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Singular Integral Equations*

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The integral equation

$$P\int_c \frac{K(\zeta',\zeta)}{\zeta'-\zeta}\varphi(\zeta')\,d\zeta' = h(\zeta)\varphi(\zeta) + f(\zeta)$$

is shown to have simple solutions obtained by standard and elementary methods if h and K have appropriate analytic properties.

I. INTRODUCTION

RECENTLY, Peters[1] has given a method to solve integral equations with kernels[2] $PK(\zeta'-\zeta)/(\zeta'-\zeta)$, where the "given" functions satisfy certain conditions. Two claims are made:

(i) In the case most discussed in the literature—K depending on only one of its two arguments—the method is simpler than the "standard"[3] one.

(ii) The method can be used to solve some equations to which the standard method is inapplicable.

The first claim is probably a matter of personal taste. Thus, the author is able to solve the problem without solving an associated Riemann–Hilbert problem. However, with the conditions imposed on the given functions the solution of the Riemann–Hilbert problem is completely elementary. It can be written down by inspection.

Of somewhat greater interest is the second claim. Due to the great variety of applications of integral equations with kernels of the indicated form, any enlargement of the class of exactly soluble problems would be of great importance. Unfortunately, as we see later, the standard method does indeed yield an exact solution for the equations discussed by Peters. Indeed, the solution is obtained possibly even more directly. The essential point is that it is not the method which yields a simple result but rather the very stringent conditions of analyticity which are imposed on the "given" functions.

In Sec. II we discuss a generalized form of the problem posed by Peters. Using the standard method this is reduced to a regular Fredholm equation. *In general* this is as far as we can go analytically. However, it is shown in Sec. III that if Peters' additional conditions are satisfied this Fredholm equation can be solved—and by elementary methods.

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[1] A. S. Peters, Commun. Pure Appl. Math. **XVIII**, 129 (1965). I am indebted to Professor C. L. Dolph for calling my attention to this article.

[2] Here and throughout this article P is to remind us that principal values are to be used when integrating the kernels.

[3] See, for example, N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff Ltd., Gröningen, The Netherlands 1953). To be precise we mean by "standard" the method described in Chap. 6 of this reference. It is introduced with the words: "This method is the one most frequently used up to the present; it was suggested (in different particular applications) by the founders of the theory of singular equations—Poincaré and Hilbert." Apparently Peters had a different definition of "standard" method in mind.

II. FORMULATION OF THE PROBLEM

We consider the equation for the unknown function φ

$$P\int_c \frac{K(\zeta',\zeta)\varphi(\zeta')\,d\zeta'}{\zeta'-\zeta} = h(\zeta)\varphi(\zeta) + f(\zeta). \tag{1}$$

Here:

(i) c is a closed contour dividing the complex plane into an interior region D_+ and an exterior region D_-. The integration is taken such that D_+ always lies to the left of c;

(ii) The functions h, f, K satisfy Hölder conditions on c;

(iii) $h(\zeta) \pm i\pi K(\zeta) \neq 0$ for ζ on c; (2)

(iv) $K(\zeta) \not\equiv 0$ for ζ on c; (3a)

where

$$K(\zeta) \equiv K(\zeta,\zeta). \tag{3b}$$

A formulation of the standard method is the following: Write

$$K(\zeta',\zeta) = \{K(\zeta',\zeta) - K(\zeta')\} + K(\zeta'). \tag{4}$$

Then Eq. (1) can be rewritten in the form

$$P\int_c \frac{\psi(\zeta')\,d\zeta'}{\zeta'-\zeta} = \frac{h(\zeta)}{K(\zeta)}\psi(\zeta) + H(\zeta), \tag{5}$$

where we have introduced the notations

$$\begin{aligned}\psi(\zeta) &= K(\zeta)\varphi(\zeta),\\ H(\zeta) &= f(\zeta) + g(\zeta),\end{aligned} \tag{6}$$

and

$$g(\zeta) = \int_c \frac{[K(\zeta') - K(\zeta',\zeta)]}{\zeta'-\zeta}\varphi(\zeta')\,d\zeta'. \tag{7}$$

We proceed as if $H(\zeta)$ in Eq. (5) were known. Let

$$N(z) = \int_c \frac{\psi(\zeta')\,d\zeta'}{\zeta'-z}. \tag{8}$$

Then, by the Plemelj formulas[3] we obtain

$$\begin{aligned}\psi(\zeta) &= \frac{N^+(\zeta) - N^-(\zeta)}{2\pi i},\\ P\int_c \frac{\psi(\zeta')\,d\zeta'}{\zeta'-\zeta} &= \frac{N^+(\zeta) + N^-(\zeta)}{2},\end{aligned} \tag{9}$$

where $N^\pm$ are the boundary values of $N(z)$ as we approach c from D_+ or D_-, respectively. Using Eq. (9) we find that Eq. (5) can be expressed as the relation between these boundary values

$$N^+(\zeta) - r(\zeta)N^-(\zeta) = 2\pi i K(\zeta)H(\zeta)/[h(\zeta) - \pi i K(\zeta)], \tag{10}$$

where

$$r(\zeta) = h(\zeta) + \pi i K(\zeta)/[h(\zeta) - \pi i K(\zeta)]. \tag{11}$$

Now let us suppose we can find a function $Y(z)$ with the properties[4]

(i) $Y(z) \equiv Y^+(z)$ is analytic and nonzero in D_+,

(ii) $Y(z) \equiv Y^-(z)$ is analytic and nonzero in D_-,

(iii) $Y^+(\zeta)/Y^-(\zeta) = r(\zeta)$, $\zeta \in c$, (12)

(iv) $Y(z) \backsim z^{-m}$ as $|z| \to \infty$.

With such a function, Eq. (10) becomes

$$\frac{N^+(\zeta)}{Y^+(\zeta)} - \frac{N^-(\zeta)}{Y^-(\zeta)} = \frac{-2\pi i K H}{h - \pi i K}\frac{1}{Y^+}. \tag{13}$$

Enumerating the analytic properties of the various functions involved and using Eq. (13) we conclude (by Liouville's theorem) that

$$\frac{N(z)}{Y(z)} + \int_c \frac{K(\zeta')H(\zeta')}{h(\zeta') - \pi i K(\zeta')}\frac{d\zeta'}{Y^+(\zeta')(\zeta'-z)} = F(z) \tag{14}$$

is a polynomial of order $m-1$.

Thus, if $m = 0$, $N(z)$ is uniquely determined. If $m > 0$, $N(z)$ is determined up to this polynomial. Finally, $m < 0$, an $N(z)$ exists if and only if additional conditions of the form

$$\int_c \frac{K(\zeta')H(\zeta')(\zeta')^i\,d\zeta'}{(h - \pi i K)Y^+} = 0. \tag{15}$$

In all three cases the following arguments are essentially the same. *For simplicity* we here limit ourselves to describing the case $m = 0$.

Then

$$N(z) = -Y(z)\int_c \frac{K(\zeta')H(\zeta')}{h(\zeta') - \pi i K(\zeta')}\frac{d\zeta'}{Y^+(\zeta')(\zeta'-z)}. \tag{16}$$

From Eq. (9) we then find [using Eq. (12)] that

$$\psi(\zeta) = \frac{h(\zeta)H(\zeta)K}{h^2 + \pi^2K^2} - \frac{Y^+(\zeta)K}{h + \pi i K}P \times \int_c \frac{K(\zeta')H(\zeta')\,d\zeta'}{[h(\zeta') - \pi i K(\zeta')]Y^+(\zeta')(\zeta'-\zeta)}, \tag{17}$$

or using Eq. (6)

$$\varphi(\zeta) = \frac{-hH(\zeta)}{\lambda^2 + \pi^2K^2} - \frac{Y^+(\zeta)}{h + \pi i K} \times P\int_c \frac{K(\zeta')H\,d\zeta'}{[h - \pi i K]Y^+(\zeta')(\zeta'-\zeta)}. \tag{18}$$

Since H involves an integral over φ this is not a

[4] The fact that an explicit integral representation for such a $Y(z)$ exists is of no importance for the considerations of this article.

solution but is rather a regular Fredholm equation for it. In general we cannot find a closed-form solution. (Many properties are, of course, obtainable from this form—e.g., existence of solutions and approximate representations.)

However, in special cases we can construct solutions. The most common such situation discussed in the literature is when $[K(\zeta') - K(\zeta', \zeta)]/(\zeta' - \zeta)$ is a polynomial in the two arguments. In this case, Eq. (18) is an equation with degenerate kernel. The solution is obtained by purely algebraic means.

A second case in which it is trivial to solve Eq. (18) is the situation described by Peters—to which we now turn our attention.

III. SOLUTION SUBJECT TO PETERS' CONDITIONS

Let us suppose that in addition to the conditions (i)–(iv) of Sec. II we also require that $h(\zeta)$, $K(\zeta', \zeta)$ be analytic in $D_+ + c$. (For K we require this in both variables.)

Now many simplifications occur. For example, to determine $Y(z)$ we note that $r(z)$ is meromorphic in D_+. It has poles at the zeros of $h - \pi iK$ and zeros at the zeros of $h + \pi iK$. Assuming for simplicity that these are all simple and labeling those of $h - \pi iK$ by β_k, $k = 1, 2, \cdots, n_2$ and those of $h + \pi iK$ by α_i, $i = 1, 2, \cdots, n_1$ we see that a suitable $Y_+(\zeta)$ is

$$Y_+(\zeta) = \frac{h + \pi iK}{h - \pi iK} \frac{\prod_{k=1}^{n_2} (\zeta - \beta_k)}{\prod_{i=1}^{n_1} (\zeta - \alpha_i)}. \tag{19}$$

From Eq. (12) we then read off that

$$Y_-(\zeta) = \frac{\prod_{k=1}^{n_2} (\zeta - \beta_k)}{\prod_{i=1}^{n_1} (\zeta - \alpha_i)}. \tag{20}$$

The index m is then just

$$n_2 - n_1. \tag{21}$$

Further, we note that it follows from Eq. (7) that $g(\zeta)$ is now analytic in $D_+ + c$. Integrals involving g are then found trivially using Cauchy's theorem and the Plemelj formula. Thus, in Eq. (18) there appears (implicitly) the integral

$$I = P \int_c \frac{K(\zeta')g(\zeta')\, d\zeta'}{[h - \pi iK]Y^+(\zeta')(\zeta' - \zeta)}. \tag{22}$$

Let

$$\mathcal{I} = \int_{c+c_1} \frac{K(\zeta')g(\zeta')\, d\zeta'}{[h - \pi iK]Y^+(\zeta')(\zeta' - \zeta)}. \tag{23}$$

Here, c_1 is taken as a small semicircle around ζ lying in D_+. By the Plemelj formula

$$\mathcal{I} = I - \frac{\pi iK(\zeta)g(\zeta)}{(h - \pi iK)Y^+(\zeta)}. \tag{24}$$

Alternately, by Cauchy's theorem

$$\mathcal{I} = \sum (2\pi i) \quad \text{(residues at poles of the integrand)}. \tag{25}$$

(By our construction these poles are just at the zeros of $h - \pi iK$.) Combining Eqs. (24) and (25) we see that I is evaluated.

From now on let us restrict ourselves to the case when $h \pm \pi iK$ have no zeros in $D_+ + c$.[5] (We emphasize that this is for simplicity and for simplicity only. No complications of principle occur in the general case—but the equations get longer.)

In this case, then,

$$I = \pi iK(\zeta)g(\zeta)/(h + \pi iK), \tag{26}$$

and Eq. (18) becomes

$$\varphi(\zeta') = \frac{-g(\zeta')}{h - \pi iK} - \frac{hf}{h^2 + \pi^2K^2} - \frac{1}{h - \pi iK} P \int_c \frac{K(\zeta'')f(\zeta'')\, d\zeta''}{[h(\zeta'') + \pi iK(\zeta'')](\zeta'' - \zeta')}. \tag{27}$$

This integral equation for φ is trivial to solve. Thus, let us multiply Eq. (27) by $[K(\zeta') - K(\zeta', \zeta)]/(\zeta' - \zeta)$ and integrate ζ' over c. The left-hand side is just $g(\zeta)$. The term on the right proportional to g is identically zero. The remaining terms are *given* functions. Hence g is determined. Returning to Eq. (27) we then see φ is given explicitly.

We find

$$g(\zeta) = -\int_c \frac{f(\zeta')}{h(\zeta') + \pi iK(\zeta')} \frac{[K(\zeta') - K(\zeta', \zeta)]\, d\zeta'}{(\zeta' - \zeta)}. \tag{28}$$

Inserting into Eq. (27) yields

$$\varphi(\zeta) = \frac{-h(\zeta)f(\zeta)}{h^2 + \pi^2K^2} - \frac{1}{h - \pi iK(\zeta, \zeta)} \times P \int_c \frac{K(\zeta', \zeta)f(\zeta')\, d\zeta'}{[h(\zeta') - \pi iK(\zeta', \zeta')](\zeta' - \zeta)}, \tag{29}$$

in agreement with Peters.[1]

IV. EXTENSIONS

Peters[6] has indicated that his method is applicable to various generalizations of Eq. (1). Of

[5] This is, of course, compatible with the earlier restriction $m = 0$.

[6] I am indebted to the referee of this paper for informing me that unpublished notes of Peters exist to this effect.

particular interest are equations of the form

$$\oint_{c:|\zeta'|=1} \frac{K_1(\zeta', \zeta)\phi(\zeta')\,d\zeta'}{(\zeta'^2 - \zeta^2)} = h(\zeta)\phi(\zeta) + f(\zeta). \tag{30}$$

The essential point is that there are now two singular points ζ and $-\zeta$ in the integral. We have not investigated, in general, whether a nontrivial modification of the standard method is necessary.

However, in this connection it may be interesting to consider a particular published[1] example of an equation of this general type.

Consider the equation

$$P \oint_{|\zeta'|=1} \frac{\zeta\phi(\zeta')\,d\zeta'}{(\zeta' - \zeta)(\zeta'\zeta - 1)} = i\lambda\phi(\zeta) + f(\zeta), \tag{31}$$

where $|\zeta| = 1$, $\zeta^2 \neq -1$, and λ is real.

Using the partial fraction decomposition

$$\frac{\zeta}{(\zeta' - \zeta)(\zeta\zeta' - 1)} = \frac{\zeta}{\zeta^2 - 1}\left\{\frac{1}{\zeta' - 1} - \frac{1}{\zeta' - \frac{1}{\zeta}}\right\}, \tag{32}$$

this becomes

$$\frac{\zeta}{\zeta^2 - 1} P\left\{\oint \frac{\phi(\zeta')\,d\zeta'}{\zeta' - \zeta} - \oint \frac{\phi(\zeta')\,d\zeta'}{\zeta' - 1/\zeta}\right\} = i\lambda\varphi(\zeta) + f(\zeta). \tag{33}$$

Greater symmetry is achieved by introducing the reciprocal of the integration variable in the second integral. We find then that the equation is

$$\frac{\zeta}{\zeta^2 - 1} P\left\{\oint \frac{\varphi(\zeta')\,d\zeta'}{\zeta' - \zeta} + \oint \frac{\zeta}{\zeta'} \frac{\varphi(1/\zeta')\,d\zeta'}{\zeta' - \zeta}\right\} = i\lambda\varphi(\zeta) + f(\zeta). \tag{34}$$

Replacing ζ by $1/\zeta$ in Eq. (34) and performing a similar change on the dummy variables gives

$$\frac{\zeta}{\zeta^2 - 1} P\left\{\oint \frac{\varphi(\zeta')\,d\zeta'}{\zeta' - \zeta} + \oint \frac{\zeta}{\zeta'} \frac{\phi(1/\zeta')\,d\zeta'}{\zeta' - \zeta}\right\} = i\lambda\varphi(1/\zeta) + f(1/\zeta). \tag{35}$$

Comparing Eqs. (34) and (35) shows that

$$\varphi\left(\frac{1}{\zeta}\right) = \varphi(\zeta) + \frac{i}{\lambda}\left[f\left(\frac{1}{\zeta}\right) - f(\zeta)\right]. \tag{36}$$

Inserting this expression for $\phi(1/\zeta)$ into Eq. (34) we see that our problem is to solve the equation

$$\frac{\zeta}{\zeta^2 - 1} P \oint \left(1 + \frac{\zeta}{\zeta'}\right) \frac{\varphi(\zeta')\,d\zeta'}{\zeta' - \zeta} = i\lambda\varphi(\zeta) + f(\zeta) + \oint \frac{i}{\lambda} \frac{\zeta}{\zeta'} \frac{[f(\zeta') - f(1/\zeta')]\,d\zeta'}{\zeta' - \zeta}. \tag{37}$$

Now, this is precisely a problem of the form we have been considering. The solution is trivial. The power of the standard method is perhaps indicated by the fact that such an equation can be solved under considerably weakened conditions. Thus, suppose λ is not a constant but is merely required to satisfy a Hölder condition on c. Our argument leading to a slightly modified form of Eq. (37) still holds. The Fredholm equation which then arises is one with a degenerate kernel. To find the solution requires only a little algebra.

V. CONCLUSION

It is hoped that it has been shown that the reason that Eq. (1) is solvable with analyticity conditions on K and f is due to the stringency of these conditions—not the choice of method. The standard method works in a quite straightforward manner.

Some indication as to how strong the analyticity requirement is can be seen if we demand that the inhomogeneous term (f) also be analytic in $D_+ + c$. With our above simplifying assumptions and following the same arguments we readily find the solution to be simply

$$\varphi(\zeta) = -f(\zeta)/[h(\zeta) - \pi i K(\zeta, \zeta)]. \tag{38}$$

Singular Solutions of Certain Integral Equations

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A class of integral equations arising in some idealized plasma problems is discussed. While these do not have solutions in the space of square-integrable functions, they do have such in an appropriate space of generalized functions. Explicit solutions are given in some special cases. It is then shown how these solutions can be used to approximate those for more general problems.

I. INTRODUCTION

IN certain idealized plasma problems one encounters[1] integral equations of the form

$$\int_S G(|\mathbf{r} - \mathbf{r}'|)f(\mathbf{r}')\,dS' = 0, \qquad \mathbf{r} \in S. \tag{1}$$

Here, G denotes the Green's function for the Helmholtz equation, i.e.,

$$(\nabla^2 - \alpha^2)G(\mathbf{r}) = -\delta(\mathbf{r}), \tag{2}$$

where explicitly,

$$G(\mathbf{r}) = e^{-\alpha r}/4\pi r. \tag{3}$$

An even more convenient form is the Fourier integral representation

$$G(\mathbf{r}) = \frac{1}{(2\pi)^3}\int \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}\,d^3k}{k^2 + \alpha^2}. \tag{4}$$

As seen in some examples given below, equations of the form of Eq. (1) have no "classical" solutions—i.e., solutions which are of class L_2. However, it is shown that there are solutions which are generalized functions. (For the idealized physical problems which result in such equations these solutions are quite acceptable.) The essential point seems to be the following: We have a certain complementarity. If the kernel of the equation is sufficiently singular, the solutions can be smooth. Conversely, if the kernel is smooth—as in our examples—the solutions are necessarily singular.

Our program is to exhibit solutions for some rather simple cases. Then it is shown how these results can be used to approximate the solutions of more complicated problems.

In Sec. II we consider the situation where S is a plane strip. While closed forms for the solution of Eq. (1) does not seem possible, we do obtain such for closely related equations. With the insight gained from these results, we are able to find the solution (Sec. IV) when the strip becomes a half-plane.

In Sec. VI we use this to show the existence and asymptotic behavior of the solution to the problem of a large strip. The opposite limiting case of a thin strip is also amenable to analytic treatment and is next discussed. How these results can be used for more general S is illustrated in Sec. VIII, where the case of a circle is considered.

II. FORMULATION OF THE STRIP PROBLEM

We consider Eq. (1) for the case where S is the region

$$a < x < b, \qquad -\infty < y < \infty, \qquad z = 0. \tag{5}$$

The integral over k_z in Eq. (4) is readily done. The resulting integral equation is

$$\int_a^b dx' \int_{-\infty}^{\infty} dy'\, G(x - x', y - y')f(x', y') = 0,$$
$$a < x < b, \qquad -\infty < y < \infty. \tag{6}$$

Here now

$$G(x, y) = \frac{1}{8\pi^2}\int \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}\,d^2k}{(k^2 + \alpha^2)^{\frac{1}{2}}}. \tag{7}$$

Noting that the equation is separable we write

$$f(x, y) = e^{-ik_0 y}f(x) \tag{8}$$

and find for $f(x)$ the equation

$$\int_a^b K(x - x')f(x')\,dx' = 0, \qquad a < x < b, \tag{9}$$

where

$$K(x) = \frac{1}{4\pi}\int_{-\infty}^{\infty} \frac{e^{-ikx}\,dk}{[k^2 + (\alpha^2 + k_0^2)]^{\frac{1}{2}}}. \tag{10}$$

Thus for all k_0 we have a problem of the same form as that with $k_0 = 0$, to which we therefore restrict ourselves.

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[1] S. Drell, H. Foley, and M. Ruderman (private communication).

It may be noted that, except for a numerical factor, $K(x) = K_0(\alpha\,|x|)$, where K_0 is the Bessel function defined by Watson.[2] Actually, however, the most useful property for our purposes is the integral representation [Eq. (101)] itself.

For orientation purposes it is convenient to consider the generalization of Eq. (9) when the kernel $K(x)$ is such that its Fourier transform $\tilde{K}$ is of the form

$$\tilde{K} \sim 1/(k^2 + \alpha^2)^\rho, \qquad \rho \text{ real}, > 0. \tag{11}$$

The motivation is threefold:

(i) As may be seen the cases $\rho = 0$ and $\rho = 1$ are trivial to solve.

(ii) In some sense the case of interest—$\rho = \frac{1}{2}$—is intermediate between these two.

(iii) If α^2 can be considered "large" one might consider as a zeroth approximation to the kernel with $\rho = \frac{1}{2}$,

$$\tilde{K} \sim 1/\alpha, \tag{12a}$$

while as a first approximation we might take

$$\tilde{K} \sim [\alpha(1 + k^2/\alpha^2)^{\frac{1}{2}}]^{-1} \approx \{\alpha[1 + (k^2/2\alpha^2)]\}^{-1}. \tag{12b}$$

Thus, these two approximations correspond to kernels of the form of Eq. (11) with $\rho = 0$ and $\rho = 1$, respectively.

III. ELEMENTARY DISCUSSION OF THE CASES $\rho = 0, 1$

If $\rho = 0$, the kernel given by Eq. (11) is such that

$$\tilde{K} = \text{const.} \tag{13}$$

Therefore

$$K[\alpha(x - x')] \sim \delta(x - x'). \tag{14}$$

The problem posed by Eq. (9) is then to find an $f(x)$ defined in the interval $a \leq x \leq b$ such that

$$0 = f(x), \qquad a < x < b. \tag{15}$$

Clearly, there are no nontrivial square-integrable solutions. If, however, generalized functions are admitted, we see that Eq. (15) says that $f(x)$ has as its support the two points a and b. The theorem of Schwartz[3] on generalized functions with point support then tells us that $f(x)$ is at most a sum of a finite number of derivatives of delta functions, i.e.,

$$f(x) = \sum_{i=0}^{N} C_i\, \delta^{(i)}(x - a) + \sum_{i=0}^{M} d_i\, \delta^{(i)}(b - x). \tag{16}$$

[2] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, New York, 1945).

[3] L. Schwartz, *Theorie des distributions* (Hermann & Cie., Paris, 1950).

Three remarks are in order:

(i) Any such f clearly solves the problem.

(ii) There are two *least singular* solutions—$\delta(x - a)$ and $\delta(x - b)$.

(iii) The *general* solution is a linear combination of these least singular solutions and their derivatives of finite order.

The case $\rho = 1$ is almost as simple. Here

$$\tilde{K} \sim (k^2 + \alpha^2)^{-1}. \tag{17a}$$

Then Eq. (9) has the form

$$\int_a^b e^{-\alpha\,|x-x'|} f(x')\, dx' = 0, \qquad a < x < b. \tag{17b}$$

We note that

$$[(-\partial^2/\partial x^2 + \alpha^2)K(\partial x)]^{\sim} = \text{const.} \tag{17c}$$

Therefore

$$[-(\partial^2/\partial x^2) + \alpha^2]K[\partial(x - x')] \sim \delta(x - x'). \tag{18}$$

Applying the operator $[-(\partial^2/\partial x^2) + \alpha^2]$ to Eq. (16) we find then that

$$f(x) = 0, \qquad a < x < b. \tag{19}$$

Again, there is no nontrivial classical solution. As a generalized function, f again has a and b as its points of support. Let us look at solutions which have only a as support.

$$\therefore \quad f(x) = \sum_{i=0}^{N} C_i\, \delta^{(i)}(x - a). \tag{20}$$

Substituting into Eq. (16) we find

$$e^{-\alpha(x-a)} \sum_{i=0}^{N} (-\alpha)^i C_i = 0. \tag{21}$$

This then yields the condition

$$\sum_{i=0}^{N} C_i(-\alpha)^i = 0. \tag{22}$$

We note that again:

(i) Here is a *least singular* solution. This occurs when only C_0, C_1 are unequal to zero. In this case

$$C_0 = \alpha C_1 \tag{23}$$

and

$$f_i(x) \sim \alpha\, \delta(x - a) + \delta'(x - a). \tag{24}$$

(ii) The general solution with point support a is a linear combination of this least singular solution and its derivatives.[4]

[4] See Appendix A.

(iii) The solutions with support b are obtained analogously.

(iv) The general solution is now just a sum of the general solutions with supports a and b, respectively.

IV. GENERAL ρ

In the cases discussed above obtaining the solutions was trivial. A few simple observations served to determine them. Here we want to show that the results are typical. To do so let us look at the special form of our Eq. (9) when $a = 0$, $b = \infty$.

The equation becomes

$$\int_0^\infty K[\alpha(x - x')]f(x')\,dx' = 0, \quad 0 < x < \infty. \tag{25}$$

Here $f(x)$ is to be determined in the interval $0 \leq x < \infty$ and explicitly we demand that $f(x)$ be a tempered distribution.[3]

Let us first specialize the results of Sec. III to the present situation.

(1) $\rho = 0$

There is a fundamental solution

$$f_1(x) = \delta(x). \tag{26}$$

The general solution is a linear combination of f_1 and its derivatives.

(2) $\rho = 1$

There is a fundamental solution

$$f_1(x) = \delta(x). \tag{27}$$

Again the general solution is a linear combination of this and its derivatives.

We turn now to the construction of solutions for a general ρ. The procedure to be followed is but a slight generalization of the usual Wiener–Hopf[5] method.

We *define*

$$f(x) = 0 \quad \text{for} \quad x < 0 \tag{28}$$

and

$$g(x) = 0 \quad \text{for} \quad x > 0.$$

Then Eq. (25) can be written in the form

$$g(x) = \int_{-\infty}^\infty K(\alpha(x - x'))f(x')\,dx', \quad -\infty < x < \infty. \tag{29}$$

Taking the Fourier transform of this equation using the convention that

$$\tilde{\phi}(k) = \frac{1}{2\pi}\int_{-\infty}^\infty e^{+ikx}\phi(x)\,dx \tag{30}$$

yields

$$\tilde{g}_-(k) = 2\pi\tilde{K}(k)\tilde{f}_+(k). \tag{31}$$

Here, specifically

$$\tilde{K}(k) = \text{const}/(k^2 + \alpha^2)^\rho. \tag{32}$$

Thus, Eq. (31) is

$$\tilde{g}_-(k) = C\tilde{f}_+(k)/(k^2 + \alpha^2)^\rho. \tag{33}$$

It may be noted that subscripts $-$ $(+)$ have been appended to remind us that $\tilde{g}(\tilde{f})$ are the boundary values of functions analytic in the lower (upper) half k-plane, respectively. Also, since we are seeking solutions which are tempered distributions, we require $\tilde{g}$, $\tilde{f}$ to have at most a polynomial behavior at infinity.

Let us factor $(k^2 + \alpha^2)^\rho$ in the form

$$(k^2 + \alpha^2)^\rho = (k + i\alpha)^\rho(k - i\alpha)^\rho. \tag{34}$$

[For nonintegral ρ the function $(k + i\alpha)^\rho$ is defined by means of a branch cut passing from $k = -i\alpha$ to ∞ in the lower half k-plane. Similarly, $(k - i\alpha)^\rho$ is defined by a branch cut in the upper half k-plane from $k = i\alpha$ to ∞.] Now Eq. (33) can be rewritten in the form

$$(k - i\alpha)^\rho\tilde{g}_-(k) = C\tilde{f}_+(k)/(k + i\alpha)^\rho. \tag{35}$$

Let us define $\Phi(k)$ by

$$\begin{aligned} \Phi(k) &= (k - i\alpha)^\rho\tilde{g}_-, && \text{Im } k < 0, \\ \Phi(k) &= C\tilde{f}_+(k)/(k + i\alpha)^\rho, && \text{Im } k > 0. \end{aligned} \tag{36}$$

Then Eq. (34) states that

$$\Phi^+ - \Phi^- = 0, \tag{37}$$

where $\Phi^\pm$ are the boundary values of Φ as the real axis is approached from above or below, respectively.

We now have enough information to determine Φ. Thus

(i) From Eq. (37) it follows that Φ is continuous across the real axis.

(ii) The analytic properties of f_+, g_-, and $(k \mp i\alpha)^\rho$ then require that Φ is analytic in the whole finite k plane.

(iii) By assumption Φ has at most a polynomial growth at infinity. Hence, we conclude from Liouville's theorem that

$$\Phi(k) = P_N(k), \tag{38}$$

where $P_N(k)$ is some polynomial. Referring back

[5] See, for example, *Fourier Transforms in the Complex Domain*, R. E. A. C. Paley and N. Wiener, Eds., (American Mathematical Society, New York, 1934).

to Eq. (36) it is then seen that the general form of $\tilde{f}_+(k)$ is

$$\tilde{f}_+(k) = (k + i\alpha)^\rho P_N(k). \tag{39}$$

Again we remark that there is a fundamental (least singular) solution. It arises from taking $N = 0$ and is

$$\tilde{f}_1(k) \sim (k + i\alpha)^\rho. \tag{40}$$

All other solutions are just polynomials in k times this. This can be translated into coordinate space. Thus, if $\tilde{\phi}(k)$ is the Fourier transform of $\phi(x)$, then $k\tilde{\phi}(k)$ is the transform of $i(\partial/\partial x)$. The above statement is then merely that the general solution is a linear combination of the fundamental solution and its derivatives.

V. EVALUATION OF THE FUNDAMENTAL SOLUTIONS

Using the Fourier inversion formula we have

$$f_1(x) = C' \int_{-\infty}^{\infty} e^{-ikx}(k + i\alpha)^\rho \, dk. \tag{41}$$

Let us first consider the case where $\rho = n$ (an integer). Then

$$f_1(x) = C' \int_{-\infty}^{\infty} e^{-ikx}(k + i\alpha)^n \, dk. \tag{42}$$

Using the noted relation between multiplication by k and differentiation with respect to x, we see that

$$\begin{aligned} f_1(x) &= C'\left(i\frac{\partial}{\partial x} + i\alpha\right)^n \int_{-\infty}^{\infty} e^{-ikx} \, dk \\ &= C\left(\alpha + \frac{\partial}{\partial x}\right)^n \delta(x). \end{aligned} \tag{43}$$

In particular we note that with $n = 0$ or 1 the previous results are again obtained.

