) be a symmetric matrix. Let $K_l{}^{(n)}$ be the cofactor of the l,l entry of (y_{ij}). Let y_{pq}, $p<q$, be a variable distinct from all other y_{ij} (except y_{qp}), and let us write $\det(y_{ij})=Ay_{pq}{}^2+By_{pq}+C$. Then

$$B^2-4AC=4K_p{}^{(n)}K_q{}^{(n)}. \tag{B.20}$$

[20] H. W. Turnbull, *The Theory of Determinants, Matrices, and Invariants* (Blackie and Son Ltd., London, 1945), 2nd edition, p. 77.

C. Dependence of F on External Masses

Källén and Wightman[2] have studied the analytic properties of the vertex function as a function of all the kinematical invariants of the process, with the invariants complex. In case of the function F, the invariants include the external masses in addition to those considered in the main part of this paper.[21] Treating all of these invariants as complex would increase the number of complex variables to six, and these may be taken as just the y_{ij} if the internal masses are held constant. We may point out that Theorem 2 (of Appendix B) applies to all the invariants of a given process, and in principle our method can also be applied to the study of F as a function of six complex variables. However, geometric complications increase rapidly with the number of dimensions. While we do not make here such a detailed study of F, we discuss for completeness the following aspects of the dependence of F on external masses: the transitions between the various cases of Sec. 3, and the analytic continuation of F to arguments $y_{ij}>1$; cf. the inequalities (1.6).

Transitions Between the Various Cases

These transitions are degenerate in the sense that some of the lines $y_{13}=\pm 1$, $L_{13}{}^{(j)}$, and $y_{24}=\pm 1$, $L_{24}{}^{(k)}$ coincide. We now describe those degenerate cases in which lines with singularities coincide, and we assume that the inequalities (1.6) hold. We give only the results. There are four types of coincidences to be considered.

(1) $\Theta\neq 2\pi$, and the sum of two adjacent angles is π. This is the transition between cases (i) and (ii) if $\Theta<2\pi$. Here, $L_{13}{}^{(1)}=-1$ or $L_{24}{}^{(1)}=-1$, and the line $y_{ik}=-1=L_{ik}{}^{(1)}$ has the property that it is not tangent to Γ, and is an asymptote which is approached at both $-\infty$ and ∞ from the region $y_{ik}<-1$.

(2) $\Theta=2\pi$, and the sum of any two adjacent angles is different from π. This is the transition between cases (ii) and (iii). Here $L_2{}^+=L_4{}^+$ and $L_1{}^+=L_3{}^+$. The curve Γ crosses the lines $y_{13}=L_2{}^+$, $y_{24}=L_1{}^+$ at their intersection $(y_{13},y_{24})=(L_2{}^+,L_1{}^+)$. The branches Γ_1 and Γ_5 are connected through the point $(L_2{}^+,L_1{}^+)$, and the surface Σ_1 does not exist. This configuration is illustrated in Fig. 11.

(3) $L_2{}^+=L_4{}^+=-1$ or $L_1{}^+=L_3{}^+=-1$ (then $\Theta=2\pi$). Let us assume for definiteness that $L_2{}^+=L_4{}^+=-1$. Then Γ consists of the line $y_{13}=-1$ and of a third degree curve. If both sets of equations hold then Γ consists of the two lines $y_{13}=-1$, $y_{24}=-1$, and of a hyperbola. This configuration is analogous to that of the equal mass case discussed in II, where we have $L_2{}^-=L_4{}^-=1$, $L_1{}^-=L_3{}^-=1$.

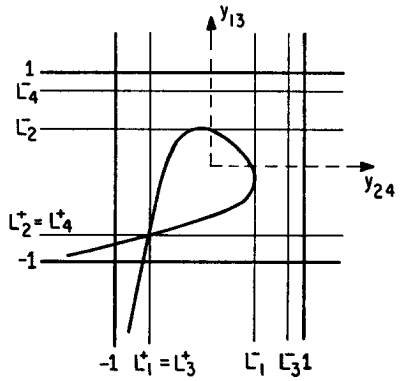

FIG. 11. The curves Γ_1 and Γ_5 when $\Theta=2\pi$.

(4) $\Theta=2\pi+2\min(\theta_{12},\theta_{23},\theta_{34},\theta_{14})$; this is the transition between cases (iii) and (iv). Here, $L_{13}{}^{(2)}=L_{13}{}^{(3)}$, $L_{24}{}^{(2)}=L_{24}{}^{(3)}$, and Γ_5 shrinks to a point.

These degenerate cases indicate the continuity that is encountered in the transitions between the various cases of Sec. 3. The singularities in these degenerate cases can be readily determined. Moreover, an examination of these degenerate cases can guide us in determining which properties of F can be carried over from one case of Sec. 3 to another.

Continuation of F to Arguments $y_{ij}>1$

If the external masses are considered to be complex variables, then the singularities of F are restricted to the hypersurfaces given by $y_{ij}=\pm 1$, in addition to those given by Eqs. (2.4a-d) and (2.6). We consider now a specific pair of indices (i,j). We conclude, as in Sec. 3, that F is singular if $y_{ij}=-1$, but if $y_{ij}=1$ it does not have a singularity of type (E^2C^1) (and associated with the boundary $x_k=x_l=0$, i, j, k, l all different). Moreover, if $y_{ij}\geq 1$ then a vertex function $F_v(y_{ik})$ for which one of the mass parameters is y_{ij} does not have a type (C^2) singularity on the boundary of the physical sheet.[22]

Now let us consider again the space of two complex variables, y_{13} and y_{24}. We see from the preceding paragraph that for $y_{ij}\geq 1-\epsilon$ (ϵ positive and sufficiently small), the only singularities of $F(y_{13},y_{24})$ with locations which vary with y_{ij} are those on the surface Σ. We obtain the locations of these singular points by analytic continuation from $y_{ij}=1-\epsilon$ of the expressions defining these points. In particular, the representation (4.1) is valid for all $y_{ij}\geq 1-\epsilon$ if it is valid for $y_{ij}=1-\epsilon$. (In one exceptional case, where the sum of the three angles other than θ_{ij} equals 2π, we must continue from the value $y_{ij}=1+\epsilon$, and the representation (4.1) is valid for all $y_{ij}\geq 1$.)

[21] The analytic dependence of the scattering amplitude on the external masses has been used in the formal proofs of dispersion relations [Bogoliubov, Medvedev, and Polivanov, lecture notes translated at the Institute for Advanced Study, Princeton, New Jersey, 1956; and H. J. Bremermann, R. Oehme, and J. G. Taylor, Phys. Rev. **109**, 2178 (1958)]. The singularities of the absorptive part which make these proofs applicable only to limited momentum transfers correspond to the singularities of the curve Γ_1 in case of the fourth order perturbation theory. (The singularities of Γ_1 can also be considered as singularities of a mass variable.) See references 3 and 8, and Sec. 4.

[22] See I and Appendix A of II. We define the physical sheet of $F_v(y_{ik})$ by $-\pi<\arg(y_{ik}-1)<\pi$, in analogy with the definition (1.8).

D. Behavior of F Near Singularities

In this appendix we determine the types of singularities which F exhibits on the various surfaces.[23] We show that, given a surface of singularities with the equation $\sigma=0$ and a point (y_{13}^0,y_{24}^0) lying on this surface, F is ordinarily of the form

$$F(y_{13},y_{24})=A(y_{13},y_{24})+B(y_{13},y_{24})f(\sigma), \qquad (D.1)$$

where the functions A and B are analytic in a neighborhood of (y_{13}^0,y_{24}^0), B is not identically zero, and $f(z)$ is one of the functions $z^{\frac{1}{2}}$, $\log z$, $z^{-\frac{1}{2}}$. If the surface $\sigma=0$ belongs to one of the degenerate cases of Appendix C, or if more than one surface of singularities passes through (y_{13}^0,y_{24}^0), then F is given by a product of factors, each of which is such as in the rhs of Eq. (D.1); e.g.,

$$F=A+B_1f_1(\sigma_1)+B_2f_2(\sigma_2)+B_3f_1(\sigma_1)f_2(\sigma_2) \qquad (D.2)$$

[cf. Eq. (D.12c)]. We note that Eqs. (D.1) and (D.2) establish the existence of singularities of F on the various surfaces of singularities described in Sec. 3.

We do not attempt to give in this appendix a systematic presentation of the subject; we only illustrate some useful techniques by means of one example. These techniques suffice to establish the forms (D.1) or (D.2) for singularities of various integrals, and in particular, for all singularities of F.

We now consider F in a neighborhood of a point (y_{13}^0,y_{24}^0), which lies on the surface of singularities $y_{13}=L_2^+$; we assume that (y_{13}^0,y_{24}^0) does not lie on any other surface of singularities, and that $L_2^+\neq -1,L_4^+$. We start with Eq. (1.3) for F, and we eliminate the δ function by integration over x_4. We next consider the integral over x_3 and its singularities of type (C^1); the result of the integration is of the form

$$\int_0^{1-x_1-x_2}\frac{dx_3}{(a_3x_3^2+b_3x_3+c_3)^2}=\frac{2a_3\log 1}{Q^{\frac{1}{2}}}+\mathfrak{R}, \qquad (D.3)$$

where we set, see Eq. (1.4)

$$D=a_3x_3^2+b_3x_3+c_3, \quad Q=b_3^2-4a_3c_3, \qquad (D.4)$$

and where $\mathfrak{R}$ is a function of x_1, x_2, and of the y_{ij}, which is regular except for those values of the arguments which result in a singularity of the integrand at an endpoint of integration. Such values, however, do not lead to a singularity at the point (y_{13}^0,y_{24}^0) specified above.