In case ρ is nonintegral we proceed in the following manner. Write

$$(k + i\alpha)^\rho = (k + i\alpha)^m (k + i\alpha)^{\rho - m}. \tag{44}$$

Here m is an integer chosen so that $-1 < \rho - m < 0$. To put this in convenient form we use the same trick as was used to get Eq. (43). Thus

$$f_1(x) = C'\left(i\frac{\partial}{\partial x} + i\alpha\right)^m \int_{-\infty}^{\infty} (k + i\alpha)^{\rho - m} e^{-ikx} \, dk. \tag{45}$$

We note that

$$\int_{-\infty}^{\infty} (k + i\alpha)^{\rho - m} e^{-ikx} \, dk = (\text{const}) e^{-\alpha x}/x^{\rho - m + 1}; \tag{46}$$

$$\therefore \; f_1(x) = C[\alpha + (\partial/\partial x)]^m e^{-\alpha x}/x^{\rho - m - 1}, \quad x \geq 0 \tag{47}$$

$$= 0, \qquad x < 0. \tag{48}$$

To recognize this distribution let us remember that these are defined as linear functionals on a space of test functions ϕ, i.e., to each ϕ we have a number (f_1, ϕ). In particular the derivative of a generalized function f—f'—is defined by

$$(f', \phi) = -(f, \phi'). \tag{49}$$

Thus, our f_1 above is

$$(f_1, \phi) = C \int_0^{\infty} \frac{e^{-\alpha x}}{x^{\rho - m + 1}} \left(\alpha - \frac{\partial}{\partial x}\right)^m \phi(x) \, dx. \tag{50}$$

Of greatest interest to us is the case $\rho = \frac{1}{2}$. Then $m = -1$ and our distribution, which we denote by $[e^{-\alpha x} x^{-3/2}]_+$ is

$$([e^{-\alpha x} x^{-\frac{3}{2}}]_+, \phi) = -2 \int_0^{\infty} \frac{e^{-\alpha x}}{x^{\frac{1}{2}}} \left(\alpha - \frac{\partial}{\partial x}\right) \phi(x) \, dx. \tag{51}$$

This can be put in the more perspicuous form by writing

$$\partial\phi(x)/\partial x = (\partial/\partial x)[\phi(x) - \phi(0)], \tag{52}$$

and integrating by parts. The result is

$$\begin{aligned} ([e^{-\alpha x} x^{-\frac{3}{2}}]_+, \phi) = \int_0^{\infty} x^{-\frac{3}{2}} e^{-\alpha x}[\phi(x) - \phi(0)] \, dx \\ - 2(2\pi)^{\frac{1}{2}}\phi(0). \end{aligned} \tag{53}$$

We note then that this fundamental solution is just the ordinary function $e^{-\alpha x}/x^{\frac{3}{2}}$ for $x > 0$, zero for $x < 0$ and is appropriately defined at $x = 0$. Indeed, this definition is such that the function is "integrable"—in the sense that we get a finite result when we put $\phi(x)$ equal to a constant. Also the modification is such that the function is *not* positive-definite. [Thus, choosing $\phi(x)$ which is of a definite sign, (f, ϕ) can have either sign.] This is to be expected. The convolution integral [Eq. (9)] of f_1 with the positive-definite kernel $K_0(\alpha\,|x|)$ could not be zero otherwise.

It may be remarked that the statement that the distribution $[e^{-\alpha x} x^{-\frac{3}{2}}]_+$ satisfies Eq. (9) is equivalent to the identity

$$\begin{aligned} &2(\alpha\pi)^{\frac{1}{2}} K_0(\alpha x) \\ &= \int_0^{\infty} x'^{-\frac{3}{2}} e^{-\alpha x'}[K_0(\alpha\,|x - x'|) - K_0(\alpha x)] \, dx'. \end{aligned} \tag{54}$$

As a check on the reasoning we verify this directly in Appendix B.

The comments on "complementarity" made in the introductory section are perhaps now clear. If ρ is large, $K(x - x')$ is smooth at $x = x'$. The

corresponding solutions are very singular.[6] Conversely, when ρ is small, K is singular at $x = x'$—and the solutions are relatively smooth. In particular, we see that the case $\rho = \frac{1}{2}$ does indeed lie between those for $\rho = 0$ and $\rho = 1$. The fundamental solution is more singular than that for $\rho = 0$ but less so than for $\rho = 1$. Indeed, except for the factor $e^{-\alpha x}$ the solution for $\rho = \frac{1}{2}$ is essentially a half-integral derivative of the delta function.

VI. EFFECTIVE SOLUTIONS FOR LARGE STRIPS

Let us return to Eq. (9). Choosing the origin to be at the midpoint of the strip and introducing dimensionless variables, this is

$$\int_{-\frac{1}{2}a}^{\frac{1}{2}a} K_0(|x - x'|)f(x')\,dx' = 0, \qquad -\tfrac{1}{2}a < x < \tfrac{1}{2}a. \tag{55}$$

[Here the correspondence with the previous notation is $\alpha(b - a) \to a$.] From Eq. (10)[7] one readily obtains as an integral representation of the Bessel function

$$K_0(|x|) = \int_1^\infty \frac{e^{-t\,|x|}\,dt}{(t^2 - 1)^{\frac{1}{2}}}. \tag{56}$$

Intuitively, the nature of the solutions for $a \gg 1$ is clear. The existence of an edge very far from a given edge should have little effect on the solution near that edge. Thus, we expect that near the edges the solutions should be much like the solutions for the half-space problems; i.e.,

$$f(x) \sim f_0^+ = A_+[e^{-(x+\frac{1}{2}a)}(x + \tfrac{1}{2}a)^{-\frac{1}{2}}]_+, \quad x \sim -\tfrac{1}{2}a$$

and (57)

$$f(x) \sim f_0^- = A_-[e^{-(\frac{1}{2}a-x)}(\tfrac{1}{2}a - x)^{-\frac{1}{2}}]_+, \quad y \sim \tfrac{1}{2}a.$$

Our procedure is to write the solution of Eq. (55) in the form

$$f = f_0^+ + f_0^- + f_1, \tag{58}$$

where we assume f_1 is a well-behaved function. We then obtain inhomogeneous Fredholm equations of the first kind to determine f_1. From these we can readily conclude that a solution of this type exists. More pragmatically, these equations permit us to obtain rapidly an asymptotic expansion of the solution for large a.

Using the fact that $f_0^\pm$ satisfy the equations

$$\int_{-\frac{1}{2}a}^{\infty} K_0(|x - x'|)f_0^+(x')\,dx' = 0, \quad -\tfrac{1}{2}a < x < \infty$$

and (59)

$$\int_{-\infty}^{\frac{1}{2}a} K_0(|x - x'|)f_0^-(x')\,dx' = 0, \quad -\infty < x < \tfrac{1}{2}a,$$

we obtain, on inserting the ansatz of Eq. (58) into Eq. (55) as an equation for f_1,

$$\int_{-\frac{1}{2}a}^{\frac{1}{2}a} K_0(|x - x'|)f_1(x')\,dx' = \int_{\frac{1}{2}a}^{\infty} K_0 f_0^+(x')\,dx' + \int_{-\infty}^{-\frac{1}{2}a} K_0 f_0^-(x')\,dx'. \tag{60}$$

We remark that the "values" of $f_0^\pm$ that are relevant in Eq. (60) are those where they are ordinary well-behaved (integrable) functions. In these regions we have the integral representations

$$f_0^+(x) = \frac{2A_+}{\pi^{\frac{1}{2}}} \int_1^\infty e^{-(x+\frac{1}{2}a)t}(t - 1)^{\frac{1}{2}}\,dt$$

and (61)

$$f_0^-(x) = \frac{2A_-}{\pi^{\frac{1}{2}}} \int_1^\infty e^{-(\frac{1}{2}a-x)t}(t - 1)^{\frac{1}{2}}\,dt.$$

Now note a convenient replication property[8] of the kernel K_0. If in any of the integrands of Eq. (60) we put $f(x') = e^{\pm tx'}$ with $1 \leq t < \infty$, all that results is a linear combination of such terms again. Thus, by explicit calculation we obtain [using the integral representation of Eq. (56)]

$$\int_{-\frac{1}{2}a}^{\frac{1}{2}a} K_0(|x - x'|)e^{\mp tx'}\,dx' = \int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}}\left[\frac{(e^{\mp tx} - e^{-t'x}e^{-\frac{1}{2}a(t' \mp t)})}{t' \mp t} + \frac{(e^{\mp tx} - e^{t'x}e^{-\frac{1}{2}a(t' \pm t)})}{t' \pm t}\right], \tag{62}$$

$$\int_{\frac{1}{2}a}^{\infty} K_0(|x - x'|)e^{-x't}\,dx' = \int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}} \frac{e^{xt'}e^{-\frac{1}{2}a(t+t')}}{t + t'} \qquad (x < \tfrac{1}{2}a), \tag{63}$$

and

$$\int_{-\infty}^{-\frac{1}{2}a} K_0(|x - x'|)e^{tx'}\,dx' = \int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}} \frac{e^{-xt'}e^{-\frac{1}{2}a(t+t')}}{t + t'} \qquad (x > -\tfrac{1}{2}a). \tag{64}$$

[6] This statement can be made more precise by considering a "function" as more singular if it can be defined only for a smaller class of test functions.

[7] Alternatively, cf. Ref. 2.

[8] See, for example, K. M. Case, Rev. Mod. Phys. **36**, 669 (1964).

This property strongly suggests that we try to represent f_1 in the form

$$f_1 = \int_1^\infty \phi_+(t)e^{-t(x+\frac{1}{2}a)}\,dt + \int_1^\infty \phi_-(t)e^{t(x-\frac{1}{2}a)}. \tag{65}$$

Note: The factors $e^{-\frac{1}{2}at}$ are appended to simplify later formulas. Also, since we are looking for f with $-\frac{1}{2}a < x < \frac{1}{2}a$ they guarantee the integrands exist if $\phi_\pm$ are moderately well behaved at infinity.

Inserting the expressions of Eqs. (61) and (65) into Eq. (60) [and using Eqs. (62)–(64)] yields

$$L = R, \tag{66}$$

where

$$\begin{aligned} L = {} & \int_1^\infty dt \int_1^\infty \frac{dt'\,\phi_+(t)e^{-\frac{1}{2}at}}{(t'^2-1)^{\frac{1}{2}}}\left[\frac{(e^{-tx} - e^{-t'x}e^{-\frac{1}{2}a(t'-t)})}{(t'-t)}\right. \\ & \left. + \frac{(e^{-tx} - e^{t'x}e^{-\frac{1}{2}a(t'+t)})}{t'+t}\right] \\ & + \int_1^\infty dt \int_1^\infty \frac{dt'\,\phi_-(t)e^{-\frac{1}{2}at}}{(t'^2-1)^{\frac{1}{2}}}\left[\frac{(e^{tx} - e^{-t'x}e^{-\frac{1}{2}a(t'+t)})}{t'+t}\right. \\ & \left. + \frac{(e^{tx} - e^{t'x}e^{-\frac{1}{2}a(t'-t)})}{t'-t}\right] \end{aligned} \tag{67}$$

and

$$\begin{aligned} R = {} & \frac{2A_+}{\pi^{\frac{1}{2}}}\int_1^\infty dt \int_1^\infty \frac{dt'\,(t-1)^{\frac{1}{2}}e^{-at}e^{xt'}e^{-\frac{1}{2}at'}}{(t'^2-1)^{\frac{1}{2}}(t+t')} \\ & + \frac{2A_-}{\pi^{\frac{1}{2}}}\int_1^\infty dt \int_1^\infty \frac{dt'\,(t-1)^{\frac{1}{2}}e^{-at}e^{-xt'}e^{-\frac{1}{2}at'}}{(t'^2-1)^{\frac{1}{2}}(t+t')}. \end{aligned} \tag{68}$$

It should be noted that in Eq. (67) there is no singularity at $t = t'$. Since, however, it is convenient to treat the individual terms separately, it is necessary to give some unique meaning to $1/(t'-t)$. Any consistent meaning will suffice. For our purposes, the principal-value interpretation is simplest. Thus from now on $1/(t'-t)$ means $P[1/(t'-t)]$.

A *sufficient* condition for Eq. (66) to be satisfied is that the coefficients of $e^{\mp tx}$, $1 \le t < \infty$, be equal. From the coefficients of e^{-tx} we obtain

$$\begin{aligned} & (t^2-1)^{\frac{1}{2}}\phi_+(t)\left\{\int_1^\infty \frac{dt'}{(t'^2-1)^{\frac{1}{2}}}\left(\frac{1}{t'-t} + \frac{1}{t'+t}\right)\right\} \\ & \quad + \int_1^\infty \frac{dt'\,\phi_+(t')}{t'-t} \\ & = \int_1^\infty \frac{e^{-at'}\,dt'}{t'+t}\left[\frac{2A_-}{\pi^{\frac{1}{2}}}(t'-1)^{\frac{1}{2}} + \phi_-(t')\right], \end{aligned} \tag{69}$$

while from the coefficients of e^{tx} we find

$$\begin{aligned} & (t^2-1)^{\frac{1}{2}}\phi_-(t)\left\{\int_1^\infty \frac{dt'}{(t'^2-1)^{\frac{1}{2}}}\left(\frac{1}{t'-t} + \frac{1}{t'+t}\right)\right\} \\ & \quad + \int_1^\infty \frac{\phi_-(t')\,dt'}{t'-t} \\ & = \int_1^\infty \frac{e^{-at'}\,dt'}{t'+t}\left[\frac{2A_+}{\pi^{\frac{1}{2}}}(t'-1)^{\frac{1}{2}} + \phi_+(t')\right]. \end{aligned} \tag{70}$$

These simplify considerably. As shown in Appendix C, the quantity in braces vanishes. Therefore, these equations are

$$P\int_1^\infty \frac{\phi_\pm(t')\,dt'}{t'-t} = \psi_\pm(t), \tag{71$^\pm$}$$

where

$$\psi_\pm(t) = \int_1^\infty \frac{e^{-at'}\,dt'}{t'+t}\left[\frac{2A_\mp}{\pi^{\frac{1}{2}}}(t'-1)^{\frac{1}{2}} + \phi_\mp(t')\right]. \tag{72}$$

If the $\psi_\pm$ of Eqs. (71$^\pm$) were known functions these would be singular integral equations of a standard form with known solutions.[9] We use these solutions to convert these equations into convenient Fredholm equations.

Thus, consider Eq. (71$^+$). Let

$$N(z) = \int_1^\infty \frac{\phi_+(t')\,dt'}{t'-z}. \tag{73}$$

Then, if $N^\pm$ denote the boundary values of N, as we approach the cut from 1 to ∞ from above and below, respectively, we have

$$\tfrac{1}{2}[N^+(t) + N^-(t)] = P\int_1^\infty \frac{\phi_+(t')\,dt'}{t'-t} \tag{74}$$

and

$$\phi^+(t) = [N^+(t) - N^-(t)]/2\pi i. \tag{75}$$

Using Eq. (74) we see that the integral Eq. (71$^+$) is

$$N^+(t) + N^-(t) = 2\psi_+(t). \tag{76}$$

With

$$X(z) = (z-1)^{\frac{1}{2}}, \tag{77}$$

this can be rewritten as

$$X^+(t)N^+(t) - X^-(t)N^-(t) = 2X^+\psi_+. \tag{78}$$

From this continuity condition and the analytic properties of $X(z)$ and $N(z)$ we conclude that

$$N(z) = \frac{1}{X(z)}\frac{1}{2\pi i}\int_1^\infty \frac{2X^+(t')\psi_+(t')\,dt'}{t'-z}. \tag{79}$$

[9] Cf., for example, N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff Ltd., Gröningen, The Netherlands, 1953).

As shown in Appendix D, we can readily evaluate the integral with respect to t'. The resulting expression for $N(z)$ is

$$N(z) = \int_1^\infty e^{-at'}\,dt'\left[\frac{2A_-}{\pi^{\frac{1}{2}}}(t'-1)^{\frac{1}{2}} + \phi_-(t')\right] \times \frac{[1 - X(-t')/X(z)]}{t' + z}. \quad (80)$$

From Eq. (75) we then find

$$\phi_+(t) = -\frac{1}{\pi}\frac{1}{(t-1)^{\frac{1}{2}}}\int_1^\infty e^{-at'}\,dt' \times \left[\frac{2A_-(t'-1)^{\frac{1}{2}}}{\pi^{\frac{1}{2}}} + \phi_-(t')\right]\frac{(t'+1)^{\frac{1}{2}}}{t'+t}. \quad (81_+)$$

In exactly the same fashion it follows that

$$\phi_-(t) = -\frac{1}{\pi}\frac{1}{(t-1)^{\frac{1}{2}}}\int_1^\infty e^{-at'}\,dt' \times \left[\frac{2A_+}{\pi^{\frac{1}{2}}}(t'-1)^{\frac{1}{2}} + \phi_+(t')\right]\frac{(t'+1)^{\frac{1}{2}}}{t'+t}. \quad (81_-)$$

These Fredholm equations can be used to demonstrate the solutions $\phi_\pm(t)$. More usefully, they can readily generate asymptotic expansions for large a.

Thus, suppose $a \gg 1$, we readily see that an iterative solution obtained by first omitting the $\phi_\pm$ on the right-hand side of Eqs. (81) yields successive terms which decrease as e^{-a} in each step. The lowest approximation is

$$\phi_\pm(t) = -\frac{1}{\pi}\frac{1}{(t-1)^{\frac{1}{2}}}\frac{2}{\pi^{\frac{1}{2}}}A_\mp\int_1^\infty \frac{e^{-at'}(t'^2-1)^{\frac{1}{2}}}{t'+t}. \quad (82)$$

For large a the integral occurring here is also readily approximated. Thus

$$\frac{2}{\pi^{\frac{1}{2}}}\int_1^\infty \frac{e^{-at'}(t'^2-1)^{\frac{1}{2}}}{t'+t}\,dt' \approx \frac{2^{\frac{1}{2}}2}{(1+t)\pi^{\frac{1}{2}}}\int_1^\infty e^{-at'}(t'-1)^{\frac{1}{2}}\,dt' = \frac{2^{\frac{1}{2}}}{1+t}\frac{e^{-a}}{a^{\frac{1}{2}}}, \quad (83)$$

$$\therefore\quad \phi_\pm(t) \approx -\frac{2^{\frac{1}{2}}}{\pi}\frac{A_\mp}{(t-1)^{\frac{1}{2}}(t+1)}\frac{e^{-a}}{a^{\frac{1}{2}}}. \quad (84)$$

With these approximations we find from Eq. (65) that

$$f_1(x) = -(e^{-a}/a^{\frac{1}{2}})[A_-g(\tfrac{1}{2}a + x) + A_+g(\tfrac{1}{2}a - x)], \quad (85)$$

where

$$g(x) = \frac{2^{\frac{1}{2}}}{\pi}\int_1^\infty \frac{e^{-xt}\,dt}{(t-1)^{\frac{1}{2}}(t+1)} \quad (86)$$

$$= e^x\{1 - \operatorname{erf}[(2x)^{\frac{1}{2}}]\}. \quad (87)$$

Of particular interest are the values of $g(x)$ for x small and large. We have

$$g(0) = 1 \quad (88)$$

and

$$g(x) \cong \frac{e^{-x}}{(2\pi x)^{\frac{1}{2}}}; \qquad x \gg 1. \quad (89)$$

Remembering that we are here considering the case $a \gg 1$, we see that

$$f_1(-\tfrac{1}{2}a) = -(e^{-a}/a^{\frac{1}{2}})\{A_- + [(A_+e^{-a})/(2\pi a)^{\frac{1}{2}}]\} \quad (90a)$$

and

$$f_1\left(\frac{a}{2}\right) = \frac{-e^{-a}}{a^{\frac{1}{2}}}\left\{\frac{A_-e^{-a}}{(2\pi a)^{\frac{1}{2}}} + A_+\right\}. \quad (90b)$$

Thus, as we had assumed, the correction term $[f_1(x)]$ is well behaved—and small.

It may be noted that continuing the iterative solutions to Eqs. $(81_\pm)$ yields improved approximations for $f_1(x)$. The successive terms decrease by a factor $O(e^{-a})$.

VII. SMALL STRIP

The case when the a of Eq. (55) is much less than unity is also amenable to a rather full analytic treatment. We note that only arguments of the kernel for values small compared to 1 occur. From the integral representation of Eq. (56) or Watson[2] we find

$$K_0(|x|) \approx -[\ln(\tfrac{1}{2}|x|) + \gamma], \qquad |x| \ll 1, \quad (91)$$

where γ is Eulers' constant.

Then we can write Eq. (55) in the form

$$\int_{-\frac{1}{2}a}^{\frac{1}{2}a}\left(\ln\frac{|x-x'|}{2} + \gamma\right)f(x')\,dx' = \int_{-\frac{1}{2}a}^{\frac{1}{2}a}\left[\ln\frac{|x-x'|}{2} + \gamma - K_0(|x-x'|)\right]f(x')\,dx', \qquad -\tfrac{1}{2}a < x < \tfrac{1}{2}a. \quad (92)$$

Our procedure closely parallels the case of the large strip. We use an iteration procedure. Thus, we first replace the "small" right-hand side by zero. After finding the solutions of the resulting homogeneous equation, we insert this in the right-hand side of Eq. (92) and solve the new inhomogeneous equation. Repeating the process yields a series solution in which successive terms are smaller and smaller. All but the first time is regular. (This is

not precisely a power series expansion. Powers of $\ln a$ also occur.)

For brevity we restrict ourselves here to the lowest approximation. The problem is to find solutions of

$$\int_{-\frac{1}{2}a}^{\frac{1}{2}a} \left(\ln \frac{|x-x'|}{2} + \gamma\right) f(x')\,dx' = 0, \qquad -\tfrac{1}{2}a < x < \tfrac{1}{2}a. \tag{93}$$

The form of Eq. (47) suggests we look for solutions which are generalized functions which can be written in the form

$$f(x) = (\partial/\partial x)h(x), \tag{94}$$

with $h(x)$ a *regular* functional satisfying a Hölder condition. Then Eq. (93) becomes

$$P\int_{-\frac{1}{2}a}^{\frac{1}{2}a} \frac{h(x')\,dx'}{x'-y} = 0, \qquad -\tfrac{1}{2}a < x < \tfrac{1}{2}a.$$

The general solution is readily shown to be

$$h(x) = C/[(\tfrac{1}{2}a)^2 - x^2]^{\frac{1}{2}}. \tag{95}$$

Hence, our solution is the functional defined by

$$(f, \phi) = -C\int_{-\frac{1}{2}a}^{\frac{1}{2}a} \frac{1}{[(\frac{1}{2}a)^2 - x^2]^{\frac{1}{2}}} \frac{\partial}{\partial x}\phi(x)\,dx. \tag{96}$$

VIII. CIRCLE

The results of the preceding sections can be used to approximate the solutions of Eq. (1) in more general situations. To illustrate we consider the case where the region S is a circle.

Then Eq. (1) is

$$\int_0^a r'\,dr' \int_0^{2\pi} d\phi'\, G(r, \phi; r', \phi')f(\mathbf{r}') = 0, \quad 0 \le r < a. \tag{97}$$

Here

$$G(r, \phi; r', \phi') = \frac{1}{8\pi^2}\int \frac{e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{(k^2+\alpha^2)^{\frac{1}{2}}}\,d^2k. \tag{98}$$

Again we note that Eq. (97) is separable. Thus, there are solutions of the form

$$f(\mathbf{r}) = f(r)e^{in\phi}. \tag{99}$$

Inserting this ansatz we find that the f_n must satisfy the equation

$$\int_0^a G_n(r, r')f_n(r')r'\,dr' = 0, \qquad 0 \le r < a, \tag{100}$$

with

$$G_n(r, r') = \int_0^\infty \frac{k\,dk}{(k^2+\alpha^2)^{\frac{1}{2}}} J_n(kr)J_n(kr'). \tag{101}$$

First let us consider the limiting situation when $\alpha a \gg 1$. In this case we expect the important regions are where the arguments of the Bessel functions are large. We approximate then by the asymptotic expansion[2]

$$J_n(x) \approx (2/\pi x)^{\frac{1}{2}} \cos(x - \tfrac{1}{2}n\pi - \tfrac{1}{4}\pi). \tag{102}$$

For the product occurring in Eq. (101) there results

$$J_n(kr)J_n(kr') \approx [1/2\pi k(rr')^{\frac{1}{2}}][(e^{ik(r-r')} + e^{-ik(r-r')}) - i(-1)^n(e^{ik(r+r')} - e^{-ik(r+r')})]. \tag{103}$$

As we have seen, it is the most singular part of the kernel which determines the solution. This is clearly the part depending on the difference $r - r'$. Thus we have the approximation

$$G_n(r, r') \approx \frac{1}{2\pi(rr')^{\frac{1}{2}}}\int_0^\infty \frac{(e^{ik(r-r')} + e^{-ik(r-r')})^{\frac{1}{2}}}{(k^2+\alpha^2)^{\frac{1}{2}}}\,dk. \tag{104}$$

Changing the k to $-k$ in the second term shows that

$$G_n(r, r') \approx K_0(\alpha\,|r-r'|)/(rr')^{\frac{1}{2}}. \tag{105}$$

Thus, with our approximations, $r^{\frac{1}{2}}f_n(r)$ satisfies the equation for a thick strip lying between 0 and a. Of the two fundamental solutions only that with the singularity at a is permissible. Thus

$$f_n(r) \approx \frac{A}{r^{\frac{1}{2}}}[e^{-\alpha(a-r)}/(a-r)^{\frac{1}{2}}]_+. \tag{106}$$

The opposite limiting case where $\alpha a \ll 1$ can also be treated simply. Thus in Eq. (3) we can neglect αr in the argument of the exponential. We find

$$G(r, \phi; r', \phi') \approx \frac{1}{4\pi}\frac{1}{[r^2 + r'^2 - 2rr'\cos(\phi - \phi')]^{\frac{1}{2}}}. \tag{107}$$

For $G_n(r, r')$ we then obtain

$$G_n \sim \int_0^{2\pi} \frac{e^{in\phi}\,d\phi}{[r^2 + r'^2 - 2rr'\cos(\phi-\phi')]^{\frac{1}{2}}}. \tag{108}$$

The most singular part of this expression is

$$G_n \approx -\frac{1}{(rr')^{\frac{1}{2}}}\ln\frac{|r-r'|}{(rr')^{\frac{1}{2}}}. \tag{109}$$

With this approximation, Eq. (100) becomes

$$\int_0^a \ln|r-r'|\,\psi(r')\,dr' = \frac{1}{2}\int_0^a (\ln r + \ln r')\psi(r')\,dr', \quad 0 \le r < a. \tag{110}$$

Here

$$\psi(r) = r^{\frac{1}{2}} f_n(r). \tag{111}$$

Suggested by our earlier results, we look for a solution where the distribution $\psi(r)$ is the derivative of an ordinary function $h(r)$ satisfying a Hölder condition. Then,

$$P \int_0^a \frac{h(r')\, dr'}{r' - r} = C, \qquad 0 \leq r < a, \tag{112}$$

where

$$C = \frac{1}{2} \int_0^a \frac{h(r')\, dr'}{r'}. \tag{113}$$

With

$$N(z) = \int_0^a \frac{h(r')\, dr'}{r' - z} \tag{114}$$

and

$$Y(z) = [(a - z)/z]^{\frac{1}{2}}, \tag{115}$$

we have

$$[N^+(r) - N^-(r)]/2\pi i = h(r), \tag{116}$$

and Eq. (112) becomes

$$Y^+N^+ - Y^-N^- = 2CY^+. \tag{117}$$

By conventional arguments[9] we conclude that

$$Y(z)N(z) = \frac{C}{2\pi i} \int_0^a \frac{2Y^+(r')\, dr'}{r' - z} \tag{118}$$

$$= C\{Y(z) + i\}. \tag{119}$$

Then

$$h(r) = \frac{iC}{2\pi i} \left[\frac{1}{Y^+(r)} - \frac{1}{Y^-(r)} \right] = (C/\pi)[r/(a - r)]^{\frac{1}{2}}. \tag{120}$$

We note that in virtue of the fact that

$$\int_0^a \frac{dr}{[r(a - r)]^{\frac{1}{2}}} = \pi, \tag{121}$$

Eq. (113) is identically satisfied.

The peculiar factor $r^{\frac{1}{2}}$ in Eq. (111) seems to make our result unacceptable. However, since we are working in cylindrical coordinates, the effect of our distributions on test functions is defined with volume element $r\, dr$.

IX. CONCLUSION

We have seen that equations like Eq. (1) have solutions—if we admit these to lie in an appropriate space of generalized functions. Exact solutions for simple cases have been found and shown to be useful for approximations in more complicated problems. Of most general interest perhaps is the complementary relation between the singular behavior of kernel and solution. In particular, the most singular part of the kernel gives the dominant behavior of the solution in limiting situations.

APPENDIX A

In Sec. III it was found that the general solution of Eq. (16) with point support a was

$$f(x) = \sum_{i=0}^{N} C_i\, \delta^{(i)}(x - a), \tag{A1}$$

where the C_i are subject to the restriction

$$\sum_{i=0}^{N} C_i(-\alpha)^i = 0. \tag{A2}$$

It was *stated* that all such are linear combinations of the fundamental solution

$$f_1(x) = \alpha\, \delta(x - a) + \delta'(x - a) \tag{A3}$$

and its derivatives. This is readily seen to be so: For the general solution given by Eq. (A1) we can regard Eq. (A2) as determining c_N when c_i ($i = 0, 1, \cdots, N - 1$) are given. On the other hand, the general linear combination of the fundamental solution and its derivatives up to order $N - 1$ is

$$\sum_{i=1}^{N} A_i[\alpha\, \delta^{(i-1)} + \delta^{(i)}]. \tag{A4}$$

Comparing with Eq. (A1) we see these agree if

$$c_i = \alpha A_{i+1} + A_i, \tag{A5}$$

where, by definition $A_0 = A_{N+1} = 0$. Thus

$$\begin{aligned} c_0 &= \alpha A_1, \\ c_1 &= \alpha A_2 + A_1, \\ &\cdots, \\ c_{N-1} &= \alpha A_N + A_{N-1}, \\ c_N &= A_N. \end{aligned} \tag{A6}$$

We are free to choose the A_i ($i = 1, 2, \cdots, N$) so that the first N of these equations are satisfied. That the last equation is satisfied will follow automatically if Eq. (A2) is fulfilled. But

$$\begin{aligned} &\sum_{i=0}^{N} (-\alpha)^i(\alpha A_{i+1} + A_i) \\ &\quad = \sum_{i=0}^{N-1} (-\alpha)^i \alpha A_{i+1} + \sum_{i=1}^{N} (-\alpha)^i A_i \\ &\quad = -\sum_{i=1}^{N} (-\alpha)^i A_i + \sum_{i=1}^{N} (-\alpha)^i A_i = 0. \end{aligned} \tag{A7}$$

APPENDIX B

In Sec. V we found that our solution of the integral Eq. (25) implied the identity

$$2\alpha\pi^{\frac{1}{2}}K_0(\alpha x) = \int_0^\infty x'^{-\frac{1}{2}}e^{-\alpha x'}[K_0(\alpha\,|x - x'|) - K_0(\alpha x)]\,dx'. \quad \text{(B1)}$$

It is perhaps illuminating to verify this identity directly. Remembering that

$$K_{\frac{1}{2}}(\alpha x) = (\pi/2\alpha x)^{\frac{1}{2}}e^{-\alpha x}, \quad \text{(B2)}$$

we see that the problem is to verify the equation

$$2^{\frac{1}{2}}\pi K_0(\alpha x) = \int_0^\infty \frac{K_{\frac{1}{2}}(\alpha x')}{x'}[K_0(\alpha\,|x - x'|) - K_0(\alpha x)]\,dx'. \quad \text{(B3)}$$

In order to evaluate the integral here it is convenient to regard

$$\int_0^\infty \text{ as } \lim_{\epsilon\to 0}\int_\epsilon^\infty.$$

(In this way we can treat the individual terms separately.)