The term $2a_3(\log 1)/Q^{\frac{1}{2}}$ is singular at $Q=0$ if and only if $\log 1\neq 0$. To determine $\log 1$, we have to examine the branches of the logarithm. When $Q=0$ and the coincident singularities of the integrand lie on the same side of the contour, or are separated from the contour, then necessarily $\log 1=0$. Let us consider now an analytic continuation such as shown in Fig. 9(a). At a singularity of type (E^1) the argument of the logarithm is 0 or 1/0, and analytic continuation around such a point leads to a different branch of the logarithm. Thus, for coincident singularities of the integrand which approach the contour from opposite sides, $\log 1=\pm 2\pi i$, and we have a singularity of the integral.

The next integration is over x_2. Integration of the function $\mathfrak{R}$ in Eq. (D.3) is complicated, but to determine the singularity of F at (y_{13}^0,y_{24}^0) we only need to consider the term $2a_3(\log 1)/Q^{\frac{1}{2}}$. We obtain

$$\int_0^{1-x_1}\frac{dx_2}{Q^{\frac{1}{2}}}=\left[\frac{2(2a_2x_2+b_2)}{(b_2^2-4a_2c_2)(a_2x_2^2+b_2x_2+c_2)^{\frac{1}{2}}}\right]_{x_2=0}^{1-x_1}, \qquad (D.5)$$

where we set

$$Q=a_2x_2^2+b_2x_2+c_2. \qquad (D.6)$$

The singularities in which we are interested come from the term in rhs of Eq. (D.5) associated with the endpoint $x_2=0$.

We are left with an integral over x_1. We know from Remark 2 of Appendix A that the entire singular part of F comes from integrating in a neighborhood of a point $x_1=x_1^0$ (of course, similar conclusions are valid for the two previous integrations, over x_3 and over x_2). In a sufficiently small neighborhood of x_1^0, the factor $(b_2^2-4a_2c_2)^{-1}$ of Eq. (D.5) is regular; this is implied by the type of singularity of F that we are investigating. Thus it suffices to consider only the following expression:

$$\sum_{n=0}^{\infty}\alpha_n\int_{x_1^0-\eta}^{x_1^0+\eta}dx_1\frac{(x_1-x_1^0)^n}{(a_1x_1^2+b_1x_1+c_1)^{\frac{1}{2}}}, \qquad (D.7)$$

where

$$\frac{2b_2}{b_2^2-4a_2c_2}=\sum_{n=0}^{\infty}\alpha_n(x_1-x_1^0)^n, \qquad c_2=a_1x_1^2+b_1x_1+c_1. \qquad (D.8)$$

The justification of our procedure presents no difficulties.[18] We may now determine the singularity of the expression (D.7) by considerations analogous to those used in the discussion of the integral over x_3.

We list below the expressions for F of the form (D.1) which apply to the various singularities (except at intersections of surfaces and in the degenerate cases). The functions A_i and B_i are analytic functions of y_{13} and y_{24} at the points under consideration.

For singularities of type (E^2C^1) we have

$$F=A_1+B_1(y_{13}+1)^{\frac{1}{2}}, \qquad (D.9a)$$

$$F=A_2+B_2(y_{24}+1)^{\frac{1}{2}}. \qquad (D.9b)$$

[23] Some results regarding the behavior of Feynman amplitudes near singularities have also been given by Eden (footnote 10), by L. D. Landau [Nuclear Physics 13, 181 (1959)], and by Mandelstam (footnote 4).

For singularities of type (E^1C^2) we have

$$F=A_3+B_3\log(y_{13}-L_j^+), \tag{D.10a}$$

$$F=A_4+B_4\log(y_{24}-L_k^+). \tag{D.10b}$$

For singularities of type (C^3) we have

$$F=A_5+B_5[\Delta(y_{13},y_{24})]^{-\frac{1}{2}}. \tag{D.11}$$

We also give the analogous forms for the vertex function $F_v(y_{13})$, where the external mass parameters are y_{12} and y_{23}. For the singularities of types (E^1C^1) and (C^2) we have, respectively,

$$F_v=A_{1v}+B_{1v}(y_{13}+1)^{\frac{1}{2}}, \tag{D.12a}$$

$$F_v=A_{2v}+B_{2v}\log(y_{13}-L_4^+). \tag{D.12b}$$

If $\theta_{12}+\theta_{23}=\pi$, $L_4^+=-1$, then we have

$$F_v=A_{3v}+B_{13v}(y_{13}+1)^{\frac{1}{2}}+B_{23v}\log(y_{13}+1)+B_{33v}(y_{13}+1)^{\frac{1}{2}}\log(y_{13}+1). \tag{D.12c}$$

It should be pointed out that the functions A_{3v} and B_{i3v} in Eq. (D.12c) may have singularities in the y_{13} plane, but the function F_v has no singularities other than at $y_{13}=-1$.