As an example we have

$$\int_0^\infty \frac{K_{\frac{1}{2}}(\alpha x')\,dx'}{x'} \approx \left(\frac{\pi}{2\alpha}\right)^{\frac{1}{2}}\int_\epsilon^\infty \frac{e^{-\alpha x'}\,dx'}{(x')^{\frac{1}{2}}} \approx \left(\frac{\pi}{2\alpha}\right)^{\frac{1}{2}}[2\epsilon^{-\frac{1}{2}} - 2(\pi\alpha)^{\frac{1}{2}} + O(\epsilon)]. \quad \text{(B4)}$$

Similarly to evaluate

$$J = \int_0^\infty K_{\frac{1}{2}}(\alpha x')K_0(\alpha\,|x - x'|)\,dx', \quad \text{(B5)}$$

we use Watson's[3] expansion

$$K_0 = \sum_{m=-\infty}^{\infty} K_m(\alpha x_>)I_m(\alpha x_<) \quad \text{(B6)}$$

(where $x_>$ and $x_<$ are the greater and lesser of x and x' respectively) and obtain

$$J = \sum_{m=-\infty}^{\infty} J_m. \quad \text{(B7)}$$

Using the differential equations for the Bessel functions we readily find

$$J_m = \frac{K_{\frac{1}{2}}(\alpha x)}{m^2 - \frac{1}{4}} + K_0(\alpha x)\left(\frac{2\pi}{\alpha}\right)^{\frac{1}{2}}\frac{\delta_{m,0}}{\epsilon^{\frac{1}{2}}} + O(\epsilon). \quad \text{(B8)}$$

The summation over m in Eq. (B7) is now simple. Thus[10]

$$\sum_{m=-\infty}^{\infty}\frac{1}{m^2 - \frac{1}{4}} = 0. \quad \text{(B9)}$$

Then

$$J = \left(\frac{2\pi}{\alpha}\right)^{\frac{1}{2}}\frac{K_0(\alpha x)}{\epsilon^{\frac{1}{2}}} + O(\epsilon). \quad \text{(B10)}$$

Combining Eqs. (B10) and (B4) we see in passing to the limit $\epsilon \to 0$ that the right-hand side of Eq. (B3) is indeed $2^{\frac{1}{2}}\pi K_0(\alpha x)$.

APPENDIX C

In Sec. VI we used the result that

$$\int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}}\left(\frac{1}{t' - t} + \frac{1}{t' + t}\right) = 0. \quad \text{(C1)}$$

To show this we consider the function $Y(z) = (z^2 - 1)^{-\frac{1}{2}}$ defined with branch cuts extending from 1 to ∞ and -1 to $-\infty$ along the real axis. Further, the function is to be positive on the top lip of the right-hand cut. Applying Cauchys' theorem we see that

$$Y(z) = \frac{1}{2\pi i}\int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}(t' - z)} + \frac{1}{2\pi i}\int_{-\infty}^{-1}\frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}(t' - z)}. \quad \text{(C2)}$$

Now, we let z approach the positive real axis at a point $t > 1$ from above and below, respectively. By the Plemelj formulas these limiting values are

$$Y^{\pm} = \frac{P}{2\pi i}\int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}(t' - t)} \pm \frac{1}{2(t^2 - 1)^{\frac{1}{2}}} + \frac{1}{2\pi i}\int_{-\infty}^{-1}\frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}(t' - t)}. \quad \text{(C3)}$$

Changing the integration variable from t' to $-t'$ in the second integral yields

$$Y^{\pm}(t) = \frac{P}{2\pi i}\int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}}\left(\frac{1}{t' - t} + \frac{1}{t' + t}\right) \pm \frac{1}{2(t^2 - 1)^{\frac{1}{2}}}. \quad \text{(C4)}$$

Adding shows that

$$\pi i[Y^+(t) + Y^-(t)] = \int_1^\infty \frac{dt'}{(t'^2 - 1)^{\frac{1}{2}}}\left(\frac{1}{t' - t} + \frac{1}{t' + t}\right). \quad \text{(C5)}$$

However, with our definition of the function $Y(z)$ we have

$$Y^+(t) + Y^-(t) = 0. \quad \text{(C6)}$$

Hence, the identity of Eq. (C1) is true.

[10] Cf. E. C. Titchmarch, *The Theory of Functions* (Oxford University Press, New York, 1939).

APPENDIX D

In Sec. VI we encountered the integral

$$\mathcal{J} = \frac{1}{2\pi i}\int_1^\infty \frac{2X^+(t')\psi_+(t')\,dt'}{t'-z}, \tag{D1}$$

where

$$X(z) = (z-1)^{\frac{1}{2}}$$

and

$$\psi_+(t') = \int_1^\infty \frac{g(t'')\,dt''}{t''+t'}. \tag{D2}$$

To evaluate the integral over t' we clearly need only

$$\mathcal{J} = \frac{1}{2\pi i}\int_1^\infty \frac{2X^+(t')\,dt'}{(t'-z)(t'+t'')}. \tag{D3}$$

Consider the function $X(z)/(z+t'')$. It has the following properties:

(i) It vanishes as $|z|^{-\frac{1}{2}}$ at infinity.

(ii) There is a branch cut extending from 1 to ∞. The boundary values as the cut is approached from above and below are opposite in sign.

(iii) There is a simple pole at $z = -t''$.

By Cauchys' theorem,

$$\frac{X(z)}{z+t''} = \frac{1}{2\pi i}\int_{c_1+c_2+c_3}\frac{X(z')\,dz'}{(z'+t'')(z'-z)}. \tag{D4}$$

Here c_1 encircles the branch cut. A large circle at infinity is labeled c_2. The pole at $-t''$ is excluded by a small circle c_3.

Now

$$\text{(i)}\quad \frac{1}{2\pi i}\int_{c_1}\frac{X(z')\,dz'}{(z'+t'')(z'-z)} = \frac{1}{2\pi i}\int_1^\infty \frac{2X^+(t')\,dt'}{(t'+t'')(t'-z)}, \tag{D5}$$

$$\text{(ii)}\quad \frac{1}{2\pi i}\int_{c_2}\frac{X(z')\,dz'}{(z'+t'')(z'-z)} = 0, \tag{D6}$$

$$\text{(iii)}\quad \frac{1}{2\pi i}\int_{c_3}\frac{X(z')\,dz'}{(z'+t'')(z'-z)} = \frac{X(-t'')}{t''+z}. \tag{D7}$$

Inserting these integrals into Eq. (D4) we see that

$$\frac{1}{2\pi i}\int_1^\infty \frac{2X^+(t')\,dt'}{(t'+t'')(t'-z)} = \frac{X(z)-X(-t'')}{t''+z}. \tag{D8}$$

A Soluble Fermi-Gas Model. Validity of Transformations of the Bogoliubov Type

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A linear soluble Fermi-gas model is used to test the validity of perturbation theory and the criteria of instability obtained by applying transformations of the Bogoliubov type. The model Hamiltonian describing the interaction of the electrons in a simple band is

$$H(\rho) = -\sum (\cos k + \rho) c_k^+ c_k + \rho \sum \cos q \; c_{k+q}^+ c_{u-q}^+ c_u c_k.$$

For a half-filled band, the energies of the low-lying states are calculated exactly, by using previous results concerning a linear chain of spins with interaction. It is shown that perturbation theory must be valid for $-1 < \rho < 1$, and, for values of ρ belonging to this range, the slope of the specific heat for $T = 0$ is calculated by direct application of Landau's theory. On the other hand, anomalous Hartree–Fock states can be built for all values of ρ, by using transformations of the Bogoliubov type, and these states are more stable than the normal Hartree–Fock state. Thus, it appears that the Bogoliubov method may lead to completely erroneous interpretations, when the coupling constants are small.

I. INTRODUCTION

DURING recent years, the general properties of Fermi systems have been studied in great detail by many physicists. The normal states are usually described in terms of quasi-particles, which are very similar to the free particles. However, there are also collective excitations in such systems, and, since the collective modes may interact with the quasi-particles, doubts have been raised against Landau's simple theory. In any case, the whole picture relies on the validity of perturbation theory and the convergence of subseries of diagram contributions, whereas, in general, these assumptions are far from completely justified. Moreover, instabilities may occur. These instabilities are usually recognized and eliminated by transformations of the Bogoliubov type. Many instabilities have been "predicted" in this way, even for very small values of the coupling constant, but again we may wonder whether the Bogoliubov method is really reliable.

For all these reasons, simple models can be very useful if they are reasonably realistic and exactly tractable. Such models can serve as a test for the approximate theories which are proposed for the description of more complicated systems. The aim of this paper is just to present such a model and to give a partial answer to the following questions: (1) What is the validity of perturbation theory? (2) Do the results of Bogoliubov transformations provide good criteria of instability for Fermi systems?

In a previous paper,[1] the behavior of a linear chain of spins (spin $\frac{1}{2}$) with nearest neighbor anisotropic interaction has been studied in detail. The Hamiltonian of the system under consideration is

$$\mathcal{H}(\rho) = \sum_{j=1}^{N} [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \rho S_j^z S_{j+1}^z], \qquad (1)$$

where S_j is the spin operator corresponding to the site j, and ρ is an anisotropy parameter which can take any real value. Moreover, it is assumed that the number N of sites is even and that the sites form a ring; thus site $N + 1$ coincides with site 1. The ground state and the first excited states of this Hamiltonian were determined by using Bethe's method, and the energies of these states calculated exactly, in the limit of infinite chains.

On the other hand, we know that, by using an appropriate transformation,[2] it is possible to change the spin Hamiltonian $\mathcal{H}(\rho)$ into a new Hamiltonian describing a linear assembly of spinless fermions, with an interaction proportional to ρ. Therefore the previous exact solutions of the spin Hamiltonian can be used to get information on the behavior of the Fermi system, for all values of the coupling constant. For completeness and in order to introduce suitable notations, we give in Sec. II the transformation which connects the two complementary forms of the Hamiltonian $\mathcal{H}(\rho)$. In Sec. III, we discuss the nature of the ground state for all values of ρ, and the validity of perturbation theory for small values of ρ. In Sec. IV, the Bogoliubov method is used to find approximate solutions of our problem, either (for $\rho > 0$) by destruction of the translational

[1] J. des Cloizeaux and M. Gaudin, J. Math. Phys. 7, 1384 (1966).

[2] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N. Y.) 16, 407 (1961).

invariance of the system, or (for $\rho < 0$) by nonconservation of the particle number. In both cases, it is shown that the method leads to unphysical results. Finally, Sec. V is devoted to a study of the excited states and to the calculation of the slope of the specific heat at $T = 0$.

II. TRANSFORMATION OF THE HAMILTONIAN $\mathcal{H}(\rho)$

The spin Hamiltonian $\mathcal{H}$ can be written as

$$\mathcal{H}(\rho) = \sum_{i=1}^{N} [\tfrac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \rho S_i^z S_{i+1}^z], \quad (2)$$

where

$$S_i^+ = S_i^x + iS_i^y, \qquad S_i^- = S_i^x - iS_i^y. \quad (3)$$

Let us introduce new operators c_i^+ and c_i, by setting

$$c_i^+ = S_i^+ \exp\left[i\pi \sum_{l=1}^{i-1} (S_l^z + \tfrac{1}{2})\right], \quad j = 1, \cdots, N,$$
$$c_i = \exp\left[-i\pi \sum_{l=1}^{i-1} (S_l^z + \tfrac{1}{2})\right] S_i^-. \quad (4)$$

These operators are Fermi operators and we can prove immediately the relations

$$[c_i^+, c_l]_+ = \delta_{il}, \qquad [c_i^+, c_l^+]_+ = [c_i, c_l]_+ = 0. \quad (5)$$

We note also that

$$S_i^z = c_i^+ c_i - \tfrac{1}{2}. \quad (6)$$

By using this relation, we can express the operators S_i^+ and S_i^- in terms of the operators c_l^+ and c_l,

$$S_i^+ = c_i^+ \exp\left[-i\pi \sum_{l=1}^{i-1} c_l^+ c_l\right],$$
$$S_i^- = \exp\left[i\pi \sum_{l=1}^{i-1} c_l^+ c_l\right] c_i. \quad (7)$$

The Hamiltonian $\mathcal{H}(\rho)$ can be written in terms of the operators c_i^+ and c_i: we get

$$\mathcal{H}(\rho) = \sum_{i=1}^{N} [\tfrac{1}{2}(c_{i+1}^+ c_i + c_i^+ c_{i+1}) + \rho(c_{i+1}^+ c_{i+1} - \tfrac{1}{2})(c_i^+ c_i - \tfrac{1}{2})] - \tfrac{1}{2}(c_N^+ c_1 + c_1^+ c_N)[\exp(i\pi n) + 1], \quad (8)$$

with

$$n = \sum_{i=1}^{N} c_i^+ c_i. \quad (9)$$

The last term both destroys the translational invariance of $\mathcal{H}(\rho)$ and introduces boundary contributions. However, as we are interested only in the bulk properties of the system in the limit of long chains, we can drop this term without significantly changing the spectrum of $\mathcal{H}(\rho)$ or the thermodynamic properties of the system. Finally, we define the Fourier transforms c_k^+ and c_k of c_i^+ and c_i by

$$c_k^+ = N^{-\frac{1}{2}} \sum_i e^{i(k+\pi)i} c_i^+, \qquad c_k = N^{-\frac{1}{2}} \sum_i e^{-i(k+\pi)i} c_i. \quad (10)$$

The Hamiltonian $\mathcal{H}(\rho)$ becomes

$$\mathcal{H}(\rho) \simeq H(\rho) = -\sum (\cos k + \rho) c_k^+ c_k + \rho N^{-1} \sum \cos q\, c_{k+q}^+ c_{u-q}^+ c_u c_k + \tfrac{1}{4} N\rho. \quad (11)$$

The number n of particles corresponding to an eigenstate of H is related to the value M of S^z [for the corresponding spin state of $\mathcal{H}(\rho)$] by

$$n = \sum c_k^+ c_k = M + \tfrac{1}{2}N. \quad (12)$$

Thus an antiferromagnetic state ($M = 0$) corresponds to a state with a half-filled band, a ferromagnetic state with $M = \pm\frac{1}{2}N$ corresponds to a state in which the band is either empty or completely full. On the other hand, we must note that the process which transforms $\mathcal{H}(\rho)$ into $H(\rho)$ does not conserve the total wavenumber.

III. NATURE OF THE GROUND STATE OF $H(\rho)$ FOR A HALF-FILLED BAND ($n = \frac{1}{2}N$)

Let us consider the ground state of $H(\rho)$ when the number of electrons is just half the number of sites. This state corresponds to the antiferromagnetic ground state of $\mathcal{H}(\rho)$ ($M = 0$). We saw in a previous paper[1] that the ground-state energy per site is a continuous function of ρ; this function is given by different analytic expressions in the three domains $\rho \leq -1$, $-1 \leq \rho \leq 1$, and $\rho \geq 1$ (see Fig. 1).

In the domain $-1 \leq \rho \leq +1$, we set

$$\rho = \cos\Theta, \qquad 0 \leq \Theta \leq \pi, \quad (13)$$

and with these notations, the ground-state energy per site is given by

$$e(\rho) = e_1(\rho) \equiv \tfrac{1}{4}\rho - \sin\Theta \int_0^\infty \left[1 - \frac{\tanh \omega\Theta}{\tanh \omega\pi}\right] d\omega. \quad (14)$$

Thus, $e(\rho)$ is an analytic function of ρ in this range. This result, which is far from being obvious *a priori* (as will be emphasized in the next section), shows that perturbation theory must be valid for $-1 < \rho < 1$. Actually, perturbation calculations have been performed by Katsura and Inawashiro,[3] who found (in our notation)

$$e(\rho) = -\frac{1}{\pi} - \frac{\rho}{\pi^2} + \left(\frac{1}{18\pi} - \frac{4}{3\pi^3}\right)\rho^2 + O(\rho^3). \quad (15)$$

[3] S. Katsura and S. Inawashiro, J. Math. Phys. 5, 1091 (1964).

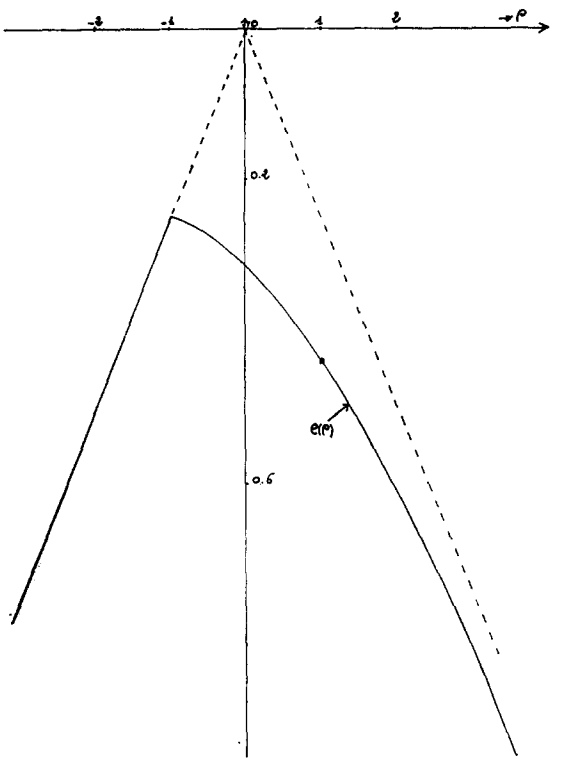

FIG. 1. Ground-state energy per site $e(\rho)$ of $H(\rho)$.

A straightforward calculation shows that the same result is obtained by expanding the function $e_1(\rho)$ given by Eq. (14), in terms of ρ.

On the other hand, perturbation theory breaks down for $|\rho| > 1$. In the domain $\rho \geq 1$, we may set

$$\rho = \cosh \Phi, \qquad \Phi > 0, \tag{16}$$

and, in this case, the ground-state energy per site is given by a different expression:

$$e(\rho) = e_2(\rho) \equiv \tfrac{1}{4}\rho - \sinh \Phi \left[\sum_{n=1}^{\infty} (1 - \tanh n\Phi) + \tfrac{1}{2} \right]. \tag{17}$$

The functions $e_1(\rho)$ and $e_2(\rho)$ differ completely from each other and therefore $e(\rho)$ is nonanalytic for $\rho = 1$. However, at this point and for real values of ρ, $e(\rho)$ and all its derivatives are continuous. It seems that this point corresponds to a transition between the normal metallic state and an insulating state. This view is supported by the appearance (for $\rho > 1$) of a gap $G(\rho)$ in the spectrum of the one-electron excitations. This gap is given by

$$G(\rho) = \sinh \Phi \sum_{-\infty}^{+\infty} \frac{(-)^n}{\cosh n\Phi} \tag{18}$$

(see Fig. 2).

This fact suggests that a good approximation for the case $\rho > 1$ might be obtained by using a transformation of the Bogoliubov type. This possibility is discussed in the next section, but, even now, we can remark that this approach seems justified if the transition at $\rho = 1$ corresponds to the appearance of long-range order when ρ becomes larger than one.

Finally, the value $\rho = -1$ is also a transition point. It is easy to show that, for $\rho \leq -1$, the ground state of $\mathcal{H}(\rho)$ is ferromagnetic ($M = \pm\frac{1}{2}N$). In this case, it is not difficult to build approximate antiferromagnetic ground states ($M = 0$), for which the mean energy per site coincides, in the limit of an infinite chain, with the ferromagnetic ground-state energy. For instance, we may assume that the spins point upward on the sites of order $1, 2, \cdots, \frac{1}{2}N$, and point downward on the sites of order $(\frac{1}{2}N + 1), \cdots, N$. This remark shows that, for $\rho < -1$, the ground state of $H(\rho)$ (with $n = \frac{1}{2}N$) is quasi-degenerate. In the ground state, all the electrons have a tendency to adhere to one another and therefore to form a drop. Thus, the point $\rho = 1$ corresponds to a liquid–gas transition, and for $\rho < -1$ we have

$$e(\rho) = e_3(\rho) = \tfrac{1}{4}\rho. \tag{19}$$

Consequently, for $\rho = -1$, $e(\rho)$ is continuous but a discontinuity appears in its derivative.

IV. HARTREE–FOCK APPROXIMATIONS AND THE NATURE OF THE GROUND STATE OF $H(\rho)$

In the sections above, it was shown that the ground state of $H(\rho)$, regular in the domain $-1 < \rho < 1$, can be obtained from the normal metallic Hartree–Fock state by perturbation theory. This normal state is, of course, the ground state of $H(0)$. Now, we want to show that, for any value of ρ

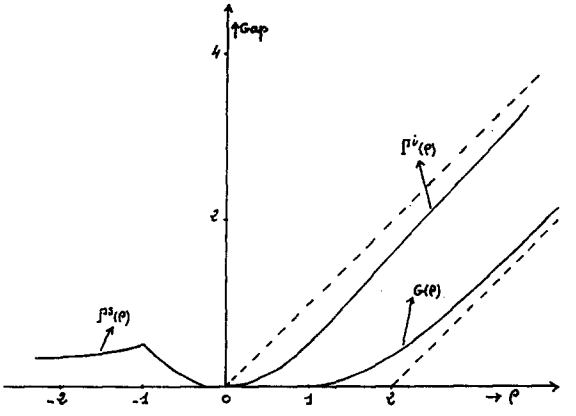

FIG. 2. Variations of the gaps $G(\rho)$, $\Gamma^i(\rho)$, and $\Gamma^s(\rho)$, where $G(\rho)$ is obtained by an exact calculation, $\Gamma^i(\rho)$ and $\Gamma^s(\rho)$ correspond to spurious instabilities.

($\rho \neq 0$), this normal Hartree–Fock state is unstable with respect to an anomalous Hartree–Fock state. For $\rho > 1$, this anomalous state is produced by destroying the translational invariance of the system, and the system then becomes an insulator with a gap appearing for all positive values of ρ. For $\rho < 1$, another kind of anomalous state is produced by nonconservation of the particle number; in this case, the system becomes superconducting, even for very small values of ρ, and again a gap appears. We just apply the methods which are currently used for predicting instabilities in Fermi systems, and the results of our transformations suggest, as usual, that the ground-state energy should not be an analytical function of ρ for $\rho = 0$.

But we know the exact result here; we know that the real ground state[4] has a normal behavior in the range $-1 < \rho < 1$, and we know that the ground-state energy per site is an anlytical function of ρ. Thus, this example shows that simple treatments using Bogoliubov transformations and Hartree–Fock approximations may be very misleading when the coupling constants appearing in the problem are small.

Now, let us build these anomalous Hartree–Fock states[5] explicitly for $\rho > 0$ and $\rho < 0$.

A. Insulating Hartree–Fock States. ($\rho > 0$)

We introduce new Fermi operators A_k^+, A_k and B_k^+, B_k by setting

$$\begin{aligned} A_k^+ &= \cos\varphi_k c_k^+ + \sin\varphi_k c_{k+\pi}^+, \\ A_k &= \cos\varphi_k c_k + \sin\varphi_k c_{k+\pi}, \end{aligned} \tag{20}$$

$$\begin{aligned} B_k^+ &= -\sin\varphi_k c_k^+ + \cos\varphi_k c_{k+\pi}^+, \\ B_k &= -\sin\varphi_k c_k + \cos\varphi_k c_{k+\pi}, \end{aligned} \tag{21}$$

where φ_k, a periodic function of k, satisfies the conditions (see Fig. 3):

$$0 < \varphi_k < \tfrac{1}{2}\pi, \quad \varphi_k = \varphi_{-k}, \quad \varphi_k + \varphi_{k+\pi} = \tfrac{1}{2}\pi. \tag{22}$$

Consequently, we have

$$\begin{aligned} A_{k+\pi}^+ &= A_k^+, \qquad A_{k+\pi} = A_k, \\ B_{k+\pi}^+ &= -B_k^+, \qquad B_{k+\pi} = -B_k. \end{aligned} \tag{23}$$

Conversely, we can write

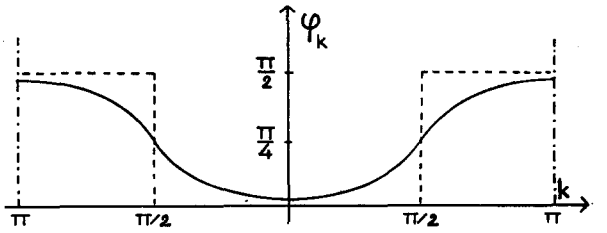

FIG. 3. Variations of φ_k with respect to the wavenumber k (schematical picture).

$$\begin{aligned} c_k^+ &= \cos\varphi_k A_k^+ - \sin\varphi_k B_k^+, \\ c_k &= \cos\varphi_k A_k - \sin\varphi_k B_k. \end{aligned} \tag{24}$$

Now, the Hamiltonian $H(\rho)$ can be expressed in terms of the new operators, and a trial ground state $|\omega_i\rangle$ is defined by

$$|\omega_i\rangle = \prod_{|k|<\frac{1}{2}\pi} A_k^+ |0\rangle, \tag{25}$$

where $|0\rangle$ is the vacuum state. The Hamiltonian $H(\rho)$ is ordered by writing the operators A_k and B_k^+ to the right of the operators A_k^+ and B_k. Then, $H(\rho)$ takes the form

$$H(\rho) = H_0^i(\rho) + H_1^i(\rho) + H_2^i(\rho), \tag{26}$$

where $H_0^i(\rho)$ is a constant, $H_1^i(\rho)$ a one-body operator and $H_2^i(\rho)$ a two-body interaction. Incidentally, we note that, if we choose $\varphi_k = 0$ for $-\frac{1}{2}\pi < k < \frac{1}{2}\pi$ and $\varphi_k = \frac{1}{2}\pi$ for $\frac{1}{2}\pi < k < \frac{3}{2}\pi$, the trial ground state $|\omega_i\rangle$ coincides with the normal Hartree–Fock state. The constant $H_0^i(\rho)$ is the expectation value of $H(\rho)$ for the state $|\omega_i\rangle$, and by minimizing this quantity, we can determine the function φ_k. We have

$$\begin{aligned} H_0^i(\rho) &= \langle\omega_i|\, H(\rho)\, |\omega_i\rangle \\ &= -\sum{}' \cos k \cos 2\varphi_k - \rho N^{-1}\Big(\sum{}' \sin 2\varphi_k\Big)^2 \\ &\quad - \rho N^{-1}\Big(\sum{}' \cos k \cos 2\varphi_k\Big)^2. \end{aligned} \tag{27}$$

Here, and in the following, the symbol $\sum'$ indicates a summation over the values of k belonging to the interval $|k| < \frac{1}{2}\pi$. The state $|\omega_i\rangle$ obtained by minimization of $H_0^i(\rho)$ is a Hartree–Fock state because the conditions

$$\partial H_0^i(\rho)/\partial\varphi_k = 0 \tag{28}$$

and

$$H_1^i(\rho)_{\text{nondiag}} = 0 \tag{29}$$

are equivalent. More explicitly, these equations imply the relations

$$\tan 2\varphi_k = \alpha/\cos k, \tag{30}$$

[4] This state is determined by using Bethe's criteria. It is assumed that the eigenstate of $\mathcal{H}(\rho)$, which is determined by using Bethe's method, coincides always with the ground state, but this fact has never been rigorously proved; however, this result can be checked in many ways.

[5] Note that the mean energy per site which will be calculated for these states, would not be changed if $H(\rho)$ was replaced by $\mathcal{H}(\rho)$.

where α, a constant, expressible in terms of sums β and γ as

$$\alpha = \beta(1 + \gamma)^{-1}, \tag{31}$$

where β and γ are given by

$$\beta = 2\rho N^{-1} \sum{}' \sin 2\varphi_k \simeq \frac{2\rho}{\pi} \int_0^{\frac{1}{2}\pi} \sin 2\varphi_k \, dk, \tag{32}$$

$$\gamma = 2\rho N^{-1} \sum{}' \cos k \cos 2\varphi_k \simeq \frac{2\rho}{\pi} \int_0^{\frac{1}{2}\pi} \cos k \cos 2\varphi_k \, dk. \tag{33}$$

Relation (30) was derived for $|k| < \frac{1}{2}\pi$, but according to Eq. (22), it is valid for all values of k. Moreover, we have

$$\sin 2\varphi_k = \alpha(\alpha^2 + \cos^2 k)^{-\frac{1}{2}}, \qquad \cos 2\varphi_k = \cos k(\alpha^2 + \cos^2 k)^{-\frac{1}{2}}. \tag{34}$$

Now, the constants β and γ can be expressed in terms of α

$$\beta = \frac{2\rho}{\pi} \int_0^{\frac{1}{2}\pi} \frac{\alpha}{(\alpha^2 + \cos^2 k)^{\frac{1}{2}}} \, dk, \tag{35}$$

$$\gamma = \frac{2\rho}{\pi} \int_0^{\frac{1}{2}\pi} \frac{\cos^2 k}{(\alpha^2 + \cos^2 k)^{\frac{1}{2}}} \, dk. \tag{36}$$

By substituting these values in Eq. (31), we find immediately the implicit equation which determines α,

$$\int_0^{\frac{1}{2}\pi} \frac{\sin^2 k}{(\alpha^2 + \cos^2 k)^{\frac{1}{2}}} \, dk = \frac{\pi}{2\rho}. \tag{37}$$

For positive values of ρ, this equation has one and only one solution. The corresponding value of $H_0^i(\rho)$ is given by

$$H_0^i(\rho) = -(N/4\rho)[2\gamma + \beta^2 + \gamma^2], \tag{38}$$

and it is not difficult to show (see Appendix A) that this quantity is smaller than the value $H_0(\rho)$ obtained for the normal Hartree–Fock state

$$H_0^i(\rho) < H_0(\rho) = -N(\pi^{-1} + \rho\pi^{-2}). \tag{39}$$

Thus, the instability of the normal Hartree–Fock state is established for all positive values of ρ. Moreover, we note that $H_0^i(\rho)$ has a singularity for $\rho = 0$.

When φ_k is given by Eqs. (30) and (37), the one-body part $H(\rho)$ takes a very simple form

$$H_1^i(\rho) = [(1 + \gamma)(\alpha^2 + \cos^2 k)^{\frac{1}{2}} + \rho]B_k^+ B_k + [(1 + \gamma)(\alpha^2 + \cos^2 k)^{\frac{1}{2}} - \rho]A_k A_k^+. \tag{40}$$

The gap corresponding to the excitations of this Hamiltonian is given by $2\Gamma^i(\rho)$

$$\Gamma^i(\rho) = (1 + \gamma)\alpha. \tag{41}$$

This function increases very slowly and for small values of ρ

$$\Gamma^i(\rho) \sim 4 \exp[-1 - \pi/2\rho], \qquad \rho \ll 1, \tag{42}$$

but, when $\rho \to \infty$, we have

$$\Gamma^i(\rho) - \rho \to 0. \tag{43}$$

Thus the functions $\Gamma(\rho)$ and $G(\rho)$ have a very similar behavior, as is shown in Fig. 2.

The preceding transformation can be easily interpreted. We know that, for large values of ρ, the ground state of $\mathcal{H}(\rho)$ becomes degenerate (in the limit $\rho \to \infty$, the spins associated with the sites point alternatively upwards and downwards). This means that, when $\rho \to \infty$, the electrons have a tendency to congregate on the sublattice formed by the sites of even (or odd) order. But partial congregation and consequently long range order may occur also for smaller values of ρ. The transformation introduced above is a mechanism which produces this effect artificially. Thus, it destroys translational symmetry. The Brillouin zone is split into two smaller zones, and consequently the system becomes an insulator.

The exact results described in the previous section indicate that a phenomenon of this nature probably occurs for $\rho > 1$, and this would explain the appearance of the gap $G(\rho)$ in this range. However, for $\rho < 1$, the artificial transformation which has been introduced above seems completely unrealistic, in spite of the instability of the normal Hartree–Fock state with respect to the anomalous insulating Hartree–Fock state. This kind of effect is probably very general and another illustration of such a phenomenon is given just below.

B. Superconducting Hartree–Fock States ($\rho < 0$)

This time, we transform $H(\rho)$ by using an ordinary Bogoliubov transformation, which amounts to binding two electrons in an antisymmetric state (symmetric coupling is forbidden by the Pauli principle and we have spinless fermions). For this purpose, we introduce the quasi-particle creation and annihilation operators b_k^+ and b_k:

$$b_k^+ = e^{\frac{1}{2}ik}(\cos\theta_k c_k + \sin\theta_k c_{-k}^+), \qquad b_k = e^{-\frac{1}{2}ik}(\cos\theta_k c_k^+ + \sin\theta_k c_{-k}), \tag{44}$$

with

$$\theta_{-k} = -\theta_k, \qquad \theta_0 = 0, \qquad \theta_{\pm\pi} = \pm\tfrac{1}{2}\pi. \tag{45}$$

The angle θ_k is determined by a minimization process, but its expected variations with respect to

k are shown in Fig. 4. For the sake of simplicity, we assume also the supplementary condition

$$\theta_k + \theta_{\pi-k} = \tfrac{1}{2}\pi. \tag{46}$$

The operators c_k^+ and c_k can be easily expressed in terms of the Fermi operators b_k^+ and b_k:

$$\begin{aligned} c_k^+ &= e^{\frac{1}{2}ik}(\cos\theta_k\, b_k - \sin\theta_k\, b_{-k}^+), \\ c_k &= e^{-\frac{1}{2}ik}(\cos\theta_k\, b_k^+ - \sin\theta_k\, b_{-k}). \end{aligned} \tag{47}$$

The trial ground state $|\omega_s\rangle$ is defined by the conditions

$$b_k\,|\omega_s\rangle = 0. \tag{48}$$

On the average, this state corresponds to a half-filled band, since we have

$$n = \sum_k \langle\omega_s|\, c_k^+ c_k\, |\omega_s\rangle = \sum_k \cos^2\theta_k = \tfrac{1}{2}N \tag{49}$$

according to assumption (46).

Now, we replace c_k^+ and c_k in $H(\rho)$ by their expressions in terms of the operators b_k^+, b_k, and we order $H(\rho)$ by putting b_k to the right of b_k^+. We obtain

$$H(\rho) = H_0^s(\rho) + H_1^s(\rho) + H_2^s(\rho), \tag{50}$$

where $H_0^s(\rho)$ is a constant, $H_1^s(\rho)$ a one-body operator, and $H_2^s(\rho)$ a two-body interaction. We have

$$\begin{aligned} H_0^s(\rho) = \langle\omega_s|\, H(\rho)\, |\omega_s\rangle &= -\sum{}' \cos k \cos 2\theta_k \\ &\quad - N^{-1}(\sum{}' \cos k \cos 2\theta_k)^2 \\ &\quad + N^{-1}(\sum{}' \sin k \sin 2\theta_k)^2. \end{aligned} \tag{51}$$

Here again, the symbol $\sum'$ indicates a summation over the range $|k| < \frac{1}{2}\pi$. The equivalent conditions

$$\partial H_0^s(\rho)/\partial\rho = 0 \tag{52}$$

and

$$H_1^s(\rho)_{\text{nondiag}} = 0 \tag{53}$$

imply the relations

$$\tan 2\theta_k = -\lambda \tan k, \tag{54}$$

where λ is a constant which can be expressed in terms of two sums μ and ν; we have

$$\lambda = \mu/(1+\nu), \tag{55}$$

where μ and ν are given by

$$\begin{aligned} \mu &= \frac{2\rho}{N}\sum{}' \sin k \sin 2\theta_k \\ &\simeq \frac{2\rho}{\pi}\int_0^{\frac{1}{2}\pi} \sin k \sin 2\theta_k\, dk, \end{aligned} \tag{56}$$

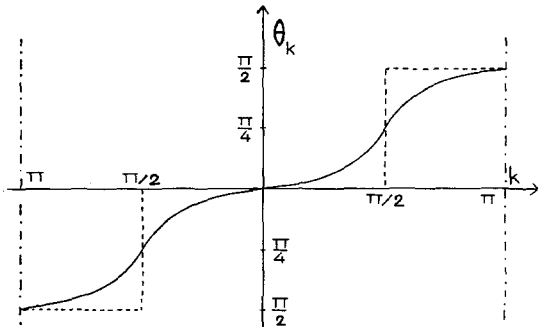

FIG. 4. Variations of θ_k with respect to the wavenumber k (schematical picture).

$$\begin{aligned} \nu &= \frac{2\rho}{N}\sum{}' \cos k \cos 2\theta_k \\ &\simeq \frac{2\rho}{\pi}\int_0^{\frac{1}{2}\pi} \cos k \cos 2\theta_k\, dk. \end{aligned} \tag{57}$$

Relation (54) was derived for $|k| < \frac{1}{2}\pi$, but according to Eq. (46) it is valid also for all values of k. (Note that θ_k is not really a periodic function of k.)

Thus we have

$$\begin{aligned} \sin 2\theta_k &= -\frac{\lambda \sin k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}, \\ \cos 2\theta_k &= \frac{\cos k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}. \end{aligned} \tag{58}$$

Now, the constants μ and ν can be expressed in terms of λ and we get

$$\mu = -\frac{2\rho}{\pi}\int_0^{\frac{1}{2}\pi} \frac{\lambda \sin^2 k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\, dk, \tag{59}$$

$$\nu = \frac{2\rho}{\pi}\int_0^{\frac{1}{2}\pi} \frac{\cos^2 k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\, dk. \tag{60}$$

By inserting these values in Eq. (55), we finally find the implicit equation which determines λ

$$\int_0^{\frac{1}{2}\pi} \frac{dk}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}} = -\frac{\pi}{2\rho}. \tag{61}$$

This equation has a unique solution for negative values of ρ. The corresponding value of $H_0^s(\rho)$ is given by

$$H_0^s(\rho) = (N/4\rho)(-2\nu + \mu^2 - \nu^2), \tag{62}$$

and it is not difficult to show that the normal Hartree–Fock state is unstable with respect to the new state $|\omega_s\rangle$ since we have (See Appendix B)

$$H_0^s(\rho) < H_0(\rho) = -N(\pi^{-1} + \rho\pi^{-2}). \tag{63}$$

On the other hand, $H_0^s(\rho)$ has a singularity for $\rho = 0$.

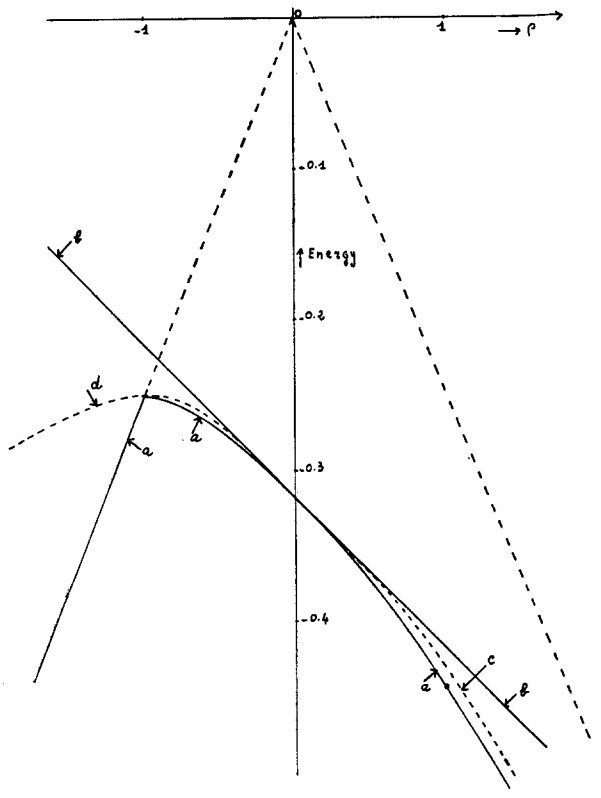

FIG. 5. (a) Ground-state energy per site $e(\rho)$ of $H(\rho)$. (b) Mean energy per site $N^{-1}H_0(\rho)$ of the normal Hartree–Fock state. (c) Mean energy per site $N^{-1}H_0'(\rho)$ of the insulating Hartree–Fock state ($\rho > 0$). (d) Mean energy per site $N^{-1}H_0^s(\rho)$ of the superconducting Hartree–Fock state ($\rho < 0$).

When θ_k is given by Eqs. (54) and (61), the one-body part of the Hamiltonian can be written as

$$H_1^s(\rho) = \sum (1 + \nu)(\cos^2 k + \lambda^2 \sin^2 k) b_k^+ b_k. \quad (64)$$

The new ground state is superconducting and a gap $\Gamma^s(\rho)$ appears in the spectrum of the elementary excitations. We have

$$\Gamma^s(\rho) = (1 + \nu)\lambda \quad \text{for} \quad -1 \leq \rho < 0 \qquad (0 < \lambda \leq 1) \quad (65)$$

and

$$\Gamma^s(\rho) = 1 + \nu \quad \text{for} \quad \rho \leq -1 \qquad (\lambda > 1). \quad (66)$$

Thus, $\Gamma^s(\rho)$ is maximum for $\rho = -1$, and indeed behaves rather strangely at this point.

On the other hand, for $-1 < \rho < 0$, the Bogoliubov transformation gives an expectation value $N^{-1}H_0(\rho)$ which does not differ much from the exact ground-state energy per site $e(\rho)$. In particular, we have

$$N^{-1}H_0^s(-1) = e(-1) = -\tfrac{1}{4}. \quad (67)$$

Moreover, a simple calculation shows that we have also

$$N^{-1}\left[\frac{d}{d\rho} H_0^s(\rho)\right]_{\rho=-1} = e'(-1 + 0) = 0. \quad (68)$$

We now see that, by using different kinds of transformations, we can build anomalous Hartree–Fock states with energies lower than the energy of the normal state, for all values of ρ ($\rho \neq 0$). Moreover, with the help of such transformations, we obtain very good approximations of the ground-state energy for $-1 < \rho < 1$, as can be seen in Fig. 5. However, we know by direct calculation that the Fermi gas has a normal behavior for $-1 < \rho < 1$ and, in particular, that the ground-state energy per site is an analytical function of ρ in the domain $|\rho| < 1$. Thus, in this case, the Bogoliubov methods fail to give good descriptions of the behavior of the system for $-1 < \rho < 1$. Therefore, we are led to believe that, in general, the application of Bogoliubov method to Fermi systems may be misleading, especially if the coupling constant is small. In particular, the results of transformations of the Bogoliubov type may suggest wrong conclusions concerning the nature of the ground state. It seems that, in general, an interaction cannot produce an instability unless it attains a definite threshold.

V. EXCITED STATES: SLOPE OF THE SPECIFIC HEAT

As the ground state of $H(\rho)$ has a normal behavior for $|\rho| < 1$, we can suppose that there is a good chance for Landau's theory to be valid in this region. On the other hand, the first excited states of $\mathfrak{IC}(\rho)$ have been determined; for each wavenumber, there are three spin waves of spin component $M = 1, 0, -1$ and these are degenerate. The excitation energy of a spin wavenumber q (with respect to the ground state) is given by

$$\eta(\rho, q) = (\pi \sin \Theta/2\Theta)\, |\sin q| \quad (69)$$

with

$$\rho = \cos \Theta, \qquad 0 < \Theta < \pi.$$

Now, we note that a spin wave of spin $M = 1$ corresponds to a one-electron excitation of $H(\rho)$. But the transformation which connects the spin operators and the fermion operators introduces a shift in the wavenumbers, and therefore the creation of an electron at the Fermi surface ($k = \pm\frac{1}{2}\pi$) must be associated with the excitation of a spin wave of wavenumber zero.

Thus, if we denote by $\epsilon(\rho, k)$ the energy of a quasi-particle of wavenumber k, we can write

$$\epsilon(\rho, k) = \eta(\rho, k - \tfrac{1}{2}\pi). \quad (70)$$

This result can be checked by perturbation; a second-order calculation gives

$$\epsilon(\rho, k) = -\cos k\left[1 + \frac{2\rho}{\pi} - \left(\frac{1}{2} - \frac{4}{\pi^2}\right)\rho^2 + \cdots\right], \tag{71}$$

and it is easy to see that this expansion agrees with Eqs. (69) and (70).

Now, from Eq. (68), we can deduce the Fermi energy $\epsilon_F(\rho)$ and the velocity $v(\rho)$ of an electron at the Fermi surface. We have

$$\epsilon_F(\rho) = \epsilon(\rho, \tfrac{1}{2}\pi) = 0, \tag{72}$$

$$v(\rho) = [\partial\epsilon(\rho, k)/\partial k]_{k=\frac{1}{2}\pi} = [\partial\eta(\rho, q)/\partial q]_{q=0}. \tag{73}$$

Thus, the Fermi energy is independent of ρ, and an exact value of the velocity $v(\rho)$ of an electron at the Fermi surface can be given for $|\rho| \leq 1$

$$\begin{aligned} v(\rho) &= (\pi \sin\Theta/2\Theta) \\ &\simeq 1 + \frac{2\rho}{\pi} - \left[\frac{1}{2} - \frac{4}{\pi^2}\right]\rho^2 + \cdots . \end{aligned} \tag{74}$$

By direct application of Landau's theory, we can now obtain the slope of the specific heat per site $C(\rho, T)$ for $T = 0$,

$$[\partial C(\rho, T)/\partial T]_{T=0} = \pi K^2/3v(\rho)$$
$$(K = \text{Boltzmann constant}).$$

With the help of the previous calculation, we can express $v(\rho)$ in terms of ρ

$$\begin{aligned} [\partial C(\rho, T)/\partial T]_{T=0} &= \tfrac{2}{3}(\Theta/\sin\Theta)K^2 \\ &= \tfrac{2}{3}K^2(1-\rho^2)^{-\frac{1}{2}}\cos^{-1}\rho \\ &\simeq \tfrac{1}{3}K^2\pi\left(1 - \frac{2\rho}{\pi} + \frac{\rho^2}{2} + \cdots\right) \end{aligned} \tag{75}$$

(See Fig. 6). In particular, we have

$$[\partial C(1, T)/\partial T]_{T=0} = \tfrac{2}{3}K^2 \tag{76}$$

and this value is in perfect agreement with the calculations of Bonner and Fisher.[6]

This result may be exact in spite of the dubious validity of the assumptions which have been used for its derivation. However, we may wonder why collective excitations of low energy (zero sound for instance) do not seem to contribute to the specific heat as they should.[7] A definite answer to this question demands a complete study of the excitations for our model. However, a few remarks can be made concerning the existence of such excitations. First, it must be realized that approximate calculations of collective modes may lead to wrong results. For instance, for $0 < \rho < 1$, the random phase approximation cannot be used for the normal state; since there exists an anomalous Hartree–Fock state of lowest energy, this approximation would lead to build collective excitations of negative energy (for instance an unstable electron-hole pair of wavenumber π), and this result obviously would be absurd. On the other hand, such a calculation does not even indicate the existence of low-lying excitations. In fact, for $\rho = 1$, Pearson and the author[8] tried to determine the eigenstates of $H(\rho)$ which, for a given wavenumber, have the lowest energy: the excited states which were found, do not seem to possess any collective character. This fact may explain the agreement between our result and the machine calculation of Bonner and Fischer.

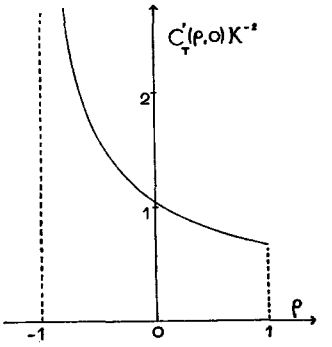

FIG. 6. Slope of the specific heat for $|\rho| \leq 1$ (exact calculation).

VI. CONCLUSION

Thus, the ground state and the first excited states of $H(\rho)$ have been studied for all values of ρ and this investigation shows clearly that perturbation theory and Landau's theory must be valid for $|\rho| < 1$; actually, many results which have been deduced from these theories have been checked by direct methods and good agreements have been obtained.

These facts are both striking and unexpected. Linear systems seem, *a priori*, very sensitive to instabilities; in fact, as was shown above, it is not difficult to predict erroneously such instabilities, by using current methods such as Bogoliubov transformations.

Consequently, doubts can be raised concerning the validity of these methods, in the case of three-dimensional systems. Hartree–Fock–Bogoliubov approximations do not seem sufficient to establish the existence of instabilities; they just give an in-

[6] J. C. Bonner and M. E. Fischer, Phys. Rev. 135, A640 (1964).

[7] The author is indebted to Dr. J. Zittartz for calling his attention on this point.

[8] J. des Cloizeaux and J. J. Pearson, Phys. Rev. 128, 2131 (1962).

dication. Moreover, the situation is not improved by introducing small corrections such as mass or charge renormalization. The preceding investigation suggests that no instabilities can occur if the coupling constant is small, but the question cannot be decided for real systems without careful examination. In any case, the present work shows that more sophisticated methods are needed in order to treat properly these problems of instabilities in Fermi systems.

ACKNOWLEDGMENTS

The author is indebted to J. F. Renardy for perturbation calculations and to Mrs. N. Tichit for numerical computations, and the author wishes to thank them for their help.

APPENDIX A

We want to prove the relation

$$2\gamma + \beta^2 + \gamma^2 > 4\pi^{-1}\rho + 4\pi^{-2}\rho^2. \tag{A1}$$

When the quantities β, γ, and ρ^{-1} are replaced by the integrals (35), (36), and (37), this condition becomes

$$\left(\int_0^{\frac{1}{2}\pi} \frac{\alpha}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk\right)^2 + \left(\int_0^{\frac{1}{2}\pi} \frac{\cos^2 k}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk\right) + 2\left(\int_0^{\frac{1}{2}\pi} \frac{\sin^2 k}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk\right)\left(\int_0^{\frac{1}{2}\pi} \frac{\cos^2 k}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk\right) > 1 + 2\int_0^{\frac{1}{2}\pi} \frac{\sin^2 k}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk, \tag{A2}$$

which is equivalent to the inequality

$$(1+\alpha^2)^{\frac{1}{2}} \int_0^{\frac{1}{2}\pi} \frac{dk}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}} > 1 + \int_0^{\frac{1}{2}\pi} \frac{\sin^2 k}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk. \tag{A3}$$

This equation can also be written

$$\int_0^{\frac{1}{2}\pi} \frac{\cos^2 k - \cos k(\alpha^2+\cos^2 k)^{\frac{1}{2}} + (1+\alpha^2)^{\frac{1}{2}} - 1}{(\alpha^2+\cos^2 k)^{\frac{1}{2}}}\,dk > 0. \tag{A4}$$

In order to prove this relation it will be sufficient to show that the integrand is positive.

For this purpose, we set

$$f(x) = x^2 - x(\alpha^2 + x^2)^{\frac{1}{2}} \tag{A5}$$

and we have:

$$f'(x) = -\frac{[(\alpha^2+x^2)^{\frac{1}{2}} - x]^2}{(\alpha^2+x^2)^{\frac{1}{2}}} < 0. \tag{A6}$$

Thus, $f(x)$ is a monotonic function of x, and this property shows the validity of the equation

$$f(\cos k) - f(1) > 0 \quad \text{for} \quad 0 < k \leq \tfrac{1}{2}\pi. \tag{A7}$$

This relation is just what we need for proving Eq. (A4), which is equivalent to the statement (A1).

APPENDIX B

We want to prove the relation

$$-2\nu + \mu^2 - \nu^2 > -4\pi^{-1}\rho - 4\pi^{-2}\rho^2 \quad \text{for} \quad \rho < 0. \tag{B1}$$

By replacing μ, ν, and ρ by the integrals of (59), (60), and (61), we get

$$\left(\int_0^{\frac{1}{2}\pi} \frac{\lambda \sin^2 k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\,dk\right)^2 - \left(\int_0^{\frac{1}{2}\pi} \frac{\cos^2 k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\,dk\right) + 2\left(\int_0^{\frac{1}{2}\pi} \frac{dk}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\right) \times \left(\int_0^{\frac{1}{2}\pi} \frac{\cos^2 k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\,dk\right) > -1 + 2\int_0^{\frac{1}{2}\pi} \frac{dk}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}. \tag{B2}$$

For $\lambda \geq 1$, this relation is trivially satisfied, and for $0 < \lambda < 1$, it is equivalent to the condition

$$(1-\lambda^2)^{\frac{1}{2}} \int_0^{\frac{1}{2}\pi} \frac{\sin^2 k}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\,dk < \int_0^{\frac{1}{2}\pi} \frac{dk}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}} - 1. \tag{B3}$$

Now, Eq. (B3) can be written in the form

$$\int_0^{\frac{1}{2}\pi} \frac{\cos k(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}} - (1-\lambda^2)^{\frac{1}{2}} \cos k - 1 + (1-\lambda^2)^{\frac{1}{2}}}{(\cos^2 k + \lambda^2 \sin^2 k)^{\frac{1}{2}}}\,dk < 0. \tag{B4}$$

In order to prove this relation, it is sufficient to show that the integrand is negative.

For this purpose, we introduce the function

$$g(x) = x[x^2(1-\lambda^2) + \lambda^2]^{\frac{1}{2}} - x^2(1-\lambda^2)^{\frac{1}{2}}. \tag{B5}$$

We have

$$g'(x) = \frac{[(x^2(1-\lambda^2)+\lambda^2)^{\frac{1}{2}} - x(1-\lambda^2)^{\frac{1}{2}}]^2}{[x^2(1-\lambda^2)+\lambda^2]^{\frac{1}{2}}} > 0. \tag{B6}$$

Thus $g(x)$ is monotonic function of x and this property shows the validity of the equation

$$g(\cos k) - g(1) < 0 \quad \text{for} \quad 0 < k \leq \tfrac{1}{2}\pi. \tag{B7}$$

This inequality implies the validity of Eq. (B4) and therefore completes the proof of the statement (B1).

The Time-Dependent Green's Function for Electromagnetic Waves in Moving Simple Media

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This paper treats the problem of radiation from sources of arbitrary time dependence in a moving medium. The medium is assumed to be lossless, with permittivity ϵ and permeability μ, and to move with constant velocity $\bar{v}$ with respect to a given inertial reference frame xyz. It is shown how the Maxwell–Minkowski equations for the electromagnetic fields in the moving medium can be integrated by means of a pair of vector and scalar potential functions analogous to those commonly used with stationary media. The wave equation associated with these potential functions is derived, and a scalar Green's function is defined to satisfy the same type of equation, with a delta-function source term $\delta(\mathbf{r} - \mathbf{r}')\,\delta(t - t')$, and the casuality condition. The solution for the Green's function is derived in closed form, by means of a Fourier integral method. The resulting Green's function is useful not only for calculating the fields from arbitrary sources in moving media, but also for its pedagogical value. It is simpler to understand the phenomenon of Cerenkov radiation using this method than it is from the conventional approach to the Cerenkov problem.

INTRODUCTION

THIS paper considers the electromagnetic radiation resulting from sources of arbitrary time dependence in a moving medium. The medium is assumed to be lossless, to be of infinite extent in all directions, and to move with a constant velocity $\mathbf{v}$ with respect to an inertial coordinate system xyz. The permittivity ϵ and permeability μ of the medium (as measured in a reference frame attached to the medium) are assumed to be constant at all frequencies and at all points of the medium.

The treatment is based on Minkowski's theory of the electrodynamics of moving media,[1] which is given by Sommerfeld[2] and which has also recently been discussed by Tai[3–6] in relation to other formulations of this subject.[7,8] The Maxwell–Minkowski equations for the electromagnetic fields in the moving medium are solved by first defining suitable vector and scalar potential functions from which the fields may be calculated. The wave equation associated with these potential functions is then derived, and the appropriate Green's function is defined. The solution for the Green's function is obtained in closed form by means of a Fourier integral method.

The resulting Green's function may be used to calculate the fields resulting from known sources of arbitrary time dependence. The special case when the sources are time-harmonic, which has been previously treated by Tai[9] and Lee and Papas,[10] is discussed. Some comments are also made concerning the pedagogical value of the result.

FORMULATION OF THE PROBLEM

Consider a lossless medium with permittivity ϵ and permeability μ (measured in a reference frame attached to the medium) moving with uniform velocity $\mathbf{v} = v\hat{z}$ with respect to a given inertial reference frame. The electromagnetic fields, as measured in the given frame, must satisfy Maxwell's equations

$$\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t, \tag{1}$$

$$\nabla \times \mathbf{H} = \partial \mathbf{D}/\partial t + \mathbf{J}, \tag{2}$$

$$\nabla \cdot \mathbf{D} = \rho, \tag{3}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{4}$$

where $\mathbf{E}$ and $\mathbf{H}$ are the electric and the magnetic field intensities, $\mathbf{D}$ and $\mathbf{B}$ the electric and magnetic flux densities, and ρ and $\mathbf{J}$ the electric source charge and current densities. All quantities are measured in MKS units.

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[2] A. Sommerfeld, *Electrodynamics* (Academic Press Inc., New York, 1952), Pts. III and IV.
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[4] C. T. Tai, Proc. IEEE **52**, 685 (1964).
[5] C. T. Tai, University of Michigan, Radiation Laboratory Report RL-310 (1965).
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[10] K. S. H. Lee and C. H. Papas, J. Math. Phys. **5**, 1668 (1964).

The motion of the medium enters the problem through the constitutive relations, which are no longer the same as those for a stationary medium, but instead are

$$\mathbf{D} = \epsilon\bar{\alpha}\cdot\mathbf{E} + \mathbf{\Omega}\times\mathbf{H} \tag{5}$$

and

$$\mathbf{B} = \mu\bar{\alpha}\cdot\mathbf{H} - \mathbf{\Omega}\times\mathbf{E}, \tag{6}$$

where $\bar{\alpha}$ is the dyadic with components

$$[\bar{\alpha}] = \begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{7}$$

and where

$$a = (1 - \beta^2)/(1 - n^2\beta^2), \tag{8}$$

$$\mathbf{\Omega} = [(n^2 - 1)\beta/c(1 - n^2\beta^2)]\hat{z}, \tag{9}$$

$$\beta = v/c, \tag{10}$$

and

$$n = (\mu\epsilon/\mu_0\epsilon_0)^{\frac{1}{2}}. \tag{11}$$

[It is assumed in Eqs. (8) and (9) that $\eta\beta \neq 1$.] ϵ_0 and μ_0 are the permittivity and permeability of free-space, and $c = (\mu_0\epsilon_0)^{-\frac{1}{2}}$ is the velocity of light in free-space. Equations (5)–(11) are Minkowski's results,[11] written in a compact form discovered by Tai.[9]

Substituting Eqs. (5) and (6) in Eqs. (1)–(4), we obtain the so-called "Maxwell–Minkowski" equations, which may be rearranged slightly and written in the form

$$\mathbf{D}_0\times\mathbf{E} = -(\partial/\partial t)(\mu\bar{\alpha}\cdot\mathbf{H}), \tag{12}$$

$$\mathbf{D}_0\times\mathbf{H} = (\partial/\partial t)(\epsilon\bar{\alpha}\cdot\mathbf{E}) + \mathbf{J}, \tag{13}$$

$$\mathbf{D}_0\cdot(\epsilon\bar{\alpha}\cdot\mathbf{E}) = \rho + \mathbf{\Omega}\cdot\mathbf{J}, \tag{14}$$

$$\mathbf{D}_0\cdot(\mu\bar{\alpha}\cdot\mathbf{H}) = 0, \tag{15}$$

where $\mathbf{D}_0$ is the differential operator

$$\mathbf{D}_0 = \nabla - \mathbf{\Omega}(\partial/\partial t). \tag{16}$$

Equations (12)–(15) may be solved by making use of vector and scalar potential functions similar to those used in ordinary electromagnetic theory for stationary media. Since

$$\mathbf{D}_0\cdot\mathbf{D}_0\times\mathbf{W} \equiv 0 \tag{17}$$

and

$$\mathbf{D}_0\times\mathbf{D}_0 U \equiv 0 \tag{18}$$

for any vector $\mathbf{W}$ and scalar U whose components have continuous second partial derivatives, a generalized Helmholtz theorem may be derived which states that, for any given vector field $\mathbf{C}$, there exists a vector field $\mathbf{F}$ and a scalar field Φ such that

$$\mathbf{C} = \mathbf{D}_0\times\mathbf{F} + \mathbf{D}_0\Phi. \tag{19}$$

$\mathbf{D}_0\times\mathbf{F}$ and $\mathbf{D}_0\Phi$ would correspond to the "rotational" and "irrotational" parts of $\mathbf{C}$ in the ordinary Helmholtz theorem.

Based on Eq. (15) and the above remarks, we may define a vector potential function $\mathbf{A}$ such that

$$\mu\bar{\alpha}\cdot\mathbf{H} = \mathbf{D}_0\times\mathbf{A}. \tag{20}$$

Then substituting this into Eq. (12) gives

$$\mathbf{D}_0\times[\mathbf{E} + \partial\mathbf{A}/\partial t] = 0, \tag{21}$$

and hence we may write

$$\mathbf{E} = -\partial\mathbf{A}/\partial t - \mathbf{D}_0\Psi, \tag{22}$$

where Ψ is a suitable scalar potential function. Substituting Eqs. (20) and (22) into Eq. (13) yields

$$\mathbf{D}_0\times[\bar{\alpha}^{-1}\cdot\mathbf{D}_0\times(\bar{\alpha}^{-1}\cdot\mathbf{A}_0)] = -\epsilon\mu(\partial^2\mathbf{A}_0/\partial t^2) - \epsilon\mu\bar{\alpha}\cdot\mathbf{D}_0\frac{\partial\Psi}{\partial t} + \mu\mathbf{J}, \tag{23}$$

where $\bar{\alpha}^{-1}$ denotes the inverse of $\bar{\alpha}$ ($\bar{\alpha}^{-1}$ always exists for $\eta\beta \neq 1$) and where we have also defined

$$\mathbf{A}_0 = \bar{\alpha}\cdot\mathbf{A}. \tag{24}$$

Next, we make use of the identity

$$\mathbf{D}_0\times[\bar{\alpha}^{-1}\cdot\mathbf{D}_0\times(\bar{\alpha}^{-1}\cdot\mathbf{A}_0)] = \frac{1}{a}[\mathbf{D}_a(\mathbf{D}_0\cdot\mathbf{A}_0) - (\mathbf{D}_a\cdot\mathbf{D}_0)\mathbf{A}_0] \tag{25}$$

with

$$\mathbf{D}_a = \frac{1}{a}\bar{\alpha}\cdot\mathbf{D}_0 = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\left(\frac{1}{a}\frac{\partial}{\partial z} - \frac{\Omega}{a}\frac{\partial}{\partial t}\right) \tag{26}$$

to write Eq. (23) in the form

$$\mathbf{D}_a(\mathbf{D}_0\cdot\mathbf{A}_0) - (\mathbf{D}_a\cdot\mathbf{D}_0)\mathbf{A}_0 = -\epsilon\mu a\frac{\partial^2\mathbf{A}_0}{\partial t^2} - \epsilon\mu a\bar{\alpha}\cdot\mathbf{D}_0\frac{\partial\Psi}{\partial t} + \mu a\mathbf{J}. \tag{27}$$

Then it is easily verified that, if we choose $\mathbf{A}_0$ and Ψ to satisfy the gauge relation

$$\mathbf{D}_0\cdot\mathbf{A}_0 = -\epsilon\mu a^2(\partial\Psi/\partial t), \tag{28}$$

then it is also true that

$$\mathbf{D}_a(\mathbf{D}_0\cdot\mathbf{A}_0) = -\epsilon\mu a\bar{\alpha}\cdot\mathbf{D}_0(\partial\Psi/\partial t), \tag{29}$$

and Eq. (27) reduces to

$$(\mathbf{D}_a\cdot\mathbf{D}_0)\mathbf{A}_0 - \epsilon\mu a(\partial^2\mathbf{A}_0/\partial t^2) = -\mu a\mathbf{J}. \tag{30}$$

[11] Reference 2, p. 282, Eq. (5).

In a similar manner, the equation for Ψ may be derived. Ψ satisfies the same type of wave equation as $\mathbf{A}_0$,

$$(\mathbf{D}_a \cdot \mathbf{D}_0)\Psi - \epsilon\mu a(\partial^2\Psi/\partial t^2) = -\frac{\rho + \boldsymbol{\Omega}\cdot\mathbf{J}}{a\epsilon}. \quad (31)$$

To solve Eqs. (30) and (31), it is appropriate to define the time-dependent Green's function $G(\mathbf{r}, t; \mathbf{r}', t')$ as the solution to the wave equation,

$$(\mathbf{D}_a \cdot \mathbf{D}_0)G - \epsilon\mu a(\partial^2 G/\partial t^2) = \delta(\mathbf{r} - \mathbf{r}')\,\delta(t - t'), \quad (32)$$

where, for brevity, we omit writing the argument of $G(\mathbf{r}, t; \mathbf{r}', t')$ explicitly, and where $\delta(r - r')$ and $\delta(t - t')$ are Dirac delta functions. G is defined to be the solution to Eq. (32) that satisfies the causality condition, i.e., $G \equiv 0$ for $t < t'$.

When the solution for G is known, the vector and scalar potentials may be calculated from

$$\mathbf{A}_0(\mathbf{r}, t) = -\mu a \iiiint \mathbf{J}(\mathbf{r}', t')G(\mathbf{r}, t; \mathbf{r}', t')\,d\mathbf{r}'\,dt' \quad (33)$$

and

$$\Psi(\mathbf{r}, t) = \frac{-1}{a\epsilon}\iiiint [\rho(\mathbf{r}', t') + \boldsymbol{\Omega}\cdot\mathbf{J}(\mathbf{r}', t')] \times G(\mathbf{r}, t; \mathbf{r}', t')\,d\mathbf{r}'\,dt', \quad (34)$$

and then the fields are given by

$$\mathbf{H} = \frac{1}{\mu}\bar{\alpha}^{-1}\cdot\mathbf{D}_0 \times (\bar{\alpha}^{-1}\cdot\mathbf{A}_0), \quad (35)$$

$$\mathbf{E} = -\bar{\alpha}^{-1}\cdot(\partial\mathbf{A}_0/\partial t) - \mathbf{D}_0\Psi. \quad (36)$$

THE SOLUTION FOR $G(r, t; r', t')$

When Eq. (32) is written out in scalar form, it is

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{1}{a}\frac{\partial^2}{\partial z^2} - 2\frac{\Omega}{a}\frac{\partial^2}{\partial t\,\partial z} + \frac{\Omega^2}{a}\frac{\partial^2}{\partial t^2} - \epsilon\mu a\frac{\partial^2}{\partial t^2}\right)G = \delta(\mathbf{r} - \mathbf{r}')\,\delta(t - t'). \quad (37)$$

We solve Eq. (37) by a Fourier integral method. [Eq. (37) may also be solved by making an affine transformation of the partial differential equation to eliminate the mixed derivative $\partial^2/\partial t\,\partial z$, and then comparing the resulting differential equation with the standard time-dependent wave equation.] We define the function $g(\mathbf{k}, \omega)$ as the four-dimensional Fourier transform of G:

$$g(\mathbf{k}, \omega) = \int^{(4)} G(\mathbf{r}, t; \mathbf{r}', t')e^{-i\mathbf{k}\cdot\mathbf{r}}e^{-i\omega t}\,d\mathbf{r}\,dt, \quad (38)$$

where $\int^{(4)} = \iiiint$. If Eq. (37) is multiplied by $e^{-i\mathbf{k}\cdot\mathbf{r}}e^{-i\omega t}$ and integrated on $\mathbf{r}$ and t, we find that

$$g(\mathbf{k}, \omega) = \frac{e^{-i\mathbf{k}\cdot\mathbf{r}'}e^{-i\omega t'}}{[\mu\epsilon a - \Omega^2/a]\omega^2 + [2\Omega k_z/a]\omega - k_x^2 - k_y^2 - (1/a)k_z^2}. \quad (39)$$

Hence, the inverse transform associated with Eq. (38) yields for G

$$G = \frac{1}{(2\pi)^4}\int^{(4)} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}e^{i\omega(t-t')}}{[\mu\epsilon a - \Omega^2/a]\omega^2 + [2\Omega k_z/a]\omega - k_x^2 - k_y^2 - (1/a)k_z^2}\,d\mathbf{k}\,d\omega. \quad (40)$$

We first evaluate the ω-integral, using contour integration. The denominator of the integral may be written as

$$\left[\mu\epsilon a - \frac{\Omega^2}{a}\right]\omega^2 + \left[\frac{2\Omega k_z}{a}\right]\omega - k_x^2 - k_y^2 - \frac{1}{a}k_z^2 = \left[\frac{n^2 - \beta^2}{c^2(1 - \beta^2)}\right][\omega - \omega_{p_1}][\omega - \omega_{p_2}], \quad (41)$$

where

$$\omega_{p_1} = -\omega_0 - \omega_1, \quad (42)$$

$$\omega_{p_2} = -\omega_0 + \omega_1, \quad (43)$$

and

$$\omega_0 = c(n^2 - 1)\beta k_z/(n^2 - \beta^2), \quad (44)$$

$$\omega_1 = \frac{c}{n^2 - \beta^2} \times \{(1 - \beta^2)[n^2k^2 - \beta^2(k_x^2 + k_y^2 + n^2k_z^2)]\}^{\frac{1}{2}}, \quad (45)$$

$$k^2 = k_x^2 + k_y^2 + k_z^2. \quad (46)$$

Thus, the poles for the ω-integration lie at ω_{p_1} and ω_{p_2} on the real axis, as shown in Fig. 1. The positions of ω_{p_1} and ω_{p_2} depend upon the other variables of integration(k_x, k_y, k_z), but for any given finite values of these variables, ω_{p_1} and ω_{p_2} are located on the real ω axis.

The path of integration for the ω-integral is along the real ω axis. For the case when $t < t'$, we may close the contour on an infinite semicircle in the lower half ω-plane. Since we want the solution for G to satisfy the causality condition, we regard

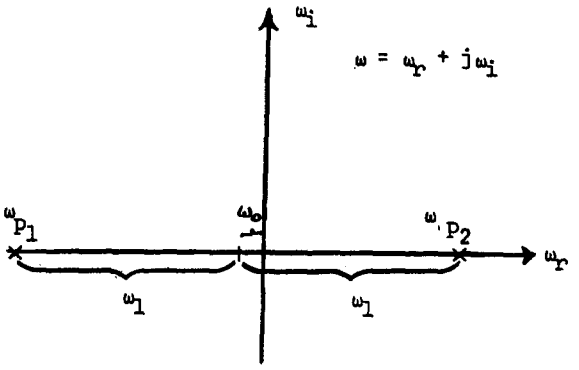

FIG. 1. Location of poles in ω-plane.

the two poles on the real ω axis as lying slightly above the real axis, in the upper half-plane. Then, of course, no poles are included in the lower half-plane and

$$G \equiv 0 \quad \text{for} \quad t < t'. \tag{47}$$

For $t > t'$, the contour may be closed on an infinite semicircle in the upper half-plane. For this case, the contour encircles the two poles at ω_{p_1} and ω_{p_2}, and the integral becomes

$$G = \frac{j}{(2\pi)^3} \int^{(3)} \frac{c^2(1-\beta^2)}{n^2-\beta^2} [\text{res}\,(\omega_{p_1}) + \text{res}\,(\omega_{p_2})] e^{j\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\, d\mathbf{k}, \tag{48}$$

where

$$\text{res}\,(\omega_{p_1}) = \exp[j\omega_{p_1}(t-t')]/(\omega_{p_1}-\omega_{p_2}) \tag{49}$$

and

$$\text{res}\,(\omega_{p_2}) = \exp[j\omega_{p_2}(t-t')]/(\omega_{p_2}-\omega_{p_1}) \tag{50}$$

are the residues in the poles at ω_{p_1} and ω_{p_2}. By Making use of the relations

$$\omega_{p_2} - \omega_{p_1} = 2\omega_1 = \frac{2c}{n^2-\beta^2}\{(1-\beta^2)[n^2k^2 - \beta^2(k_x^2+k_y^2+n^2k_z^2)]\}^{\frac{1}{2}} \tag{51}$$

and

$$\exp[j\omega_{p_2}(t-t')] - \exp[j\omega_{p_1}(t-t')] = 2j\exp[-j\omega_0(t-t')]\sin[\omega_1(t-t')], \tag{52}$$

G may be written

$$G = \frac{-1}{(2\pi)^3} c(1-\beta^2) \times \int^{(3)} \frac{e^{-j\omega_0(t-t')}\sin[\omega_1(t-t')]e^{j\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{\{(1-\beta^2)[n^2k^2-\beta^2(k_x^2+k_y^2+n^2k_z^2)]\}^{\frac{1}{2}}}\, d\mathbf{k}. \tag{53}$$

To eliminate the radical in the denominator, we define the new variables of integration

$$k_1 = (n^2-\beta^2)^{\frac{1}{2}}k_x, \tag{54}$$

$$k_2 = (n^2-\beta^2)^{\frac{1}{2}}k_y, \tag{55}$$

and

$$k_3 = [n^2(1-\beta^2)]^{\frac{1}{2}}k_z. \tag{56}$$

Then

$$\{(1-\beta^2)[n^2k^2 - \beta^2(k_x^2+k_y^2+n^2k_z^2)]\}^{\frac{1}{2}} = (1-\beta^2)^{\frac{1}{2}}k_0, \tag{57}$$

where

$$k_0 = (k_1^2+k_2^2+k_3^2)^{\frac{1}{2}}. \tag{58}$$

Also,

$$\omega_1 = [c(1-\beta^2)^{\frac{1}{2}}/(n^2-\beta^2)]k_0 \tag{59}$$

so that

$$\sin[\omega_1(t-t')] = \sin(\mathcal{K}k_0\tau), \tag{60}$$

where

$$\mathcal{K} = c(1-\beta^2)^{\frac{1}{2}}/(n^2-\beta^2), \tag{61}$$

and

$$\tau = t - t'. \tag{62}$$

Furthermore,

$$\omega_0 = [c(n^2-1)\beta/(n^2-\beta^2)]k_3 \tag{63}$$

$$= \gamma k_3, \tag{64}$$

where γ is defined to be

$$\gamma = c(n^2-1)\beta[n(n^2-\beta^2)(1-\beta^2)^{\frac{1}{2}}]^{-1}, \tag{65}$$

so that

$$e^{-j\omega_0(t-t')} = e^{-j\gamma k_3\tau}. \tag{66}$$

Finally, we define

$$\mathbf{r}_1 = x_1\hat{x} + y_1\hat{y} + z_1\hat{z}, \tag{67}$$

with

$$x_1 = x/(n^2-\beta^2)^{\frac{1}{2}}, \tag{68}$$

$$y_1 = y/(n^2-\beta^2)^{\frac{1}{2}}, \tag{69}$$

$$z_1 = z/[n^2(1-\beta^2)]^{\frac{1}{2}}; \tag{70}$$

then with

$$\mathbf{k}_0 = k_1\hat{x} + k_2\hat{y} + k_3\hat{z}, \tag{71}$$

$$e^{j\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = e^{j\mathbf{k}_0\cdot(\mathbf{r}_1-\mathbf{r}_1')}. \tag{72}$$

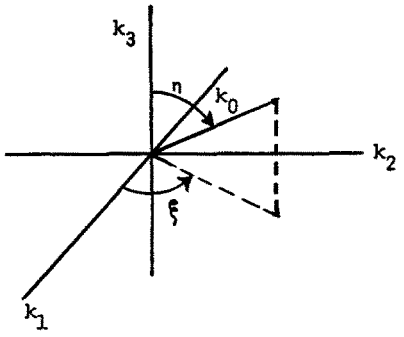

FIG. 2. The angles η and ξ.

Substituting these relations into Eq. (53) gives for G

$$G = -\frac{1}{(2\pi)^3}\frac{c}{n(n^2-\beta^2)} \times \int^{(3)} \frac{1}{k_0} e^{-j\gamma k_0 \tau} \sin(\mathcal{K}k_0\tau) e^{j\mathbf{k}_0\cdot(\mathbf{r}_1-\mathbf{r}_1')}\, d\mathbf{k}_0. \quad (73)$$

To evaluate this integral, it is convenient to change the integration into spherical coordinates. We let

$$k_1 = k_0 \sin\eta\cos\xi, \quad (74)$$

$$k_2 = k_0 \sin\eta\sin\xi, \quad (75)$$

$$k_3 = k_0\cos\eta, \quad (76)$$

where the angles η and ξ are as shown in Fig. 2. We also change the vector $\mathbf{r}_1 - \mathbf{r}_1'$ into spherical coordinates:

$$x_1 - x_1' = R_1 \sin\theta\cos\phi, \quad (77)$$

$$y_1 - y_1' = R_1 \sin\theta\sin\phi, \quad (78)$$

$$z_1 - z_1' = R_1\cos\theta, \quad (79)$$

where θ and ϕ are shown in Fig. 3. With this change of variables, G becomes

$$G = \frac{-1}{(2\pi)^3}\frac{c}{n(n^2-\beta^2)}\int_{k_0=0}^{\infty} I(k_0)\sin(\mathcal{K}k_0\tau)k_0\, dk_0, \quad (80)$$

where $I(k_0)$ contains the "angle" integrals

$$I(k_0) = \int_{\eta=0}^{\pi}\int_{\xi=0}^{2\pi} \exp\{jk_0R_1[\sin\eta\sin\theta\cos(\xi-\phi) + \cos\eta\cos\theta]\}\exp(-j\gamma k_0\tau\cos\eta)\sin\eta\, d\eta\, d\xi. \quad (81)$$

The $I(k_0)$ integral may be cast into a standard form by defining two new variables R_2 and θ_2 such that

$$R_2\sin\theta_2 = R_1\sin\theta, \quad (82)$$

$$R_2\cos\theta_2 = R_1\cos\theta - \gamma\tau. \quad (83)$$

For any given values of R_1, θ, and $\gamma\tau$, it may be seen from Fig. 4 that there always exist values for R_2 and θ_2 which satisfy Eqs. (82) and (83).

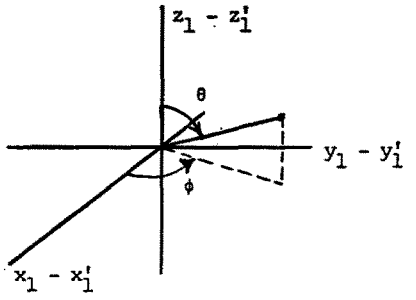

FIG. 3. The angles θ and ϕ.

Substituting Eqs. (82) and (83) into Eq. (81) gives

$$I(k_0) = \int_{\eta=0}^{\pi}\int_{\xi=0}^{2\pi} \exp\{jk_0R_1[\sin\eta\sin\theta_2\cos(\xi-\phi) + \cos\eta\cos\theta_2]\}\sin\eta\, d\eta\, d\xi \quad (84)$$

$$= 4\pi\frac{\sin(k_0R_2)}{k_0R_2}. \quad (85)$$

With this result in Eq. (80), we have for G:

$$G = \frac{-1}{2\pi^2}\frac{c}{n(n^2-\beta^2)R_2} \times \int_{k_0=0}^{\infty}\sin(k_0R_2)\sin(\mathcal{K}k_0\tau)\, dk_0. \quad (86)$$

Taking advantage of the fact that

$$\sin(k_0R_2)\sin(\mathcal{K}k_0\tau)$$

is an even function of k_0 about $k_0 = 0$, we may include a factor of $\frac{1}{2}$ and write the limits of integration as $-\infty$ to $+\infty$. Then writing $\sin(k_0R_2)$ and $\sin(\mathcal{K}k_0\tau)$ in terms of exponentials, we find that G splits into a sum of four integrals, each of which can be evaluated by means of the Fourier transform relation

$$\int_{-\infty}^{\infty} e^{\pm jxv}\, dx = 2\pi\,\delta(y). \quad (87)$$

Thus G is given by

$$G = \frac{1}{8\pi\mathcal{K}R_2}\frac{c}{n(n^2-\beta^2)}\left[\delta\left(\tau+\frac{R_2}{\mathcal{K}}\right) - \delta\left(\tau-\frac{R_2}{\mathcal{K}}\right) + \delta\left(\tau+\frac{R_2}{\mathcal{K}}\right) - \delta\left(\tau-\frac{R_2}{\mathcal{K}}\right)\right]. \quad (88)$$

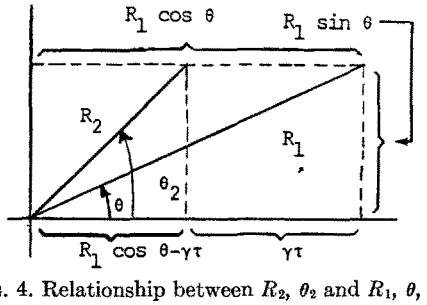

FIG. 4. Relationship between R_2, θ_2 and R_1, θ, $\gamma\tau$.

Since this solution actually applies only for $\tau = t - t' > 0$, the arguments of the delta functions $\delta(\tau + R_2/\mathfrak{C})$ are never zero. Hence these terms do not contribute to the solution and we have

$$G = \frac{-1}{4\pi\mathfrak{C}R_2}\frac{c}{n(n^2-\beta^2)}\,\delta\left(\tau - \frac{R_2}{\mathfrak{C}}\right). \tag{89}$$

Finally, if we define the new "radius" R_0

$$R_0 = \left\{(x-x')^2 + (y-y')^2 + \frac{n^2-\beta^2}{n^2(1-\beta^2)}\left[z - z' - \frac{n^2-1}{n^2-\beta^2}v\tau\right]^2\right\}^{\frac{1}{2}}, \tag{90}$$

then one can show, after a certain amount of algebra, that

$$\mathfrak{C}R_2 = \frac{c(1-\beta^2)^{\frac{1}{2}}}{(n^2-\beta^2)^{\frac{1}{2}}}R_0, \tag{91}$$

$$\frac{R_2}{\mathfrak{C}} = \left[\frac{1-(\beta/n)^2}{1-\beta^2}\right]^{\frac{1}{2}}\frac{R_0}{v_0}, \tag{92}$$

where

$$v_0 = (\mu\epsilon)^{-\frac{1}{2}} \tag{93}$$

is the phase velocity of a wave in the medium, as seen from a frame fixed in the medium. Thus, the final solution for G is

$$G = -\frac{1}{4\pi}\left[\frac{1-(\beta/n)^2}{1-\beta^2}\right]^{\frac{1}{2}}\frac{1}{R_0} \times \delta\left\{\tau - \left[\frac{1-(\beta/n)^2}{1-\beta^2}\right]^{\frac{1}{2}}\frac{R_0}{v_0}\right\}. \tag{94}$$

As a check on the algebra, we notice that, for either $\beta = 0$ or $n = 1$, G reduces to

$$G = -\frac{1}{4\pi R_0}\,\delta(\tau - R_0/v_0), \tag{95}$$

where

$$R_0 = [(x-x')^2 + (y-y')^2 + (z-z')^2]^{\frac{1}{2}}, \tag{96}$$

which is known to be the solution to the time-dependent wave equation

$$\nabla^2 G - \frac{1}{v_0^2}\frac{\partial^2 G}{\partial t^2} = \delta(\mathbf{r}-\mathbf{r}')\,\delta(t-t'). \tag{97}$$

INTERPRETATION OF THE RESULT

Recalling that (x', y', z') represents the source point and (x, y, z) the observation point, it is clear from Eq. (90) that R_0 is the "radius" between the point $(x', y', z' + [(n^2-1)/(n^2-\beta^2)]v\tau)$ and the observation point (x, y, z), with the z-axis dimensions scaled by the factor $(n^2-\beta^2)^{\frac{1}{2}}/n^2(1-\beta^2)$. (This scaling is associated with the Lorentz contraction occurring in this axis.) Thus, the solution for G given in Eq. (94) represents an expanding "spherical shell". The center of the shell is located not at the source point, but at the point $z = z' + [(n^2-1)/(n^2-\beta^2)]v\tau$ on the z axis. In other words, the entire shell is "dragged" along by the velocity of the medium. At a given time interval $\tau = t - t'$ after the source impulse occurs, the equation of the shell is

$$R_0 = \left[\frac{1-\beta^2}{1-(\beta/n)^2}\right]^{\frac{1}{2}} v_0(t-t'). \tag{98}$$

Furthermore, the shell is attenuated by the factor $1/R_0$ as it propagates outward.

To see how the shape of the shell depends on the velocity of the medium, consider first the case where the medium is not moving. Then, after a certain time interval, the shell would have the appearance shown in Fig. 5, i.e., it would be an actual sphere about the source point. Next, suppose the medium is moving, but moves slowly enough so that $n\beta = v/v_0 < 1$. Then, after the same time interval, the shell would have the appearance shown in Fig. 6. The center of the shell is now at the point $z' + [(n^2-1)/(n^2-\beta^2)]v(t-t')$, rather than at the source point z'. [It is interesting to note that the center of the shell does not keep up with the

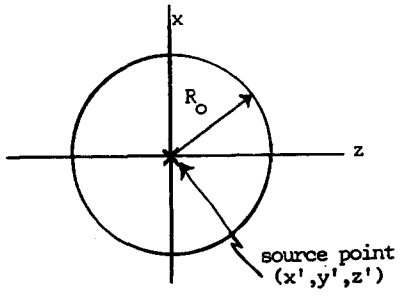

Fig. 5. Expanding spherical shell for $\eta\beta = 0$.

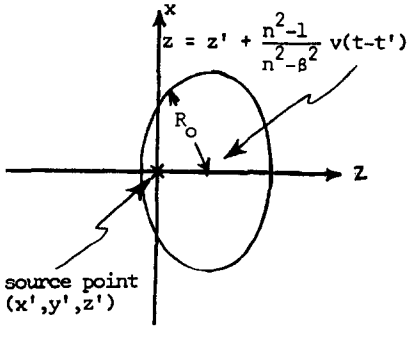

FIG. 6. Expanding "spherical" shell for $0 < \eta\beta < 1$.

medium. The center of the shell moves with velocity $\mathbf{v}[(n^2 - 1)/(n^2 - \beta^2)]$, whereas the medium moves with velocity $\mathbf{v}$.] Also, the shell is flattened in the z axis, so it is actually an oblate spheroid. It does, however, propagate away from the source point in all directions; the source point is inside the shell. Finally, consider the case where the medium moves with a high enough velocity so that $\eta\beta = v/v_0 > 1$. For this case, the entire shell is dragged to the right of the source point, as shown in Fig. 7. The source point is outside the shell. As the shell expands and moves to the right, it stays at all times inside a cone of interior half-angle θ_0, the intersection of which with the xz-plane is shown by the dashed line in Fig. 7. It is not difficult to show that the cone half-angle is specified by

$$\cos\theta_0 = [(n^2\beta^2 - 1)/\beta^2(n^2 - 1)]^{\frac{1}{2}}. \qquad (99)$$

Thus, for $\eta\beta = v/v_0 = 1$, the "cone" is actually the entire half-space $z > z'$. For $\eta\beta > 1$, the cone angle decreases as the velocity of the medium increases. Of course, for $\eta\beta < 1$, there is no cone; the shell propagates away from the source in all directions.

One useful application of these results is that they provide a simple way of understanding the phenomenon of Cerenkov radiation. It is well known that, a point charge moving through a dielectric medium with constant velocity v excites nonradiating fields if $v < v_0$ and radiating fields if $v > v_0$. The entire character of the fields changes at the critical velocity $v = v_0$. The customary procedure for studying this problem is to solve for the fields as measured in a reference frame stationary with respect to the medium. The fields are constructed by a Fourier integral method, and the resulting evaluation of the integral is different, depending on whether $v < v_0$ or $v > v_0$. However, if we study this problem from the reference frame of the charge, rather than that of the medium, the Green's function given above can be used to find the fields, and the reason for the entirely different forms of solution for $v < v_0$ and $v > v_0$ is quite obvious.

To be specific, suppose we postulate a point charge of q_0 coulombs, located at the origin and is suddenly "turned on" at $t = 0$; i.e., suppose

$$\rho(x, y, z, t) = q_0\,\delta(\mathbf{r})u(t), \qquad (100)$$

where $u(t)$ denotes a unit step function occurrring at $t = 0$. When this is substituted in Eq. (31) for the scalar potential, it is seen that Ψ at any given point in space is just the time integral of the Green's function G.

Consider first the case where $\eta\beta = v/v_0 < 1$.

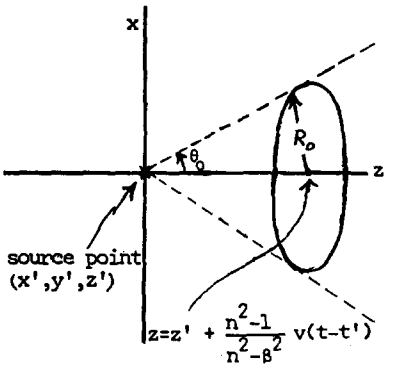

FIG. 7. Expanding "spherical" shell for $\eta\beta > 1$.

In this situation the shell propagates away from the source point in all directions. The scalar potential Ψ, the time integral of G, then has the form of an electrostatic potential inside the shell and zero outside. At any given point in space, after a sufficient time interval, the wavefront passes through that point, and eventually the wavefront becomes infinitely remote from the source in all directions. Sooner or later, the field becomes electrostatic at any given point.

Now, contrast this with the case where $\eta\beta = v/v_0 > 1$. For this case the shell lies entirely to the right of the source. Both sides of the shell propagate away from the source in the same direction. At any given point in space, Ψ is again the time integral of G. If we choose a point outside the cone, clearly the sphere never gets there. Ψ, and hence the fields, are identically zero in this region. If we choose a point inside the cone, first one side of the spherical shell and then the other side arrives there. Hence, Ψ undergoes two step discontinuities, one as each side of the shell arrives. Finally, after both discontinuities occur, there are no further discontinuities, and Ψ assumes an electrostatic behavior. At a given instant of time, we thus have the situation shown in Fig. 8. Here, Ψ_1 represents the value of Ψ after the first discontinuity, and Ψ_2 represents the value after the second discontinuity.

Clearly, in this case, the discontinuity in Ψ, which exists on the boundary of the cone, never leaves the vicinity of the source. This situation accounts

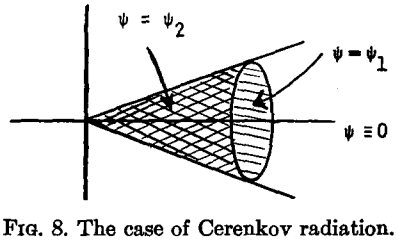

FIG. 8. The case of Cerenkov radiation.

for the presence of "radiation"-type fields; no matter how long we wait, there is always a wave front (the boundary of the cone) in the vicinity of the source.

Of course, these comments come as no surprise to any one already familiar with the phenomenon of Cerenkov radiation. However, the author feels that this approach to the subject affords a simpler way of teaching about Cerenkov radiation than does the conventional approach.

One final remark is appropriate. It is also of interest to solve for the Green's function associated with the harmonic time dependence. If we assume a source with time dependence $e^{j\omega t}$, the equation for the harmonic Green's function may be obtained by replacing "$\partial/\partial t$" in Eq. (37) with "$j\omega$". Denoting the harmonic Green's function by $g(\mathbf{r};\mathbf{r}')$, we have

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{1}{a}\frac{\partial^2}{\partial z^2}-\frac{2j\omega\Omega}{a}\frac{\partial}{\partial z}-\frac{\omega^2\Omega^2}{a}+\omega^2\mu\epsilon a\right)g(\mathbf{r};\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \quad (101)$$

This problem has been solved by Tai,[9] and also by Lee and Papas,[10] and the result, for the case $\eta\beta < 1$, is

$$g(\mathbf{r};\mathbf{r}') = \frac{a^{\frac{1}{2}}}{4\pi}e^{jka^{\frac{1}{2}}R_a}e^{j\omega\Omega(z-z')}/R_a, \quad (102)$$

where

$$R_a = [(x-x')^2 + (y-y')^2 + a(z-z')^2]^{\frac{1}{2}}, \quad (103)$$

and, for the case $\eta\beta > 1$, the result is

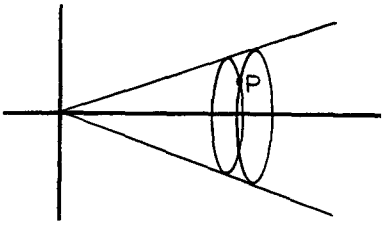

FIG. 9. The two spherical wavefronts through point P.

$$g(\mathbf{r};\mathbf{r}') = \begin{cases} -\dfrac{1}{2\pi}(|a|)^{\frac{1}{2}}e^{j\omega\Omega(z-z')}\dfrac{\cos k(|a|)^{\frac{1}{2}}R_a'}{R_a'} : \\ \qquad\qquad |a|^{\frac{1}{2}}(z-z') > r, \\ 0 : \qquad\qquad |a|^{\frac{1}{2}}(z-z') < r, \end{cases} \quad (104)$$

where

$$R_a' = [|a|(z-z')^2 - r^2]^{\frac{1}{2}} \quad (105)$$

and

$$r^2 = (x-x')^2 + (y-y')^2. \quad (106)$$

Tai obtained this solution by reducing the differential equation to a two-dimensional Klein–Gordon equation, whose solution is known. Lee and Papas approached the problem from the standpoint of Foruier analysis, similar to what we have done here.

The solution to this equation can also be obtained from the time-dependent Green's function by evaluating the integral

$$g(r;r')e^{j\omega t} = \int_{t'=-\infty}^{t} e^{j\omega t'}G(\mathbf{r},\, t;\mathbf{r}',\, t')\, dt', \quad (107)$$

which is straightforward, but rather tedious, to carry out. For the case $\eta\beta > 1$, and for points inside the Cerenkov cone, there are two values of t' for which the delta function contained in G contributes to the integral. The two values of t' are the retarded times associated with the two "spheres" which can be drawn through a given point P inside the Cerenkov cone as shown in Fig. 9. The interference between these two spheres is responsible for the standing-wave behavior of $(g\mathbf{r};\mathbf{r}')$ in this region. For $\eta\beta < 1$, there is only one value of t' for which the delta function in the argument of Eq. (107) contributes, and hence $g(\mathbf{r};\mathbf{r}')$ for this case exhibits the usual traveling-wave behavior associated with outward-propagating waves.

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Propagation of Correlations in a Boltzmann Gas*

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New results are obtained on the propagation of correlations in a Boltzmann gas on the scale of the mean free path and the collisional time scale which appear to support M. Green's conjecture on this subject.

INTRODUCTION

In the past few years much research[1-6] has been carried out on just how the Boltzmann equation follows from the Liouville equation, and on how higher-order corrections to the Boltzmann equation are found.[7-12] In the present paper, these questions are re-examined by using the multiple time- and space-scale approach[13,14] which follows from the well-known Bogoliubov–Krylov technique of nonlinear mechanics.

The major new results which emerge from the present analysis follow from a careful examination of the behavior of the first-order correction to the two-particle correlation function. It is found that this function exhibits a variety of different types of behavior, among which are two different kinds of singular behavior. We have shown that, by removing the secular behavior of this function, a condition on the zeroth-order correlation function is obtained. This condition determines its behavior on the collisional time scale and the mean free path space scale. This leads to the verification of Green's conjecture[8] concerning the zeroth-order correlation functions. In addition, we have found singular behavior for small relative velocities of an integrable kind. The corrections arising from the singular region of phase-space have been shown to be of higher order than the terms kept in the present analysis.

Finally, we demonstrate that the Choh–Uhlenbeck corrections to the Boltzmann equation do drive the system to thermal equilibrium if we assume that there is no secular behavior.

I. THE BASIC EQUATIONS AND EXPANSION PROCEDURE

The starting point for the calculation is the BBGKY hierarchy governing the reduced distribution functions f_s.

$$\left[\frac{\partial}{\partial t} + \sum_{i=1}^{s} \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} - \frac{1}{m} \sum_{i=1}^{s} \sum_{j=1}^{s'} \frac{\partial \phi(|\mathbf{x}_{ij}|)}{\partial \mathbf{x}_i} \cdot \frac{\partial}{\partial \mathbf{v}_i}\right] f_s = \frac{n}{m} \int d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \frac{\partial \phi(|\mathbf{x}_{i,s+1}|)}{\partial \mathbf{x}_i} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{v}_i}, \qquad s = 1, 2 \cdots, \tag{1.1}$$

where

$$\mathbf{x}_{ij} = \mathbf{x}_i - \mathbf{x}_j. \tag{1.2}$$

The notation is the same as that in Ref. 13. It is convenient to measure lengths in units of r_0, the range of the interaction potential ϕ, and to measure time in units of r_0/v_{av}, the time of a binary interaction, with v_{av}, a typical particle velocity.

The Boltzmann regime is characterized by strong interactions and dilute systems. Thus, we introduce the expansion parameter ϵ, such that

$$nr_0^3 = \epsilon, \quad \langle\phi\rangle/mv_{\mathrm{av}}^2 \sim 1, \quad \epsilon \ll 1 \tag{1.3}$$

with $\langle\phi\rangle$ the characteristic strength of the potential.

Rewriting (1.1) in dimensionless units but retain-

* A preliminary account of this work was reported in Bull. Am. Phys. Soc. 10, 531 (1965).

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ing the same labels as above, we obtain

$$\left[\frac{\partial}{\partial t} + \sum_{i=1}^{s} \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} - \sum_{i=1}^{s} \sum_{j=1}^{s'} \frac{\partial \phi(|\mathbf{x}_{ij}|)}{\partial \mathbf{x}_i} \cdot \frac{\partial}{\partial \mathbf{v}_i}\right] f_s$$

$$= \epsilon \int d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \frac{\partial \phi(|\mathbf{x}_{i,s+1}|)}{\partial \mathbf{x}_i} \cdot \frac{\partial}{\partial \mathbf{v}_i} f_{s+1}. \quad (1.4)$$

In the following, we assume that the potential is repulsive and that the ensemble is spatially homogeneous. Introducing the definitions

$$\Theta(ij) = \frac{\partial \phi(|\mathbf{x}_{ij}|)}{\partial \mathbf{x}_i} \cdot \left(\frac{\partial}{\partial \mathbf{v}_i} - \frac{\partial}{\partial \mathbf{v}_j}\right) \quad (1.5)$$

and

$$H(1, \cdots, s) = \sum_{i=1}^{s} \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} - \sum_{i=1}^{s} \sum_{j>1}^{s} \Theta(ij), \quad (1.6)$$

$$\left[\frac{\partial}{\partial t} + H(1, \cdots, s)\right] f_s$$

$$= \epsilon \int d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \Theta(i, s+1) f_{s+1}. \quad (1.7)$$

Our object is to seek an asymptotic solution of (1.7) for small ϵ. We know[1] that a simple power series in ϵ does not suffice and that a more complicated asymptotic representation must be found. The multiple time and space scale procedure assumes that an expansion of the form

$$f_s = f_s^{(0)}(\mathbf{x}_1, \cdots, \mathbf{x}_s, \mathbf{v}_1, \cdots, \mathbf{v}_s, t, \epsilon\mathbf{x}_1, \cdots, \epsilon\mathbf{x}_s, \epsilon t, \epsilon^2\mathbf{x}_1, \cdots, \epsilon^2\mathbf{x}_s, \epsilon^2 t, \cdots)$$
$$+ \epsilon f_s^{(1)}(\mathbf{x}_1, \cdots, \mathbf{x}_s, \mathbf{v}_1, \cdots, \mathbf{v}_s, t, \epsilon\mathbf{x}_1, \cdots, \epsilon\mathbf{x}_s, \epsilon t, \epsilon^2\mathbf{x}_1, \cdots, \epsilon^2\mathbf{x}_s, \epsilon^2 t, \cdots)$$
$$+ \epsilon^2 f_s^{(2)}(\mathbf{x}_1, \cdots, \mathbf{x}_s, \mathbf{v}_1, \cdots, \mathbf{v}_s, t, \epsilon\mathbf{x}_1, \cdots, \epsilon\mathbf{x}_s, \epsilon t, \epsilon^2\mathbf{x}_1, \cdots, \epsilon^2\mathbf{x}_s, \epsilon^2 t, \cdots) + \cdots \quad (1.8)$$

adequately represents the solution. The initial conditions on the f_s must also be expanded as in (1.8).

It is often convenient to introduce correlation functions g_s in a recursive manner

$$f_2(1\ 2) = f_1(1) f_1(2) + g_2(1\ 2),$$
$$f_3(1\ 2\ 3) = f_1(1) f_1(2) f_1(3) + \sum_P f_1(1) g_2(2\ 3) + g_3(1\ 2\ 3), \quad \text{etc.} \quad (1.9)$$

It is assumed that all the g_s vanish at $t = 0$ so that the initial state is one of complete chaos and only correlations arising from interactions is present in the system.

II. THE LOWEST-ORDER BEHAVIOR

The lowest-order equations which follow from (1.7) are

$$[\partial/\partial t + H^{(0)}(1, \cdots, s)] f_s^{(0)} = 0. \quad (2.1)$$

Thus, for $s = 1$, we find

$$\partial f_1^{(0)}/\partial t = 0 \quad (2.2)$$

and for $s \geq 2$

$$f_s^{(0)} = \exp[-H^{(0)}(1, \cdots, s)t] f_s^{(0)} \quad (t = 0, \epsilon t, \cdots). \quad (2.3)$$

Throughout the paper, we indicate explicitly [as in (2.3)] only those arguments of functions which need special attention drawn to them.

The operator

$$S_{-t}(1, \cdots, s) \equiv \exp[-H^{(0)}(1, \cdots, s)t] \quad (2.4)$$

was first introduced by Bogoliubov[1] and has been extensively studied by Cohen.[11] Briefly, it replaces the phase-space coordinates of the s particles by their values at time zero which are calculated using the trajectories generated by $H^{(0)}(1, \cdots, s)$.

For $s = 2$, (2.3) becomes, upon using (1.9),

$$g_2^{(0)}(t, \epsilon t, 12) = [S_{-t}(12) - 1] f_1^{(0)}(1, \epsilon t) f_1^{(0)}(2, \epsilon t) + S_{-t}(12) g_2^{(0)}(t = 0, \epsilon t, 12). \quad (2.5)$$

We first note the appearance of the nonphysical function $g_2^{(0)}(t = 0, \epsilon t, 12)$ in (2.5). Such functions are a characteristic feature of the procedure used here and arise in a characteristic way. In the present instance, in solving (2.1) on the t and $\mathbf{x}_{12}$ scales, it was implicitly assumed that the variations in ϵt and $\epsilon\mathbf{x}_{12}$ were negligible. The error committed is of order ϵ as long as t and $\mathbf{x}_{12}$ are of order unity. The general nature of this type of expansion is such that these errors are corrected order by order. In another interpretation of this procedure,[14] the arguments of the functions on the various scales are assumed to be independent variables in the strict sense. In the present paper, we do not take this point of view but rather require that we be as near as possible to the physical "line", defined by $t_0, \epsilon t_1, \epsilon^2 t_2, \cdots$ with $t_0 = t_1 = t_2 \cdots = t$.

We next note that (2.5) predicts a long-range finite correlation on the $\mathbf{x}_{12}$ scale in certain cases, even if $g_2^{(0)}(t = 0, \epsilon t)$ vanishes. This phenomenon occurs when the two particles undergo a collision in the remote past, so that $(S_{-t} - 1)$ does not vanish. We see that this region of phase space gives rise to secular behavior in the next order. Note that in thermal equilibrium, $g_2^{(0)}(t)$ has a finite range, since, with $f_1^{(0)}$ Maxwellian and energy conservation, $g_2^{(0)}$ vanishes for $t \gg |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$.

To next order (1.7) gives

$$\left[\frac{\partial}{\partial t} + H^{(0)}(1, \cdots, s)\right] f_s^{(1)} + \left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] f_s^{(0)} = \int d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \Theta(i, s+1) f_{s+1}^{(0)}, \quad (2.6)$$

where

$$H^{(1)}(1, \cdots, s) = \sum_{i=1}^{s} \mathbf{v}_i \cdot \frac{\partial}{\partial \epsilon \mathbf{x}_1}. \quad (2.7)$$

In particular, for $s = 1$, we have

$$\frac{\partial f_1^{(1)}}{\partial t} + \frac{\partial f_1^{(0)}}{\partial \epsilon t} = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) f_2^{(0)}(t, \epsilon t, 12). \quad (2.8)$$

Upon integrating (2.8), we find explicit secular behavior on the t scale, which is removed by requiring

$$\frac{\partial f_1^{(0)}}{\partial \epsilon t} = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) f_2^{(0)}(\infty, \epsilon t, 12). \quad (2.9)$$

Therefore, we also get from (2.8)

$$\frac{\partial f_1^{(1)}}{\partial t} = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) \times [f_2^{(0)}(t, \cdots) - f_2^{(0)}(\infty, \cdots)]. \quad (2.10)$$

In order to demonstrate that the decomposition of (2.8) into (2.9) and (2.10) is valid, we must show that acceptable behavior for the time development of $f_1^{(0)}$ in ϵt and $f_1^{(1)}$ in t results. In contradistinction to other treatments of this problem, we cannot in fact demonstrate this here, since we have no knowledge of $g_2^{(0)}(t = 0, \epsilon t)$ and further we cannot obtain any information on it in this order of approximation. We must therefore proceed to the next order and, among other things, look for a determination of $g_2^{(0)}(t = 0, \epsilon t)$.

III. BEHAVIOR OF $f_2^{(1)}$

In this section, we examine the behavior of $f_2^{(1)}$ in those regions of phase space where $|\mathbf{v}_{12}|$ is of order unity and $|\mathbf{x}_{12}|$ is larger than unity (greater than r_0). It is seen that the analysis falls naturally into examining times $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$ and times $t > |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$.

We start from (2.6) which for $s = 2$ reads

$$\left[\frac{\partial}{\partial t} + H^{(0)}(12)\right] f_2^{(1)} + \left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(12)\right] f_2^{(0)} = \int d\mathbf{x}_3\, d\mathbf{v}_3\, [\Theta(13) + \Theta(23)] f_3^{(0)}. \quad (3.1)$$

The formal solution of (3.1) is

$$f_2^{(1)}(t) = S_{-t}(12) f_2^{(1)}(t = 0, \epsilon t) + \int_0^t dt'\, S_{-(t-t')}(12) \left\{ -\left(\frac{\partial}{\partial \epsilon t} + \mathbf{v}_{12} \cdot \frac{\partial}{\partial \epsilon \mathbf{x}}\right) f_2^{(0)}(t', \epsilon t) + \int d\mathbf{x}_3\, d\mathbf{v}_3\, [\Theta(13) + \Theta(23)] f_3^{(0)}(t', \epsilon t, 123) \right\}. \quad (3.2)$$

We now define

$$S_{-t}(123, i3) \equiv e^{-H(123, i3)t} \quad (3.3)$$

and

$$H(123, i3) = H^{(0)}(123) + \Theta(i3). \quad (3.4)$$

Thus, using (2.3), (2.9), (3.3), and (3.4), we can rewrite (3.2) as

$$\begin{aligned} f_2^{(1)}(t) &= S_{-t}(12) f_2^{(1)}(0, \epsilon t) \\ &+ \int_0^t dt'\, S_{-(t-t')}(12) \Big[\int d\mathbf{x}_3\, d\mathbf{v}_3\, (\Theta(13) \\ &\times \{ [S_{-t'}(123) - S_{-t'}(123, 23)] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ &+ [S_{-t'}(123, 23) - S_{-\infty}(13)] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ &+ S_{-t'}(123) [f_3^{(0)}(0, \epsilon t) - f_1^{(0)} f_1^{(0)} f_1^{(0)}] \\ &- S_{-\infty}(13) g_2^{(0)}(t = 0, 13) f_1^{(0)}(2) \} \\ &+ \Theta(23) \{ [S_{-t'}(123) - S_{-t'}(123, 13)] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ &+ [S_{-t'}(123, 13) - S_{-\infty}(23)] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ &+ S_{-t'}(123) [f_3^{(0)}(0, \epsilon t) - f_1^{(0)} f_1^{(0)} f_1^{(0)}] \\ &- S_{-\infty}(23) g_2^{(0)}(t = 0, 23) f_1^{(0)}(1) \}) \\ &- \left(\frac{\partial}{\partial \epsilon t} + \mathbf{v}_{12} \cdot \frac{\partial}{\partial \epsilon \mathbf{x}}\right) [f_2^{(0)}(t', \epsilon t) - f_1^{(0)}(1) f_1^{(0)}(2)] \Big]. \end{aligned} \quad (3.5)$$

Equation (3.5) consists of five groups of terms which we consider separately below.

The first of these is

$$I_1 = \int_0^t dt'\, S_{-(t-t')}(12) \int d\mathbf{x}_3\, d\mathbf{v}_3\, (\{\Theta(13)[S_{-t'}(123) - S_{-t'}(123, 23)] + \Theta(23)[S_{-t'}(123) - S_{-t'}(123, 13)]\} f_1^{(0)} f_1^{(0)} f_1^{(0)}). \quad (3.6)$$

It is clear that the [13] and [23] terms behave similarly so that we only explicitly consider the [13] terms. First note that $\Theta(13)$ provides the restriction $|\mathbf{x}_{13}| \leq 1$ and that the S operators cancel if for all t', $0 \leq t' \leq t$, $|\mathbf{x}_{23}| > 1$. Thus, $|\mathbf{x}_{23}|$ must be less than unity at some time during the integration. If particles [2] and [3] interact at time $\bar{t} < t' \leq t$ and particles [1] and [3] interact at time t', these conditions are satisfied. We denote this trajectory by [23]–[13].

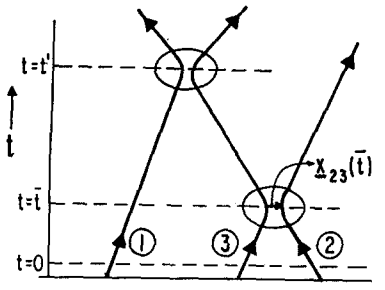

FIG. 1. The [23]–[13] trajectories.

Other interaction sequences such as [23]–[12]–[13] and [12]–[23]–[13] are also possible, but they are shown below to yield smaller contributions to (3.6) as t becomes large.

Figure 1 shows the sequence [23]–[13]. Note from the figure that

$$\mathbf{x}_{23}(t') \simeq \mathbf{v}_{23}(t' - \bar{t}) + \mathbf{x}_{23}(\bar{t}). \tag{3.7}$$

Thus, for the sequence to occur, $\bar{t}$ must be such that

$$|\mathbf{x}_{23} - \mathbf{v}_{23}(t' - \bar{t})| < 1, \tag{3.8}$$

since $\mathbf{x}_{23}(\bar{t}) \sim 1$.

We picture the cone of allowed velocities in relative coordinate space in Fig. 2. From Fig. 2 we conclude that the solid angle of allowable relative velocities is

$$d\Omega \sim \frac{1}{|\mathbf{x}_{23}|^2}. \tag{3.9}$$

We further assume that

$$\Theta(13)[S_{-t'}(123) - S_{-t'}(123, 23)]f_1^{(0)}(1)f_1^{(0)}(2) \sim 1 \tag{3.10}$$

for those values of $\mathbf{x}_3$ and $\mathbf{v}_3$ for which the integrand does not vanish. Thus, the contribution to I_1 is

$$\int_0^t dt'\, S_{-(t-t')}(12) \int_{|\mathbf{x}_{13}|<1} d\mathbf{x}_{13} \int_{d\Omega} f(\mathbf{v}_3)\, d\mathbf{v}_3. \tag{3.11}$$

Further,

$$\mathbf{v}_3 = \mathbf{v}_2 - \mathbf{v}_{23} \simeq \mathbf{v}_2 - |\mathbf{v}_{23}|\hat{x}_{23}, \quad \hat{x}_{23} = \mathbf{x}_{23}/|\mathbf{x}_{23}| \tag{3.12}$$

and

$$\mathbf{x}_{23} = -\mathbf{x}_{12} + \mathbf{x}_{13} \simeq -\mathbf{x}_{12} \tag{3.13}$$

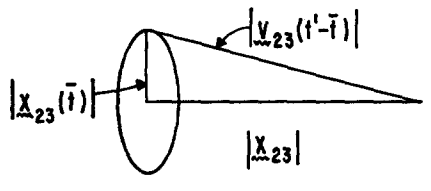

FIG. 2. Cone of allowed velocities.

so that we may write (3.11) as

$$\int_0^t dt'\, S_{-(t-t')}(12)\, \frac{1}{|\mathbf{x}_{12}|^2} \times \int f(\mathbf{v}_2 + |\mathbf{v}_{23}|\,\hat{x}_{12})\, |\mathbf{v}_{23}|^2\, d\,|\mathbf{v}_{23}|. \tag{3.14}$$

We note that, for trajectories for which $|\mathbf{x}_{12}| > 1$ for all time,

$$H^{(0)}(12) = \mathbf{v}_{12}\cdot\partial/\partial\mathbf{x}_{12}.$$

The expression (3.14) then becomes

$$\int_0^t \frac{dt'}{|\mathbf{x}_{12} - \mathbf{v}_{12}(t - t')|^2} \sim \frac{1}{v_{12}^2 t}, \quad t > \frac{|\mathbf{x}_{12}|}{|\mathbf{v}_{12}|}, \tag{3.15}$$

upon assuming that the velocity integration in (3.14) yields a quantity of order unity.

When we consider the other interaction sequences such as [23]–[12]–[13], etc., it is clear that the solid angle of relative velocities is

$$d\Omega \sim |\mathbf{x}_{12}(t')|^{-2}\, |\mathbf{x}_{23}(\bar{t})|^{-2} \sim |\mathbf{x}_{12}(t')|^{-4} \tag{3.16}$$

so that a faster decay than $1/t$ results. We conclude therefore that the dominant behavior of I_1 is a $1/t$ decay.

The next group of terms in (3.5) is

$$I_2 = \int_0^t dt'\, S_{-(t-t')}(12) \int d\mathbf{x}_3\, d\mathbf{v}_3 \times \{\Theta(13)[S_{-t'}(123, 23) - S_{-\infty}(13)] + \Theta(23)[S_{-t'}(123, 13) - S_{-\infty}(23)]\} f_1^{(0)} f_1^{(0)} f_1^{(0)}. \tag{3.17}$$

Again, we only treat the [13] terms explicitly. Introducing the change of variables

$$\mathbf{x}_1' = \mathbf{x}_1, \quad \mathbf{x}_{12} = \mathbf{x}_1 - \mathbf{x}_2, \quad \mathbf{x}_{13} = \mathbf{x}_1 - \mathbf{x}_3 \tag{3.18}$$

enables us to write

$$H^{(0)}(12) = H_r(12) + \mathbf{v}_1\cdot\left(\frac{\partial}{\partial\mathbf{x}_{13}} + \frac{\partial}{\partial\mathbf{x}_1'}\right) \tag{3.19}$$

with the relative operator given by

$$H_r(12) = \mathbf{v}_{12}\cdot\frac{\partial}{\partial\mathbf{x}_{12}} - \Theta(12). \tag{3.20}$$

We also have

$$H^{(0)}(123) = H_r(12) + H_r(13) + v_1\cdot\frac{\partial}{\partial x_1'} - \Theta(23). \tag{3.21}$$

Using the above relations, we can carry out the time integration for some of the terms in (3.17) with the result that the [13] contribution to I_2 becomes

$$\int d\mathbf{x}_{13}\, d\mathbf{v}_3 \{\exp[-H_r(12) - H_r(13)]t - \exp[-H_r(12)t]\} f_1^{(0)} f_1^{(0)} f_1^{(0)} + \int_0^t dt' \exp[-H_r(12)(t-t')] \times \int d\mathbf{x}_{13}\, d\mathbf{v}_{13}\, \mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} \{\exp[-H_r(12) - H_r(13)]t' - \exp[-H_r(13)t_\infty]\} f_1^{(0)} f_1^{(0)} f_1^{(0)}. \quad (3.22)$$

It is clear that the first integral in (3.22) is finite. The second integral in (3.22) may be written as

$$\int_0^t dt' \exp[-H_r(12)(t-t')] \int d\mathbf{x}_{13\perp}\, d\mathbf{v}_3\, |\mathbf{v}_{13}| \times \{\exp[-H_r(12) - H_r(13)]t' - \exp[-H_r(13)t_\infty]\}_{\mathbf{x}_{13\parallel}=-\infty}^{\mathbf{x}_{13\parallel}=+\infty} f_1^{(0)} f_1^{(0)} f_1^{(0)}. \quad (3.23)$$

The trajectories appropriate for consideration of (3.23) are shown in Fig. 3. The upper limit of the $\mathbf{x}_{13\parallel}$ integration in (3.23) yields a finite result. We see this by phase-space arguments similar to those used for treating (3.6). However, if no [12] interaction occurs, then the argument differs and is similar to that following (7.2). For the lower limit, we note that $H_r(13)$ effectively vanishes since the [13] interaction has not yet occurred. Thus (3.23) becomes

$$-\int_0^t d\tau \exp[-H_r(12)\tau] \int d\mathbf{x}_{13\perp}\, d\mathbf{v}_{13}\, |\mathbf{v}_{13}| \times \exp\{[-H_r(12)(t-\tau)] - 1\} f_1^{(0)} f_1^{(0)} f_1^{(0)}. \quad (3.24)$$

For $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$, $H_r(12)$ commutes with $|\mathbf{v}_{13}|$ and (3.24) becomes

$$-\int_0^t d\tau \int d\mathbf{x}_{13\perp}\, d\mathbf{v}_{13}\, |\mathbf{v}_{13}| \{\exp[-H_r(12)t] - \exp[-H_r(12)\tau]\} f_1^{(0)} f_1^{(0)} f_1^{(0)}, \quad (3.25)$$

which clearly vanishes. For $t > |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$, (3.24) may be written

$$-\left(\int_0^{|\mathbf{x}_{12}|/|\mathbf{v}_{12}|} d\tau + \int_{|\mathbf{x}_{12}|/|\mathbf{v}_{12}|}^t d\tau\right) \times \exp[-H_r(12)\tau] \int d\mathbf{x}_{12}\, d\mathbf{v}_{13}\, |\mathbf{v}_{13}| \times \{\exp[-H_r(12)(t-\tau)] - 1\} f_1^{(0)} f_1^{(0)} f_1^{(0)}. \quad (3.26)$$

The first term of (3.26) is just

$$-\frac{|\mathbf{x}_{12}|}{|\mathbf{v}_{12}|} \int d\mathbf{x}_{13}\, d\mathbf{v}_{13}\, |\mathbf{v}_{13}| \times [\exp(-H_r t) - 1] f_1^{(0)} f_1^{(0)} f_1^{(0)}, \quad (3.27)$$

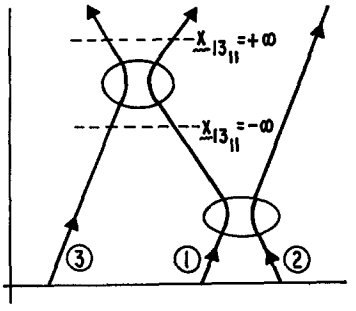

FIG. 3. Trajectories for Eq. (3.23).

which is spatially secular. The second term of (3.26) is

$$-\int_{|\mathbf{x}_{12}|/|\mathbf{v}_{12}|}^t d\tau \int d\mathbf{x}_{13}\, d\mathbf{v}_{13} \times \exp[-H_r(12)\tau]\, |\mathbf{v}_{13}| \times \exp[+H_r(12)\tau]\{\exp[-H_r(12)t] - \exp[-H_r(12)\tau]\} f_1^{(0)} f_1^{(0)} f_1^{(0)}, \quad (3.28)$$

which vanishes in the same manner as (3.25).

We see therefore that I_2 is finite for $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$ but exhibits secular behavior for $t > |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$. It should be noted that, in the examination of I_2 (and I_3 to follow), we have treated the integrals as if the limits of integration were independent of $\mathbf{x}_{13}$ or $\mathbf{x}_{23}$. In the Appendix we show that this neglect is justified, since the additional contributions arising from the limits of integration all cancel.

The next group of terms we consider is

$$I_3 = \int_0^t dt'\, S_{-(t-t')}(12) \int d\mathbf{x}_3\, d\mathbf{v}_3 \times [\Theta(13) + \Theta(23)] S_{-t'}(123) \times [f_3^{(0)}(0, \epsilon t) - f_1^{(0)}(1) f_1^{(0)}(2) f_1^{(0)}(3)]. \quad (3.29)$$

We use (1.9), (3.20), and (3.21) to carry out some of the time integrations in (3.29) with the result

$$I_3 = \int d\mathbf{x}_3\, d\mathbf{v}_3 \{\exp[-H^{(0)}(123)t] - \exp[-H_r(12)t]\}[\sum_P f_1^{(0)} g_2^{(0)}(0, \epsilon t) + g_3^{(0)}(0, \epsilon t)] + \int_0^t dt' \exp[-H_r(12)(t-t')] \times \int d\mathbf{x}_{13}\, d\mathbf{v}_3 \left[\mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} - \Theta(23)\right] \times \exp[-H^{(0)}(123)t'] \times [\sum_P f_1^{(0)} g_2^{(0)}(0, \epsilon t) + g_3^{(0)}(0, \epsilon t)]. \quad (3.30)$$

The first integral in (3.30) is finite because both the integrand and the range of integration in $\mathbf{x}_3$

are finite. The $\Theta(23)$ contribution in (3.30) is also finite because, if $|\mathbf{x}_{12}|$ is of order unity, the $H_r(12)$ operator can only act for a finite time. If $|\mathbf{x}_{12}|$ is large, then $|\mathbf{x}_{23}|$ must also be large and $\Theta(23)$ then vanishes.

In order to proceed with the analysis, we are forced to make assertions on the behavior of the correlation functions and then demonstrate *a posteriori* that they are correct. We assume here that $g_2^{(0)}(t = 0, \epsilon t)$ is finite in the region of phase space corresponding to the two particles having already collided and is zero elsewhere. The rationale for this assumption follows from the discussion after (2.5), where we concluded that $g_2^{(0)}(t, \epsilon t)$ was finite in this range of phase space. We make a similar assertion for $g_3^{(0)}(t = 0, \epsilon t)$, i.e., it is only nonzero in the region of phase space corresponding to two successive binary interactions having occurred involving all three particles.

Thus, we examine the remaining terms in (3.30)

$$\int_0^t dt' \exp\left[-H_r(12)(t-t')\right] \int d\mathbf{x}_{13}\, d\mathbf{v}_3\, \mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} \times \exp\left\{-[H_r(12) + H_r(13) - \Theta(23)]t'\right\} \times [f_1^{(0)}(1)g_2^{(0)}(23) + f_1^{(0)}(2)g_2^{(0)}(13) + f_1^{(0)}(3)g_2^{(0)}(12) + g_3^{(0)}(123)], \tag{3.31}$$

and conclude that the terms involving integration over particle [3] must be nonsecular. This follows, since, over most of the range of integration, they are, in fact, zero and the range in which they are nonzero is of order $1/|\mathbf{x}_{13}|^2$. The only possible secular term in (3.31) is thus

$$\int_0^t dt' \exp\left[-H_r(12)(t-t')\right] \int d\mathbf{x}_{13\perp}\, d\mathbf{v}_3\, |\mathbf{v}_{13}| \times \exp\left\{-[H_r(12) + H_r(13) - \Theta(23)]t'\right\} \times f_1^{(0)}(3)g_2^{(0)}(t = 0, \epsilon t, 12)\Big|_{|\mathbf{x}_{13}|=-\infty}^{|\mathbf{x}_{13}|=+\infty}. \tag{3.32}$$

The contribution from the upper limit in (3.32) vanishes since the operators stream the arguments of $g_2^{(0)}$ into the region of phase space for which it vanishes. This can be seen from Fig. 4 since the [13] interaction changes $\mathbf{v}_1$ by a quantity of order unity and $\mathbf{x}_{12}$ is also changed by order unity.

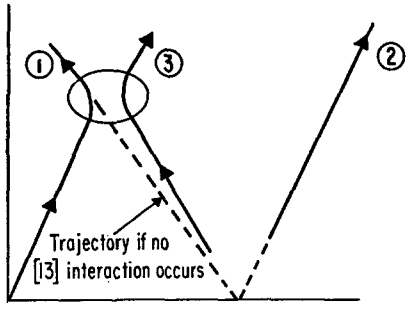

FIG. 4. Trajectories for $\mathbf{x}_{13\parallel} = +\infty$ in Eq. (3.32).

For the lower limit of (3.32), we refer to Fig. 3 and note that both operators $\Theta(13)$ and $\Theta(23)$ vanish. Thus, $\partial/\partial\mathbf{x}_{13}$ reduces to the identity operator and (3.32) becomes

$$-\int_0^t dt' \exp\left[-H_r(12)(t-t')\right] \int d\mathbf{x}_{13\perp}\, d\mathbf{v}_3\, |\mathbf{v}_{13}| \times \exp\left[-H_r(12)t'\right] f_1^{(0)}(3)g_2^{(0)}(12, 0, \epsilon t). \tag{3.33}$$

It is then clear that, for $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$, (3.33) becomes

$$-t\left(\int_{|\mathbf{x}_{13}|\le 1} d\mathbf{x}_{13\perp}\, d\mathbf{v}_3\, |\mathbf{v}_{13}|\, f_1^{(0)}(3)\right) \times \exp\left[-H_r(12)t\right] g_2^{(0)}(t = 0, \epsilon t, 12) \tag{3.34}$$

and is secular.

The next group of terms is

$$I_4 = -\int_0^t dt'\, S_{-(t-t')}(12) \int d\mathbf{x}_3\, d\mathbf{v}_3 \times [\Theta(13)S_{-\infty}(13)g_2^{(0)}(13)f_1^{(0)}(2) + \Theta(23)S_{-\infty}(23)g_2^{(0)}(23)f_1^{(0)}(1)]. \tag{3.35}$$

This expression clearly vanishes since the $S_{-\infty}$ operators project the coordinates into the region of phase space for which $g_2^{(0)}$ vanishes.

The last group of terms in (3.5) may be written

$$I_5 = -\int_0^t d\tau\, S_{-\tau}(12)\left(\frac{\partial}{\partial \epsilon t} + \mathbf{v}_{12}\cdot\frac{\partial}{\partial \epsilon \mathbf{x}_{12}}\right) \times [f_2^{(0)}(t-\tau, \epsilon t) - f_1^{(0)}(1)f_1^{(0)}(2)]. \tag{3.36}$$

For $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$, the S operator commutes with $\mathbf{v}_{12}$, so that (3.36) becomes

$$-\int_0^t d\tau \left(\frac{\partial}{\partial \epsilon t} + \mathbf{v}_{12}\cdot\frac{\partial}{\partial \epsilon \mathbf{x}_{12}}\right) \times [f_2^{(0)}(t, \epsilon t) - S_{-\tau}f_1^{(0)}(1)f_1^{(0)}(2)]. \tag{3.37}$$

Further, we note that

$$S_{-\tau}f_1^{(0)}f_1^{(0)} = f_1^{(0)}f_1^{(0)}, \quad 0 \le \tau \le t, \quad t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}| \tag{3.38}$$

so (3.36) becomes

$$-t\left(\frac{\partial}{\partial \epsilon t} + \mathbf{v}_{12}\cdot\frac{\partial}{\partial \epsilon \mathbf{x}}\right) \times \exp\left[-H^{(0)}(12)t\right] g_2^{(0)} \quad (t = 0, \epsilon t, 12), \tag{3.39}$$

which is secular.

IV. PROPAGATION OF CORRELATIONS

We now want to collect all the secular terms in $f_2^{(1)}$ and require that their sum vanish so that in fact $f_2^{(1)}$ exhibits regular behavior. We first demonstrate that, if we remove the secular behavior for $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$, we also remove it for $t > |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$.

To prove this statement, we write (3.1) in the form

$$\left[\frac{\partial}{\partial t} + H^{(0)}(12)\right] f_2^{(1)}(t) = A(t) \tag{4.1}$$

and solve this to get

$$f_2^{(1)}(t) = \exp\left[-H^{(0)}(12)(t - t_0) f_2^{(1)}(t_0)\right] + \int_{t_0}^{t} dt' \exp\left[-H^{(0)}(12)(t - t')\right] A(t'). \tag{4.2}$$

The trajectories contributing to (4.2) are shown in Fig. 5. Now choose

$$t_0 = t - |\mathbf{x}_{12}|/|\mathbf{v}_{12}| - 1 \tag{4.3}$$

and write (4.2) as

$$f_2^{(1)}(t) = \exp\left[-H^{(0)}(12)(1 + |\mathbf{x}_{12}|/|\mathbf{v}_{12}|)\right] \times f_2^{(1)}(t - 1 - |\mathbf{x}_{12}|/|\mathbf{v}_{12}|) + \left(\int_{t-1-|\mathbf{x}_{12}|/|\mathbf{v}_{12}|}^{t+1-|\mathbf{x}_{12}|/|\mathbf{v}_{12}|} dt' + \int_{t+1-|\mathbf{x}_{12}|/|\mathbf{v}_{12}|}^{t} dt'\right) \exp\left[-H^{(0)}(12)(t - t')\right] A(t'). \tag{4.4}$$

The last term in (4.4) can be transformed so that (4.4) becomes

$$f_2^{(1)}(t) = \exp\left[-H^{(0)}(12)(1 + |\mathbf{x}_{12}|/|\mathbf{v}_{12}|)\right] \times f_2^{(1)}(t - 1 - |\mathbf{x}_{12}|/|\mathbf{v}_{12}|) + \int_{t-1-|\mathbf{x}_{12}|/|\mathbf{v}_{12}|}^{t+1-|\mathbf{x}_{12}|/|\mathbf{v}_{12}|} dt' \exp\left[-H^{(0)}(12)(t - t')\right] A(t') + \int_{0}^{-1+|\mathbf{x}_{12}|/|\mathbf{v}_{12}|} d\tau \exp\left[-H^{(0)}(12)\tau\right] A(t - \tau). \tag{4.5}$$

The corresponding expression of $f_2^{(1)}$ for $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$ may be written

$$f_2^{(1)}(t) = \exp\left[-H^{(0)}(12)t\right] f_2^{(1)}(0) + \int_{0}^{t} d\tau \exp\left[-H^{(0)}(12)\tau\right] A(t - \tau). \tag{4.6}$$

We see that the first term of (4.5) projects $f_2^{(1)}$ into the phase-space region which does not lead to secular behavior. The second term of (4.5) is clearly of order unity. The last term of (4.5) is the same function of $(|\mathbf{x}_{12}|/|\mathbf{v}_{12}|) - 1$ that the last term of (4.6) is of t. Thus if (4.6) is rid of secular behavior, (4.5) does not exhibit secularities.

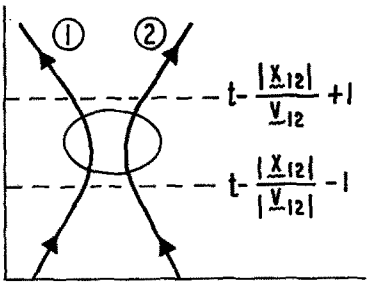

FIG. 5. Trajectories for Eq. (4.2).

Upon collecting all the secular terms for $t < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|$, we have

$$\left(\frac{\partial}{\partial \epsilon t} + \mathbf{v}_{12} \cdot \frac{\partial}{\partial \epsilon \mathbf{x}}\right) \exp\left[-H^{(0)}(12)t\right] g_2^{(0)}(t = 0, 12) + \sum_{i=1}^{2} \left[\int_{|\mathbf{x}_{i3}| \le 1} d\mathbf{x}_{i3\perp}\, d\mathbf{v}_3\, |\mathbf{v}_{i3}|\, f_1^{(0)}(3)\right] \times \exp\left[-H^{(0)}(12)t\right] g_2^{(0)}(0, 12) = 0, \tag{4.7}$$

which describes the propagation of correlations on the collisional time scale and the mean free path length scale. The quantity

$$\nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t) = \sum_{i=1}^{2} \int_{|\mathbf{x}_{i3}| \le 1} d\mathbf{x}_{i3\perp}\, d\mathbf{v}_3\, |\mathbf{v}_{i3}|\, f_1^{(0)}(3) \tag{4.8}$$

is clearly the effective collision frequency of particles [1] and [2] with [3].

We solve (4.7) and have

$$\exp\left[-H^{(0)}(12)t\right] g_2^{(0)}[\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, t = 0, \epsilon\mathbf{x}_{12}, \epsilon t] = \exp\left[-\int_{\epsilon t_0}^{\epsilon t} \nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t')\, d\epsilon t'\right] \times \exp\left[-H^{(0)}(12)t\right] g_2^{(0)}[\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, t = 0, \epsilon\mathbf{x}_{12} - \epsilon\mathbf{v}_{12}(t - t_0), \epsilon t_0], \tag{4.9}$$

where ϵt_0 is an arbitrary initial time. The result (4.9) is easily generalized to

$$\exp\left[-H^{(0)}(12)(t - \tilde{t})\right] g_2^{(0)}[\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, \tilde{t}, \epsilon\mathbf{x}_{12}, \epsilon t] = \exp\left[-\int_{\epsilon t_0}^{\epsilon t} \nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t')\, d\epsilon t'\right] \times \exp\left[-H^{(0)}(12)(t - \tilde{t})\right] g_2^{(0)}[\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, \tilde{t}, \epsilon\mathbf{x}_{12} - \epsilon\mathbf{v}_{12}(t - t_0), \epsilon t_0] \tag{4.10}$$

with the restriction

$$(t - \tilde{t}) < |\mathbf{x}_{12}|/|\mathbf{v}_{12}|, \tag{4.11}$$

which was imposed in obtaining (4.9). In view of (4.11), we can let the $H^{(0)}(12)$ operators act in

(4.10) and get

$$g_2^{(0)}[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t}), \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \epsilon\mathbf{x}_{12}, \epsilon t] = \exp\left[-\int_{\epsilon t_0}^{\epsilon t} \nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t')\, d\epsilon t'\right] \times g_2^{(0)}[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t}), \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \epsilon\mathbf{x}_{12} - \epsilon\mathbf{v}_{12}(t - t_0), \epsilon t_0]. \quad (4.12)$$

It is clear that we have the freedom to return to the physical "line" by choosing

$$t_0 = \bar{t}. \quad (4.13)$$

Thus, we simply rewrite (4.12) as

$$g_2^{(0)}[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t}), \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \epsilon\mathbf{x}_{12}, \epsilon t] = \exp\left[-\int_{\epsilon\bar{t}}^{\epsilon t} \nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t')\, d\epsilon t'\right] \times g_2^{(0)}[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t}), \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \epsilon\mathbf{x}_{12} - \epsilon\mathbf{v}_{12}(t - \bar{t}), \epsilon\bar{t}]. \quad (4.14)$$

Equation (4.14) can be put into a more transparent form by noting from (2.1) that

$$g_2^{(0)}[\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, t, \epsilon\mathbf{x}_{12}, \epsilon t] = \{\exp[-H^{(0)}(12)(t - \bar{t})] - 1\} f_1^{(0)} f_1^{(0)}(2) + \exp[-H^{(0)}(12)(t - \bar{t})] \times g_2^{(0)}(\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \epsilon t, \epsilon\mathbf{x}_{12}). \quad (4.15)$$

However, with the restriction (4.11), the *ff* term in (4.15) vanishes while the other term on the right-hand side of (4.15) is identical to the left-hand side of (4.14). Thus, (4.14) may be written as

$$g_2^{(0)}(\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, t, \epsilon\mathbf{x}_{12}, \epsilon t) = \exp\left[-\int_{\epsilon\bar{t}}^{\epsilon t} \nu(\epsilon t')\, d\epsilon t'\right] g_2^{(0)}[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t}), \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \epsilon\mathbf{x}_{12} - \epsilon\mathbf{v}_{12}(t - \bar{t}), \epsilon t]. \quad (4.16)$$

We can carry this one step further by projecting $g_2^{(0)}$ into the region of phase space for which it vanishes by assumption. To accomplish this we use (4.15) in the form

$$g_2^{(0)}\{\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t}), \mathbf{v}_1, \mathbf{v}_2, \bar{t}, \times \epsilon[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t})], \epsilon\bar{t}\} = (\exp\{-H^{(0)}[\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t})](\bar{t} - \tau)\} - 1) f_1^{(0)}(1) f_1^{(0)}(2), \quad (4.17)$$

where

$$\bar{t} - \tau > |\mathbf{x}_{12} - \mathbf{v}_{12}(t - \bar{t})|/|\mathbf{v}_{12}| + O(1/|\mathbf{v}_{12}|) \quad (4.18)$$

and we have written the arguments of $H^{(0)}(12)$ explicitly to avoid confusion.

Thus, we finally obtain

$$g_2^{(0)}(\mathbf{x}_{12}, \mathbf{v}_1, \mathbf{v}_2, t, \epsilon t, \epsilon\mathbf{x}_{12}) = \exp\left[-\int_{\epsilon\bar{t}}^{\epsilon t} \nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t')\, d\epsilon t'\right] \times (\exp\{-H^{(0)}[\mathbf{x} - \mathbf{v}(t - \bar{t})] \times (\bar{t} - \tau)\} - 1) f_1^{(0)}(1, \epsilon\bar{t}) f_1^{(0)}(2, \epsilon\bar{t}). \quad (4.19)$$

The result (4.19) is pleasing physically since it shows that the correlation is generated by the collision of two particles and then sticks out long thin arms in phase space until a collision with a third particle occurs which causes it to decay exponentially. A conjecture of Green[8] appears to be in accord with this picture. It is interesting to note that the result (4.19) supports the Bogoliubov hypothesis that higher-correlation functions become functionals of the one-particle function. We see, however, that it is not a functional of f_1 at the same time but rather there is a history dependence.

We conclude, therefore, that we have removed the secular behavior of $f_2^{(1)}$ subject to the assumptions made earlier on the phase-space behavior of the correlation functions.

V. VERIFICATION OF PHASE-SPACE ASSUMPTIONS

We now want to demonstrate that there is a consistent solution of the equations of the hierarchy which has the properties we assumed earlier for the correlation functions, subject to the initial conditions of chaos at time zero. We therefore drop the assumption that $g_s^{(0)}$ vanishes unless there have been s binary interactions and are thus forced to consider all the equations of the hierarchy jointly since, in principle, $g_{s-1}^{(0)}$ depends on $g_s^{(0)}$, etc.

We obtain from (2.6)

$$f_s^{(1)}(t) = \exp[-H^{(0)}(1, \cdots, s)(t - t_0)] f_s^{(1)}(t_0) + \int_{t_0}^{t} dt' \exp[-H^{(0)}(1, \cdots, s)(t - t')] \times \left\{\int_{|\mathbf{x}_i, s+1| \le 1} d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \Theta(i, s+1) f_{s+1}^{(0)}(t') - \left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] f_s^{(0)}(t')\right\}. \quad (5.1)$$

Our object is to remove the secular terms from (5.1), and in so doing, obtain an equation of evolution for $g_s^{(0)}$ which is free of our earlier assumption. We find it easier to solve the dynamical problem piecewise than to consider the whole problem all at once. Thus, we assume that, during the time interval $t - t_0$

(which is order unity but numerically greater than unity), none of the s particles is interacting. We then join such solutions across an interaction interval, τ, of order unity. The rationale follows from our earlier observations that secular behavior arises in $t - t_0$ intervals and that τ intervals contribute terms of order unity.

We now substitute (2.3) into (5.1) and write

$$(t - t_0)\left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] f_s^{(0)}$$
$$= -f_s^{(1)}(t) + \exp[-H^{(0)}(1, \cdots, s)(t - t_0)] f_s^{(1)}(t_0)$$
$$+ \int_{t_0}^{t} dt' \exp[-H^{(0)}(1, \cdots, s)(t - t')]$$
$$\times \left[\int_{|\mathbf{x}_i, s+1| \leq 1} d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \Theta(i, s+1) f_{s+1}^{(0)}(t')\right]. \tag{5.2}$$

Since we wish to collect only the secular terms from the right-hand side of (5.2), we lump all the nonsecular terms into a quantity called N_s. We assume that $f_s^{(1)}(t_0)$ is not secular and that we remove the secularities from $f_s^{(1)}(t)$. Thus, the first two terms on the right-hand side of (5.2) are put in N_s. It is convenient to introduce coordinates relative to $\mathbf{x}_i$ and write

$$H^{(0)}(1, \cdots, s) \equiv H_s(i)$$
$$= \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} + \sum_{j=1, j\neq i}^{s} \mathbf{v}_{ij} \cdot \frac{\partial}{\partial \mathbf{x}_{ij}} - \sum_{i=1}^{s} \sum_{j>i}^{s} \Theta(ij) \tag{5.3}$$

and

$$H^{(0)}(1, \cdots, s+1) \equiv H_{s+1}(i) = H_s(i)$$
$$+ \mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}} - \sum_{j=1}^{s} \Theta(j, s+1). \tag{5.4}$$

Equation (5.2) may then be written

$$(t - t_0)\left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] f_s^{(0)}$$
$$= \sum_{i=1}^{s} \int_{t_0}^{t} dt' \left\{\exp[-H_s(i)(t - t')]\right.$$
$$\times \int_{|\mathbf{x}_i, s+1| \leq 1} d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \left[-H_{s+1}(i) + H_s(i)\right.$$
$$\left. + \mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}} - \sum_{j=1, j\neq i}^{s} \Theta(j, s+1)\right]$$
$$\left. \times \exp[-H_{s+1}(i)(t' - t_0)] f_{s+1}^{(0)}(t_0)\right\} + N_s. \tag{5.5}$$

Note that the $\Theta(j, s+1)$ terms can be included in N_s, since the time interval over which they act is limited and thus they produce no secular behavior.

We then carry out some of the time integrations in (5.5) and have

$$(t - t_0)\left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] f_s^{(0)}$$
$$= \sum_{i=1}^{s} \int_{|\mathbf{x}_i, s+1| \leq 1} d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1} \{\exp[-H_{s+1}(i)(t - t_0)]$$
$$- \exp[-H_s(i)(t - t_0)]\} f_{s+1}^{(0)}(t_0)$$
$$+ \sum_{i=1}^{s} \int_{t_0}^{t} dt' \exp[-H_s(i)(t - t')]$$
$$\times \int_{|\mathbf{x}_i, s+1| \leq 1} d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1}\, \mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}}$$
$$\times \exp[-H_{s+1}(i)(t' - t_0)] f_{s+1}^{(0)}(t_0) + N_s. \tag{5.6}$$

It is clear that the first group of terms on the right-hand side of (5.6) now should be put into N_s.

It is convenient to add and subtract terms in (5.6) to try to mirror the earlier calculation. We therefore write

$$(t - t_0)\left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] f_s^{(0)}$$
$$= \sum_{i=1}^{s} \int_{t_0}^{t} dt' \exp[-H_s(i)(t - t')]$$
$$\times \int_{|\mathbf{x}_i, s+1| \leq 1} d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1}\, \mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}}$$
$$\times \exp\left\{-\left[H_s(i) + \mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}}\right.\right.$$
$$\left.\left. - \Theta(i, s+1) - \sum_{j=1, j\neq i}^{s} \Theta(j, s+1)\right](t' - t_0)\right\}$$
$$\times \{f_1^{(0)}(s+1) f_1^{(0)}(i) f_{s-1}^{(0)}(t_0)$$
$$+ f_1^{(0)}(s+1)[f_s^{(0)}(t_0) - f_1^{(0)}(i) f_{s-1}^{(0)}(t_0)]$$
$$+ [f_{s+1}^{(0)}(t_0) - f_1^{(0)}(s+1) f_s^{(0)}(t_0)]\} + N_s. \tag{5.7}$$

We first note that, in effect, the last term in the exponential operator in (5.7) can be thrown into N_s, since it is only nonzero if both the ith- and the jth-particles interact with the $(s+1)$ particle. In the treatment of $f_2^{(1)}$, we saw that such configurations do not yield secular behavior.

To proceed with the analysis of (5.7), we next note that, since the s particles do not interact with each other, (5.3) reduces to

$$H_s(i) = \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} + \sum_{j=1, j\neq i}^{s} \mathbf{v}_{ij} \cdot \frac{\partial}{\partial \mathbf{x}_{ij}}. \tag{5.8}$$

Further, in our present coordinate system, $f_1^{(0)}(s+1)$, $f_1^{(0)}(i)$, and $f_{s-1}^{(0)}(t_0)$ are all independent of $\mathbf{x}_i$. Thus, $H_s(i)$ and $\mathbf{v}_{i,s+1} \cdot \partial/\partial \mathbf{x}_{i,s+1} - \Theta(i, s+1)$ may be

regarded as commuting operators. Therefore, the first term in the integrand of (5.7) may be written as

$$\sum_{i=1}^{s}\int_{t_0}^{t}dt'\int_{|\mathbf{x}_{i,s+1}|\leq 1}d\mathbf{x}_{s+1}\,d\mathbf{v}_{s+1}\,\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}$$
$$\times\exp\left\{-\left[\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right](t'-t_0)\right\}$$
$$\times f_1^{(0)}(s+1)f_1^{(0)}(i)f_{s-1}^{(0)}(t_0). \tag{5.9}$$

From the second group of terms in (5.7), we get

$$\sum_{i=1}^{s}\int_{t_0}^{t}dt'\exp\left[-H_s(i)(t-t')\right]$$
$$\times\int_{|\mathbf{x}_{i,s+1}|\leq 1}d\mathbf{x}_{i,(s+1)\perp}\,d\mathbf{v}_{s+1}\,|\mathbf{v}_{i,s+1}|$$
$$\times\exp\left\{-\left[H_s(i)+\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}\right.\right.$$
$$\left.\left.-\Theta(i,s+1)\right](t'-t_0)\right\}f_1^{(0)}(s+1)$$
$$\times[f_s^{(0)}(t_0)-f_1^{(0)}(i)f_{s-1}^{(0)}(t_0)]\big|_{|\mathbf{x}_{i,(s+1)\parallel}=-\infty}^{|\mathbf{x}_{i,(s+1)\parallel}=+\infty}. \tag{5.10}$$

The upper limit in (5.10) can possibly contribute a secular term. In the lower limit, we note that $\mathbf{v}_{i,s+1}\cdot\partial/\partial\mathbf{x}_{i,s+1}-\Theta(i,s+1)$ acts in the exponential to yield the identity operator, and, upon using (5.8), we can bring the $H_s(i)$ operator through. The lower limit of (5.10) can thus be written

$$\sum_{i=1}^{s}\int_{t_0}^{t}dt'\int_{|\mathbf{x}_{i,s+1}|\leq 1}d\mathbf{x}_{i,(s+1)\perp}\,d\mathbf{v}_{s+1}\,|\mathbf{v}_{i,s+1}|$$
$$\times f_1^{(0)}(s+1)[f_s^{(0)}(t)-f_1^{(0)}(i)f_{s-1}^{(0)}(t)]|_{\mathbf{x}_{i,(s+1)\parallel}=-\infty}. \tag{5.11}$$

It is advantageous to force this expression to resemble (5.9) and we thus insert the identity operator to get

$$\sum_{i=1}^{s}\int_{t_0}^{t}dt'\int_{|\mathbf{x}_{i,s+1}|\leq 1}d\mathbf{x}_{i,(s+1)\perp}\,d\mathbf{v}_{s+1}\,|\mathbf{v}_{i,s+1}|$$
$$\times\exp\left\{-[\mathbf{v}_{i,s+1}\cdot\partial/\partial\mathbf{x}_{i,s+1}-\Theta(i,s+1)](t'-t_0)\right\}$$
$$\times f_1^{(0)}(s+1)[f_s^{(0)}(t)-f_1^{(0)}(i)f_{s-1}^{(0)}(t)]|_{\mathbf{x}_{i,(s+1)\parallel}=-\infty}. \tag{5.12}$$

We can further undo the $\mathbf{x}_{i,(s+1)\parallel}$ integration and rewrite (5.12) with a correction term from the upper limit. Rather than pausing to do this here, we collect all the results and simply rewrite (5.7) as

$$(t-t_0)\left[\frac{\partial}{\partial\epsilon_t}+H^{(1)}(1,\cdots,s)\right]f_s^{(0)}$$
$$=\sum_{i=1}^{s}\int_{t_0}^{t}dt'\int_{|\mathbf{x}_{i,s+1}|\leq 1}d\mathbf{x}_{s+1}\,d\mathbf{v}_{s+1}\,\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}$$
$$\times\exp\left\{-\left[\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right](t'-t_0)\right\}$$
$$\times f_1^{(0)}(s+1)f_s^{(0)}(t)+R_s+N_s, \tag{5.13}$$

where

$$R_s=\sum_{i=1}^{s}\int_{t_0}^{t}dt'\exp\left[-H_s(i)(t-t')\right]$$
$$\times\left(\int d\mathbf{x}_{i,s+1}\,d\mathbf{v}_{s+1}\,|\mathbf{v}_{i,s+1}|\exp\left\{-\left[H_s(i)\right.\right.\right.$$
$$\left.\left.\left.+\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right](t'-t_0)\right\}\right.$$
$$\times f_1^{(0)}(s+1)(f_s^{(0)}(t_0)-f_1^{(0)}(i)f_{s-1}^{(0)}(t_0))\big|^{|\mathbf{x}_{i,(s+1)\parallel}=+\infty}$$
$$+\int d\mathbf{x}_{s+1}\,d\mathbf{v}_{s+1}\,d\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}\exp\left\{-\left[H_s(i)\right.\right.$$
$$\left.\left.+\mathbf{v}_i\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right](t'-t_0)\right\}$$
$$\left.\times[f_{s+1}^{(0)}(t_0)-f_1^{(0)}(s+1)f_s^{(0)}(t_0)]\right)$$
$$-\sum_{i=1}^{s}\int_{t_0}^{t}dt'\int d\mathbf{x}_{i,(s+1)\perp}\,d\mathbf{v}_{s+1}\,|\mathbf{v}_{i,s+1}|$$
$$\times\exp\left\{-\left[\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right](t'-t_0)\right\}$$
$$\times f_1^{(0)}(s+1)[f_s^{(0)}(t)-f_1^{(0)}(i)f_{s-1}^{(0)}(t)]|^{|\mathbf{x}_{i,(s+1)\parallel}=+\infty}. \tag{5.14}$$

Next, we note that the operator

$$\exp\left\{-\left[\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right](t'-t_0)\right\}, \tag{5.15}$$

occurring in (5.13), describes the usual two-particle interaction and, for

$$t'-t_0>1, \tag{5.16}$$

we can replace (5.15) by

$$\exp\left\{-\left[\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right]t_\infty\right\}. \tag{5.17}$$

Thus, we may rewrite (5.13) as

$$\left[\frac{\partial}{\partial\epsilon t}+H^{(1)}(1,\cdots,s)\right]f_s^{(0)}$$
$$=\sum_{i=1}^{s}\int d\mathbf{x}_{s+1}\,d\mathbf{v}_{s+1}\,\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}$$
$$\times\exp\left\{-\left[\mathbf{v}_{i,s+1}\cdot\frac{\partial}{\partial\mathbf{x}_{i,s+1}}-\Theta(i,s+1)\right]t_\infty\right\}$$
$$\times f_1^{(0)}(s+1)f_s^{(0)}(t)+\frac{R_s+N_s}{(t-t_0)}. \tag{5.18}$$

If we now substitute the cluster expansion in (5.18) there results

$$\left[\frac{\partial}{\partial \epsilon t} + H^{(1)}(1, \cdots, s)\right] g_s^{(0)}$$
$$= \sum_{i=1}^{s} \int d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1}\, \mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}}$$
$$\times \exp\left\{-\left[\mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}} - \Theta(i, s+1)\right] t_\infty\right\} f_1^{(0)}(s+1) g_s^{(0)}(t)$$
$$+ F_s\{R_s\} + G_s\{N_s\}, \tag{5.19}$$

where F_s and G_s are functionals of the R_s and N_s, respectively. We do not write out the explicit expressions for F_s and G_s here but simply note that they are complicated sums of products of the R's and N's involving j particles with $1 \leq j \leq s$.

From (2.1) we have, for the time interval $t - t_0$,

$$\left[\frac{\partial}{\partial t} + H^{(0)}(1, \cdots, s)\right] g_s^{(0)} = 0. \tag{5.20}$$

Thus, combining (5.19) and (5.20) we get

$$\frac{\partial g_s^{(0)}}{\partial t} + H^{(0)}(1, \cdots, s) g_s^{(0)}$$
$$+ \epsilon \frac{\partial g_s^{(0)}}{\partial \epsilon_t} + \epsilon H^{(1)}(1, \cdots, s) g_s^{(0)}$$
$$= -\epsilon \nu(\mathbf{v}_1 \cdots \mathbf{v}_s, \epsilon t) g_s^{(0)}$$
$$+ \epsilon F'\{R_s\} + \epsilon G\{N_s\}. \tag{5.21}$$

In writing (5.21) we have defined the generalized collision frequency

$$\nu(\mathbf{v}_1, \cdots, \mathbf{v}_s, \epsilon t) = \sum_{i=1}^{s} \int d\mathbf{x}_{(s+1)\perp}\, d\mathbf{v}_{s+1}\, |\mathbf{v}_{i,s+1}|$$
$$\times \exp\left\{-\left[\mathbf{v}_{i,s+1} \cdot \frac{\partial}{\partial \mathbf{x}_{i,s+1}} - \Theta(i, s+1)\right] t_\infty\right\} f_1^{(0)}(s+1)\Big|_{\mathbf{x}_{i,(s+1)\parallel} = -\infty}. \tag{5.22}$$

The expression on the right-hand side of (5.22) evaluated at $x_{i,(s+1)\parallel} = +\infty$ has been lumped with F to become F'.

The piecing procedure for solving the complete problem then consists of using (5.21) in the intervals in which the s particles are not interacting, and then using (2.1) in the intervals in which they do interact. Clearly, for a finite number of interactions, we introduce a relative error of order ϵ in this way since we have used (2.1) rather than an equation good to one higher order in ϵ as is (5.21). This relative error does not influence the outcome of the proof, however, since we wish to make statements concerning a zeroth-order quantity.

In addition to the piecing procedure, we use an iterative procedure to solve (5.21). The lowest-order approximation consists of neglecting $F'\{R_s\}$ in (5.21). Note that the interval can be as long as $t - t_0 \sim 1/\epsilon$. Now, $G\{N_s\}$ certainly has at least one term which behaves as $1/(t - t_0)$ while all the others behave as

$$\frac{1}{(t - t_0)^p}, \quad 1 < p \leq s. \tag{5.23}$$

Therefore, the $G\{N_s\}$ terms can at best produce a term which is of order ϵ in $(g_s^{(0)})_0$ after integrating for a time of order $1/\epsilon$. We proceed to the next iterate by substituting $(g_s^{(0)})_0$ into $F'\{R_s\}$. By carefully examining R_s in (5.14) using arguments analogous to those used earlier for $f_2^{(1)}$, we can conclude that no secular terms are produced. Thus, $F'\{R_s\}$ actually behaves in the same fashion as the $G\{N_s\}$ terms did in the lowest approximation. We therefore see that the equations governing $(g_s^{(0)})_1$ are essentially identical to the equations for $(g_s^{(0)})_0$. The net effect is, then, that, as far as the present proof is concerned, we can simply drop the F' and G terms from consideration and we need not iterate at all.

We can now return to (5.21) and, for $s = 2$, we have

$$\frac{\partial g_2^{(0)}}{\partial t} + H^{(0)}(12) g_2^{(0)} + \epsilon \frac{\partial g_2^{(0)}}{\partial \epsilon t} + \epsilon H^{(1)}(12) g_2^{(0)}$$
$$= -\epsilon \nu(\mathbf{v}_1, \mathbf{v}_2, \epsilon t) g_2^{(0)}. \tag{5.24}$$

Note now that (5.24) holds in all regions of phase space and for time intervals in which particles [1] and [2] do not interact with each other. However, we can now apply (5.24) to the situation in which

$$g_2^{(0)}(t = 0, \epsilon t = 0, 1, 2) = 0, \tag{5.25}$$

and we see that it remains zero until an interaction takes place. During the time of interaction we use

$$\frac{\partial g_2^{(0)}}{\partial t} + H^{(0)}(12) g_2^{(0)} = -\Theta(12) f_1^{(0)} f_1^{(0)} \tag{5.26}$$

which then creates the correlation.

Thus, the above arguments have related $g_2^{(0)}$ to its physical initial value and have demonstrated that the assumption that $g_2^{(0)}$ vanishes in the region of phase space corresponding to no previous interaction is, in fact, correct. As a by-product, we have also obtained (5.21) for the s particle correlations, and can thus describe the long-time, long-space behavior of all the correlations.

VI. BEHAVIOR OF $f_2^{(1)}$ FOR $|\mathbf{v}_{12}| \ll 1$

On physical grounds, we are led to suspect that some sort of singular behavior arises for $|\mathbf{v}_{12}| \ll 1$, since two particles might then stay together for times comparable to the time between collisions. We therefore investigate here the nature of this singular behavior. We assume that $\mathbf{v}_{12}$ is small and that the range in configuration space is limited by

$$\phi(|\mathbf{x}_{12}|) \leq \tfrac{1}{2}(v_{12}^2). \tag{6.1}$$

A crude estimate of the behavior of $f_2^{(1)}$ follows from (3.2) under these assumptions. We may assume that the integrand of the t' integration is of order unity for

$$|\exp[-H^{(0)}(12)(t-t')]\mathbf{x}_{12}| \sim 1. \tag{6.2}$$

For such configurations, the interval in t' for which this is so is of order $|\mathbf{v}_{12}|^{-1}$ which indicates that $f_2^{(1)}$ varies as $|\mathbf{v}_{12}|^{-1}$ for $|\mathbf{v}_{12}| \ll 1$.

To treat this more formally, we scale the variables in the usual manner of asymptotic analysis. We write

$$\mathbf{v}_{12} = \epsilon^{\delta}\tilde{\mathbf{v}}_{12}, \quad \tilde{\mathbf{v}}_{12} \sim 1. \tag{6.3}$$

Assuming that (6.1) holds, we have

$$\phi(|\mathbf{x}_{12}|) \sim \epsilon^{2\delta}\tilde{\phi}(|\mathbf{x}_{12}|), \quad \tilde{\phi}(|\mathbf{x}_{12}|) \sim 1. \tag{6.4}$$

We then write (2.1) for $s = 2$ in the form

$$\left[\frac{\partial}{\partial t} + \mathbf{v}_{12}\cdot\frac{\partial}{\partial \mathbf{x}_{12}} - \frac{\partial\phi}{\partial \mathbf{x}_{12}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)\right] g_2^{(0)} = \frac{\partial\phi}{\partial \mathbf{x}_{12}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right) f_1^{(0)}(1) f_1^{(0)}(2). \tag{6.5}$$

Introducing the variables

$$\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2, \quad \mathbf{V} = \mathbf{v}_1 + \mathbf{v}_2 \tag{6.6}$$

enables us to write

$$\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2} = 2\frac{\partial}{\partial \mathbf{v}_{12}} \tag{6.7}$$

and, by Taylor expansion,

$$f_1^{(0)}\begin{pmatrix}\mathbf{v}_1\\ \mathbf{v}_2\end{pmatrix} = f_1^{(0)}(\tfrac{1}{2}\mathbf{V}) \pm \tfrac{1}{2}\mathbf{v}_{12}\cdot\nabla_{\mathbf{v}} f_1^{(0)} + \tfrac{1}{8}\mathbf{v}_{12}\mathbf{v}_{12} : \nabla_{\mathbf{v}}\nabla_{\mathbf{v}} f_1^{(0)} + \cdots. \tag{6.8}$$

We now rewrite (6.5) in the scaled variables and require that all the terms remain in the scaled version. This yields

$$\left(\frac{\partial}{\partial \tilde{t}} + \tilde{\mathbf{v}}_{12}\cdot\frac{\partial}{\partial \mathbf{x}_{12}} - 2 - \frac{\partial\tilde{\phi}}{\partial \mathbf{x}_{12}}\cdot\frac{\partial}{\partial \tilde{\mathbf{v}}_{12}}\right)\tilde{g}_2^{(0)} = \frac{1}{2}\frac{\partial\tilde{\phi}}{\partial \mathbf{x}_{12}}\cdot\frac{\partial}{\partial \mathbf{v}_{12}} \times \left[f_1^{(0)}\left(\frac{\mathbf{V}}{2}\right)\tilde{\mathbf{v}}_{12}\tilde{\mathbf{v}}_{12} : \nabla_{\mathbf{v}}\nabla_{\mathbf{v}} f_1^{(0)} - (\tilde{\mathbf{v}}_{12}\cdot\nabla_{\mathbf{v}} f_1^{(0)})^2\right] \tag{6.9}$$

with the additional scaling

$$g_2^{(0)} = \epsilon^{2\delta}\tilde{g}_2^{(0)} \tag{6.10}$$

and

$$d\tilde{t}/dt = \epsilon^{\delta}. \tag{6.11}$$

We next turn to (3.1) and write it in the form

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_{12}\cdot\frac{\partial}{\partial \mathbf{x}_{12}} - 2\frac{\partial\phi}{\partial \mathbf{x}_{12}}\cdot\frac{\partial}{\partial \mathbf{v}_{12}}\right) f_2^{(1)} = H(f_3^{(0)}) - \frac{\partial f_2^{(0)}}{\partial \epsilon t} - \mathbf{v}_{12}\cdot\frac{\partial f_2^{(0)}}{\partial \epsilon \mathbf{x}_{12}}. \tag{6.12}$$

We note that the second term on the right-hand side of (6.12) is clearly of order unity, while $H(f_3^{(0)})$ is at best of order unity. The third term is

$$\mathbf{v}_{12}\cdot\frac{\partial}{\partial \epsilon \mathbf{x}} f_2^{(0)} = \epsilon^{3\delta}\tilde{\mathbf{v}}_{12}\cdot\frac{\partial\tilde{g}_2^{(0)}}{\partial \epsilon \mathbf{x}}. \tag{6.13}$$

The scaled version of (6.12) is then

$$\epsilon^{\delta}\left(\frac{\partial}{\partial \tilde{t}} + \tilde{\mathbf{v}}_{12}\cdot\frac{\partial}{\partial \mathbf{x}_{12}} - 2\frac{\partial\tilde{\phi}}{\partial \mathbf{x}_{12}}\cdot\frac{\partial}{\partial \tilde{\mathbf{v}}_{12}}\right) f_2^{(1)} = O(1), \tag{6.14}$$

which indicates that

$$f_2^{(1)} = \tilde{f}_2^{(1)}/\epsilon^{\delta} \tag{6.15}$$

and verifies the crude estimate of the behavior of $f_2^{(1)}$.

We next examine the question of whether, for some value of δ, the ϵ expansion used in the paper becomes invalid. The ratio

$$\epsilon f_2^{(1)}/g_2^{(0)} \sim \epsilon^{1-3\delta} \tag{6.16}$$

becomes of order unity for $\delta = \frac{1}{3}$. We then must examine the contribution to f_1 arising from $f_2^{(1)}$ and compare it with the contribution from $g_2^{(0)}$. The contribution is

$$\int_{v_{12}=0}^{v_{12}\sim\epsilon^{\frac{1}{3}}} d\mathbf{v}_{12} \int_{\phi(|\mathbf{x}_{12}|)\leq v_{12}^2} d\mathbf{x}_{12} \times \frac{\partial\phi}{\partial \mathbf{x}_{12}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right) f_2^{(1)}. \tag{6.17}$$

The spatial volume of integration is of order unity for $\mathbf{x}_{12}$ determined by (6.1). Further,

$$\frac{\partial\phi}{\partial \mathbf{x}_{12}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right) \sim 2\frac{\partial\tilde{\phi}}{\partial \mathbf{x}_{12}}\cdot\frac{\partial\tilde{f}_2^{(1)}}{\partial \tilde{\mathbf{v}}_{12}} \sim 1. \tag{6.18}$$

Thus, the integral in (6.17) is of order

$$\int_{v_{12}=0}^{v_{12}\sim\epsilon^{\frac{1}{3}}} |v_{12}|^2\, d\mathbf{v}_{12} \sim \epsilon. \tag{6.19}$$

We therefore conclude that, although $f_2^{(1)}$ diverges for $|\mathbf{v}_{12}| \ll 1$, the contribution to the kinetic equation

for f_1 is of higher order in ϵ and, thus, the original ordering is not upset for $\delta \geq \frac{1}{3}$.

VII. THE BOLTZMANN AND CHOH-UHLENBECK RESULTS

We can now go back and point out the connection between the present work and the Boltzmann and Choh–Uhlenbeck results.

To this end, we first go back to (2.9) and (2.10) and write them as

$$\frac{\partial f_1^{(0)}}{\partial \epsilon t} = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) S_{-\infty}(12) \times [f_1^{(0)} f_1^{(0)} + g_2^{(0)}(0, \epsilon t, 12)] \tag{7.1}$$

and

$$\frac{\partial f_1^{(1)}}{\partial t} = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12)(S_{-t} - S_{-\infty}) \times [f_1^{(0)} f_1^{(0)} + g_2^{(0)}(t = 0, \epsilon t, 12)]. \tag{7.2}$$

In considering (7.1) we immediately note that the $S_{-\infty}$ operator projects the arguments of $g_2^{(0)}$ into the phase-space region in which it vanishes. As for the ff term in (7.1), we note that Bogoliubov[1] has demonstrated that this is just another version of the standard Boltzmann collision integral. The H theorem then guarantees the behavior of $f_1^{(0)}$.

We next turn to (7.2). The $\Theta(12)$ operator restricts $\mathbf{x}_{12}$ to be of order unity at time t or the integral vanishes. Trajectories which have $\mathbf{x}_{12}(t) \sim 1$ at time t and $\mathbf{x}_{12}(0) \sim 1$ are the only ones which contribute to the integral. Thus, we require

$$|\mathbf{x}_{12}(t) - \mathbf{x}_{12}(0)| < 1 \tag{7.3}$$

or, estimating,

$$|\mathbf{v}_{12}|\, t < 1. \tag{7.4}$$

We can write (7.2) as

$$\frac{\partial f_1^{(1)}}{\partial t} = \frac{\partial}{\partial \mathbf{v}_1} \cdot \int d\mathbf{v}_{12}\, \mathbf{F}(\mathbf{v}_{12}), \tag{7.5}$$

where the vector $\mathbf{F}$ vanishes if $|\mathbf{v}_{12}| > 1/t$ and is at most of order unity if $|\mathbf{v}_{12}| < 1/t$. Thus,

$$\partial f_1^{(1)}/\partial t \sim t^{-3} \tag{7.6}$$

and this contribution is well behaved as t becomes large.

We have then justified the original decomposition of (2.8) into (2.9) and (2.10) and have demonstrated that the standard Boltzmann result obtains.

The next order result is, from (1.7),

$$\frac{\partial f_1^{(2)}}{\partial t} + \frac{\partial f_1^{(1)}}{\partial \epsilon t} + \frac{\partial f_1^{(0)}}{\partial \epsilon^2 t} = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) f_2^{(1)}(t, \epsilon t, \epsilon^2 t). \tag{7.7}$$

Upon removing secular behavior, we get

$$\frac{\partial f_1^{(1)}}{\partial \epsilon t}(\infty, \epsilon t, \epsilon^2 t) + \frac{\partial f_1^{(0)}}{\partial \epsilon^2 t}(\epsilon t, \epsilon^2 t) = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) f_2^{(1)}(\infty, \epsilon t, \epsilon^2 t) \tag{7.8}$$

and

$$\frac{\partial f_1^{(2)}}{\partial t} + \frac{\partial f_1^{(1)}}{\partial \epsilon t}(t, \epsilon t, \epsilon^2 t) - \frac{\partial f_1^{(1)}}{\partial \epsilon t}(\infty, \epsilon t, \epsilon^2 t) = \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12)[f_2^{(1)}(t, \epsilon t, \epsilon^2 t) - f_2^{(1)}(\infty, \epsilon t, \epsilon^2 t)]. \tag{7.9}$$

We, of course, expect that (7.8) provides corrections to the Boltzmann equation and that (7.9) describes the quick approach to the collisional time scale.

From (3.1), we get

$$\begin{aligned} f_2^{(1)}(t) = {} & \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t - t')] \int d\mathbf{x}_3\, d\mathbf{v}_3 \\ & \times [\Theta(13) + \Theta(23)] \exp[-H^{(0)}(123)(t' - t_0)] f_3^{(0)} \\ & - \exp[-H^{(0)}(12)(t - t_0)] \int_{t_0}^{t} dt' \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13) \\ & \times \exp[-H^{(0)}(13) t_\infty] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ & - \exp[-H^{(0)}(12)(t - t_0)] \int_{t_0}^{t} dt' \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(23) \\ & \times \exp[-H^{(0)}(23) t_\infty] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ & + \exp[-H^{(0)}(12)(t - t_0)] f_2^{(1)}(t_0) - \int_{t_0}^{t} dt' \\ & \times \exp[-H^{(0)}(12)(t - t')] \mathbf{v}_{12} \cdot \frac{\partial}{\partial \epsilon \mathbf{x}} f_2^{(0)}(t'). \end{aligned} \tag{7.10}$$

In writing (7.10) we have used (7.1) and the fact that the $S_{-\infty}$ operator projects $g_2^{(0)}$ into the region in which it vanishes.

For substitution into (7.8), we need $f_2^{(1)}$ for $|\mathbf{x}_{12}| \leq 1$ and for t large. We note that $f_2^{(1)}$ itself cannot possibly be secular in this range of phase space since $\mathbf{x}_{12}$ cannot possibly be parallel to $\mathbf{v}_{12}$. However, contributions to $f_2^{(1)}$ can arise from correlation functions whose arguments are such that $\mathbf{x}_{12}$ was parallel to $\mathbf{v}_{12}$ at some time. In principle, we then should use the correlations corrected for the exponential behavior that we found earlier. This is one of the essential differences between the present treatment and earlier treatments of this problem.

The last term on the right-hand side of (7.10) then vanishes, since the $\epsilon\mathbf{x}$ derivative of $g_2^{(0)}$ is only

nonzero if $\mathbf{x}_{12}$ is parallel to $\mathbf{v}_{12}$. We can now rewrite (7.10) in the form

$$
\begin{aligned}
f_2^{(1)} &= \int d\mathbf{x}_3\, d\mathbf{v}_3 \{\exp[-H^{(0)}(123)(t-t_0)] \\
&\quad - \exp[-H^{(0)}(12)(t-t_0)]\} f_1^{(0)} f_1^{(0)} f_1^{(0)} \\
&\quad + \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t')] \int d\mathbf{x}_3\, d\mathbf{v}_3\, \mathbf{v}_3 \cdot \frac{\partial}{\partial \mathbf{x}_3} \\
&\quad \times \exp[-H^{(0)}(123)(t'-t_0)] f_1^{(0)} f_1^{(0)} f_1^{(0)} \\
&\quad + \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t')] \int d\mathbf{x}_3\, d\mathbf{v}_3 \\
&\quad \times [\Theta(13) + \Theta(23)] \exp[-H^{(0)}(123)(t'-t_0)] \\
&\quad \times [f_1^{(0)}(3) g_2^{(0)}(12) + f_1^{(0)}(2) g_2^{(0)}(13) \\
&\quad + f_1^{(0)}(1) g_2^{(0)}(23) + g_3^{(0)}(123)] \\
&\quad - \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t_0)] \Big[\int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13) \\
&\quad \times (\{\exp[-H^{(0)}(13)(t_\infty - t_0)] \\
&\quad - \exp[-H^{(0)}(13)(t'-t_0)]\} \\
&\quad + \exp[-H^{(0)}(13)(t'-t_0)) f_1^{(0)} f_1^{(0)} f_1^{(0)} \\
&\quad + \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(23) (\{\exp[-H^{(0)}(23)(t_\infty - t_0)] \\
&\quad - \exp[-H^{(0)}(23)(t'-t_0)]\} \\
&\quad + \exp[-H^{(0)}(23)(t'-t_0)]) f_1^{(0)} f_1^{(0)} f_1^{(0)} \Big] \\
&\quad + \exp[-H^{(0)}(12)(t-t_0)] f_2^{(1)}(t_0). \qquad (7.11)
\end{aligned}
$$

The second term on the right-hand side of (7.11) vanishes under the assumption that t is less than $|\mathbf{x}_3|/|\mathbf{v}_3|$, since the upper and lower limits of the $\mathbf{x}_{3\parallel}$ integration are then identical.

We next consider the term

$$
\begin{aligned}
&-\int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t_0)] \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13) \\
&\qquad \times \exp[-H^{(0)}(13)(t'-t_0)] f_1^{(0)} f_1^{(0)} f_1^{(0)}, \qquad (7.12)
\end{aligned}
$$

which can be written

$$
\begin{aligned}
&\int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t_0)] \int d\mathbf{x}_3\, d\mathbf{v}_3\, H^{(0)}(13) \\
&\qquad \times \exp[-H^{(0)}(13)(t'-t_0)] f_1^{(0)} f_1^{(0)} f_1^{(0)}. \qquad (7.13)
\end{aligned}
$$

The term in the $\mathbf{x}_{13\parallel}$ integration which would add to (7.13) in obtaining it from (7.12) vanishes for the same reason as given above after (7.11). We can now integrate (7.13) and get

$$
\begin{aligned}
&\int d\mathbf{x}_3\, d\mathbf{v}_3 \{\exp[-H^{(0)}(12)(t-t_0)] \\
&\qquad - \exp[-H^{(0)}(12)(t-t_0)] \\
&\qquad \times \exp[-H^{(0)}(13)(t-t_0)]\} f_1^{(0)} f_1^{(0)} f_1^{(0)}. \qquad (7.14)
\end{aligned}
$$

Clearly, the terms involving particles [2] and [3] can be handled in the same way. Thus, (7.11) becomes

$$
\begin{aligned}
f_2^{(1)} &= \int d\mathbf{x}_3\, d\mathbf{v}_3 \{\exp[-H^{(0)}(123)(t-t_0)] \\
&\quad + \exp[-H^{(0)}(12)(t-t_0)] - \exp[-H^{(0)}(12)(t-t_0)] \\
&\quad \times \exp[-H^{(0)}(13)(t-t_0)] - \exp[-H^{(0)}(12)(t-t_0)] \\
&\quad \times \exp[-H^{(0)}(23)(t-t_0)]\} f_1^{(0)} f_1^{(0)} f_1^{(0)} \\
&\quad - \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t_0)] \int d\mathbf{x}_3\, d\mathbf{v}_3 \\
&\quad \times (\Theta(13) \{\exp[-H^{(0)}(13)(t_\infty - t_0)] \\
&\quad - \exp[-H^{(0)}(13)(t'-t_0)]\} \\
&\quad + \Theta(23) \{\exp[-H^{(0)}(23)(t_\infty - t_0)] \\
&\quad - \exp[-H^{(0)}(23)(t'-t_0)]\}) f_1^{(0)} f_1^{(0)} f_1^{(0)} \\
&\quad + \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t')] \int d\mathbf{x}_3\, d\mathbf{v}_3 \\
&\quad \times [\Theta(13) + \Theta(23)] \exp[-H^{(0)}(123)(t'-t_0)] \\
&\quad \times [f_1^{(0)}(3) g_2^{(0)}(12) + f_1^{(0)}(2) g_2^{(0)}(13) \\
&\quad + f_1^{(0)}(1) g_2^{(0)}(23) + g_3^{(0)}(123)] \\
&\quad + \exp[-H^{(0)}(12)(t-t_0)] [f_1^{(0)}(1) f_1^{(1)}(t_0, \epsilon t, 2) \\
&\quad + f_1^{(0)}(2) f_1^{(1)}(t_0, \epsilon t, 1) + g_2^{(1)}(t_0)]. \qquad (7.15)
\end{aligned}
$$

Now consider the contribution to (7.15) arising from

$$
\begin{aligned}
&\int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t-t')] \\
&\quad \times \int d\mathbf{x}_3\, d\mathbf{v}_3\, [\Theta(13) + \Theta(23)] \\
&\quad \times \exp[-H^{(0)}(123)(t'-t_0)] f_1^{(0)}(3) g_2^{(0)}(12). \qquad (7.16)
\end{aligned}
$$

A typical set of trajectories contributing to (7.16) is shown in Fig. 6. The same figure with [1] and [2] interchanged is also appropriate. Note that there is a [12] interaction prior to t_0 and there is thus a nonzero value for $g_2^{(0)}(12)$. Further, there is a [13] or [23] interaction as required by the presence of $\Theta(13) + \Theta(23)$. Finally $|\mathbf{x}_{12}| \leq 1$ at time t. We note that the distance $\overline{BC}$ is of order $\mathbf{v}_1(t - t_0) \sim \overline{AC}$. Thus, assuming the integrand of the phase-space integration to be of order unity, the integral itself

is of order $1/|\mathbf{v}_1|^2(t - t_0)^2$ because of the solid angle. The further t' integration then yields the behavior $(t - t_0)^{-1}$. It is clear that if a greater number of binary interactions had occurred in the interval $t - t_0$ which still satisfied the above restrictions, a result would have been obtained which vanished more rapidly than $(t - t_0)^{-1}$.

The terms

$$\int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t - t')] \int d\mathbf{x}_3\, d\mathbf{v}_3 \times \{\Theta(13) \exp[-H^{(0)}(123)(t' - t_0)] f_1^{(0)}(1) g_2^{(0)}(23) + \Theta(23) \exp[-H^{(0)}(123)(t' - t_0)] f_1^{(0)}(2) g_2^{(0)}(13)\} \tag{7.17}$$

also yield a behavior of $(t - t_0)^{-1}$ from arguments similar to those given above. Figure 7 illustrates the trajectories appropriate for carrying out the details. Of course, [1] and [2] can be interchanged.

We can dispose of the terms arising from $g_3^{(0)}(123)$ immediately by noting that, at least two binary interactions must have occurred prior to t_0 for these terms to be finite. From solid angle consideration these terms vanish faster than $(t - t_0)^{-1}$.

We finally consider the terms

$$\int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t - t')] \int d\mathbf{x}_3\, d\mathbf{v}_3 \times \{\Theta(13) \exp[-H^{(0)}(123)(t' - t_0)] f_1^{(0)}(2) g_2^{(0)}(13) + \Theta(23) \exp[-H^{(0)}(123)(t' - t_0)] f_1^{(0)}(1) g_2^{(0)}(23)\} \tag{7.18}$$

and rewrite the first term in (7.18) as

$$\begin{aligned} &\int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t - t_0)] \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13) \\ &\times \exp[-H^{(0)}(13)(t' - t_0)] g_2^{(0)}(13) f_1^{(0)}(2) \\ &+ \int_{t_0}^{t} dt' \{\exp[-H^{(0)}(12)(t - t')] \\ &- \exp[-H^{(0)}(12)(t - t_0)]\} \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13) \\ &\times \exp[-H^{(0)}(13)(t' - t_0)] g_2^{(0)}(13) f_1^{(0)}(2) \\ &+ \int_{t_0}^{t} dt' \exp[-H^{(0)}(12)(t - t')] \int d\mathbf{x}_3\, d\mathbf{v}_3 \\ &\times \Theta(13) \{\exp[-H^{(0)}(123)(t' - t_0)] \\ &- \exp[-H^{(0)}(13)(t' - t_0)]\} g_2^{(0)}(13) f_1^{(0)}(2). \end{aligned} \tag{7.19}$$

The expression

$$G = \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13) \times \exp[-H^{(0)}(13)(t' - t_0)] g_2^{(0)}(13) f_1^{(0)}(2) \tag{7.20}$$

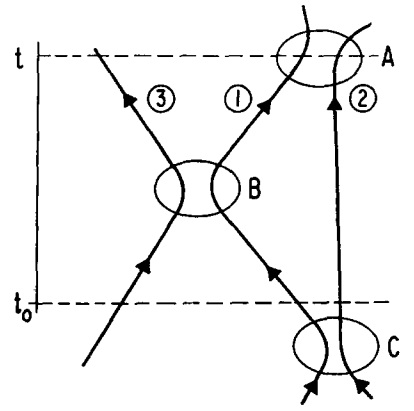

FIG. 6. Trajectories for Eq. (7.16).

clearly depends on $\mathbf{v}_1$ and $\mathbf{v}_2$ but not on $\mathbf{x}_{12}$. Then,

$$\{\exp[-H^{(0)}(12)(t - t')] - \exp[-H^{(0)}(12)(t - t_0)]\} G(\mathbf{v}_1, \mathbf{v}_2) = 0 \tag{7.21}$$

for $|\mathbf{x}_{12}| < 1$, if both operators project G into the phase-space region before a [12] interaction occurs. Thus, (7.21) is true if both

$$t - t' > 1/|\mathbf{v}_{12}|, \qquad t - t_0 > 1/|\mathbf{v}_{12}|. \tag{7.22}$$

We thus conclude that the second line of (7.19) vanishes faster than $(t - t_0)^{-3}$. This follows from the argument that (7.22) forces us to consider $t \approx t'$ in order to get a nonzero contribution. Then, substituting t for t' in the $\exp[-H^{(0)}(13)(t' - t_0)]$ operator yields

$$|\mathbf{v}_{13}| < (t - t_0)^{-1} \tag{7.23}$$

in order that $g_2^{(0)}(13)$ is not projected into the region in which it vanishes. We thus find at least a $(t - t_0)^{-3}$ decay from the velocity integration alone.

A typical nonvanishing trajectory contributing

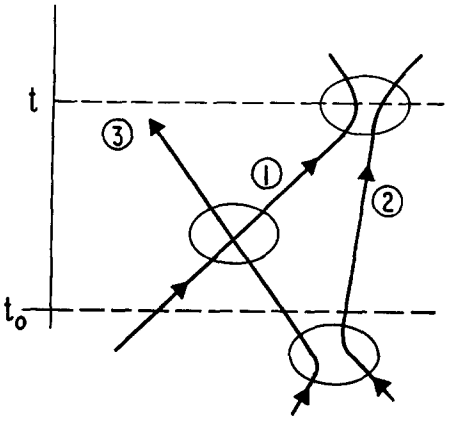

FIG. 7. Trajectories for Eq. (7.17).

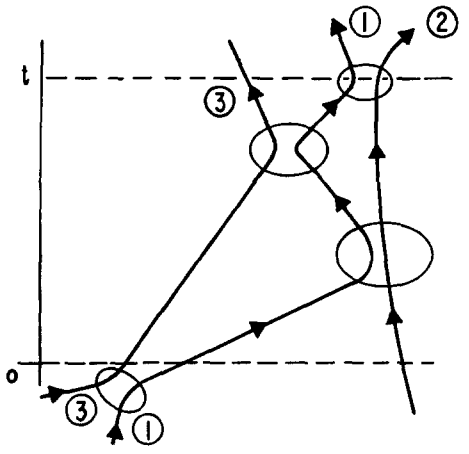

FIG. 8. Trajectories for the third line in Eq. (7.19).

to the third line of (7.19) is shown in Fig. 8. We see that there must be a [13] interaction prior to t_0 to keep $g_2^{(0)}(13)$ nonzero and there must be a [13] interaction in the interval $t - t_0$ because of $\Theta(13)$. We also require a [12] interaction at time t and a [12] or [32] interaction so that the H operators do not cancel. By comparison with the previous cases, we see that this contribution certainly decay at least as $(t - t_0)^{-1}$ and most probably faster.

In view of the above, we may write (7.15) as

$$\begin{aligned} f_2^{(1)}(t) = \int d\mathbf{x}_3\, d\mathbf{v}_3 \{ & \exp[-H^{(0)}(123)(t-t_0)] \\ & - \exp[-H^{(0)}(12)(t-t_0)] \exp[-H^{(0)}(13)(t-t_0)] \\ & - \exp[-H^{(0)}(12)(t-t_0)] \exp[-H^{(0)}(23)(t-t_0)] \\ & + \exp[-H^{(0)}(12)(t-t_0)]\} f_1^{(0)} f_1^{(0)} f_1^{(0)} \\ & + \exp[-H^{(0)}(12)(t-t_0)][f_1^{(0)}(2) f_1^{(1)}(t_0, \epsilon t, 1) \\ & + f_1^{(0)}(1) f_1^{(1)}(t_0, \epsilon t, 2) + g_2^{(1)}(t_0, \epsilon t)] \\ & + \exp[-H^{(0)}(12)(t-t_0)] \int_{t_0}^{t} dt' \int d\mathbf{x}_3\, d\mathbf{v}_3 \\ & \times (\Theta(13)\{\exp[-H^{(0)}(13)(t'-t_0)] \\ & - \exp[-H^{(0)}(13)(t_\infty - t_0)]\}[f_1^{(0)}(1) f_1^{(0)}(3) \\ & + g_2^{(0)}(13, t_0)] f_1^{(0)}(2) + \Theta(23)\{\exp[-H^{(0)}(23)(t'-t_0)] \\ & - \exp[-H^{(0)}(23)(t_\infty - t_0)]\}[f_1^{(0)}(2) f_1^{(0)}(3) \\ & + g_2^{(0)}(23, t_0)] f_1^{(0)}(1)) + A(t-t_0) + B(t-t_0). \end{aligned} \tag{7.24}$$

Here $A(t - t_0)$ includes all the terms which behave as $(t - t_0)^{-1}$, while B includes those which decay faster than $(t - t_0)^{-1}$.

We then finally get

$$\begin{aligned} & \lim_{t-t_0\to\infty} \frac{\partial f_1^{(1)}}{\partial \epsilon t} + \frac{\partial f_1^{(0)}}{\partial \epsilon^2 t} \\ & = \lim_{t-t_0\to\infty} \int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12) \exp[-H^{(0)}(12)(t-t_0)] \\ & \times [f_1^{(0)}(1) f_1^{(1)}(2) + f_1^{(0)}(2) f_1^{(1)}(1)] \\ & + \int d\mathbf{x}_2\, d\mathbf{v}_2\, d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(12)\{\exp[-H^{(0)}(123)(t-t_0)] \\ & - \exp[-H^{(0)}(12)(t-t_0)] \exp[-H^{(0)}(13)(t-t_0)] \\ & - \exp[-H^{(0)}(12)(t-t_0)] \exp[-H^{(0)}(23)(t-t_0)] \\ & + \exp[-H^{(0)}(12)(t-t_0)]\} f_1^{(0)}(1) f_1^{(0)}(2) f_1^{(0)}(3), \end{aligned} \tag{7.25}$$

which is the standard Choh–Uhlenbeck result.

However, we note that in obtaining (7.25) we have dropped the term

$$\lim_{t-t_0\to\infty} \exp[-H^{(0)}(12)(t-t_0)] g_2^{(1)}(t_0) \tag{7.26}$$

by assuming it to vanish. In fact, we get no information on $g_2^{(1)}(0)$ in this order and, in principle, must determine it by going to next order. We also observe that the term $A(t - t_0)$ produces an error of order ϵ only if we require $t - t_0 \sim 1/\epsilon$. This also entails computing to higher order to examine the ϵt dependence of the various functions involved. These higher-order calculations are not done here but have been carried out in a paper to appear subsequently. The results verify that (7.25) is correct.

We next turn to the time evolution of the system predicted by (7.25). To do this we need some information which follows from the Boltzmann equation (7.1). We know that as $\epsilon t \to \infty$, we have

$$\begin{aligned} f_1^{(0)} \to n^{(0)} & \left(\frac{m}{2\pi\kappa T^{(0)}}\right)^{\frac{3}{2}} \\ & \times \exp\left[-\frac{m}{2\kappa T^{(0)}} (\mathbf{v} - \mathbf{V}^{(0)})^2\right], \end{aligned} \tag{7.27}$$

where

$$\begin{aligned} n^{(0)} &= \int d\mathbf{v}\, f_1^{(0)}, \\ n^{(0)}\mathbf{V}^{(0)} &= \int d\mathbf{v}\, \mathbf{v} f_1^{(0)}, \\ \frac{3}{2}\frac{n^{(0)}\kappa T^{(0)}}{m} &= \frac{1}{2}\int d\mathbf{v}\, (v - V^{(0)})^2 f_1^{(0)}. \end{aligned} \tag{7.28}$$

Further, it follows from (7.1) that for all ϵt

$$\frac{\partial n^{(0)}}{\partial \epsilon t} = \frac{\partial \mathbf{V}^{(0)}}{\partial \epsilon t} = \frac{\partial T^{(0)}}{\partial \epsilon t} = 0. \tag{7.29}$$

From (7.25), we have

$$\frac{\partial n^{(1)}}{\partial \epsilon t} + \frac{\partial n^{(0)}}{\partial \epsilon^2 t} = 0,$$

$$\frac{\partial}{\partial \epsilon t}(n^{(0)}\mathbf{V}^{(1)} + n^{(1)}\mathbf{V}^{(0)}) + \frac{\partial}{\partial \epsilon^2 t}\mathbf{n}^{(0)}V^{(0)} = 0,$$

$$\frac{\partial}{\partial \epsilon t}(\tfrac{3}{2}n^{(0)}\kappa T^{(1)} + \tfrac{3}{2}n^{(1)}\kappa T^{(0)}) + \frac{\partial}{\partial \epsilon^2 t}(\tfrac{3}{2}n^{(0)}\kappa T^{(0)})$$

$$= -\int d\mathbf{v}_1\, d\mathbf{v}_2\, d\mathbf{v}_3\, d\mathbf{x}_2\, d\mathbf{x}_3\, \mathbf{v}_1 \cdot \frac{\partial \phi}{\partial \mathbf{x}_{12}}$$

$$\times [S_{-\infty}(123) - S_{-\infty}(12)S_{-\infty}(13)$$

$$- S_{-\infty}(12)S_{-\infty}(23) + S_{-\infty}(12)]f_1^{(0)}f_1^{(0)}f_1^{(0)} \equiv Q. \quad (7.30)$$

By secularity removal, (7.30) yields

$$\frac{\partial n^{(1)}}{\partial \epsilon t} = \frac{\partial \mathbf{V}^{(1)}}{\partial \epsilon t} = \frac{\partial n^{(0)}}{\partial \epsilon^2 t} = \frac{\partial \mathbf{V}^{(0)}}{\partial \epsilon^2 t} = \frac{\partial T^{(0)}}{\partial \epsilon^2 t} \quad (7.31)$$

and

$$\tfrac{3}{2}n^{(0)}\kappa \frac{\partial T^{(1)}}{\partial \epsilon t} = Q. \quad (7.32)$$

We can now return to (7.25) and consider integrating it with respect to ϵt to search for secular behavior. In the limit as $\epsilon t \to \infty$ we know that

$$\partial f_1^{(0)}/\partial \epsilon^2 t \to 0, \quad (7.33)$$

since $f_1^{(0)}$ takes on the form (7.27) and (7.31) holds. We also know that the Choh–Uhlenbeck triple collision term vanishes if $f_1^{(0)}$ is Maxwellian. Thus, the only secularity producing term in (7.25) is

$$\int d\mathbf{x}_2\, d\mathbf{v}_2\, \Theta(12)S_{-\infty}(12)[f_1^{(0)}(\infty, 1)f_1^{(1)}(\infty, \infty, 2)$$

$$+ f_1^{(0)}(\infty, 2)f_1^{(1)}(\infty, \infty, 1)], \quad (7.34)$$

which must therefore be set equal to zero. This leads to

$$f_1^{(1)}(\infty, \infty) = f_1^{(0)}(\infty)(\alpha + \boldsymbol{\beta}\cdot\mathbf{v} + \gamma v^2) \quad (7.35)$$

which we recognize is simply a perturbed Maxwellian, with α, $\boldsymbol{\beta}$, and γ determined by normalization. We therefore conclude that, if (7.25) has a well-behaved (secularity-free) solution, the system does tend to thermal equilibrium, although we have not found a formal H theorem. It is of interest to note from (7.33) that the system apparently prefers not to evolve on the $\epsilon^2 t$ scale, and that we can, at least to this order, assume that an asymptotic representation is achieved without an $\epsilon^2 t$ dependence.

VIII. CONCLUSIONS

We have seen that it is possible to remove secular behavior to the order we have gone and obtain significant information on the long-time, long-space behavior of the various functions in so doing. We have also seen that the singular behavior for $|\mathbf{v}_{12}| \ll 1$ does not influence our results to the order we have gone.

At first glance one might think that some of the above conclusions contradict well-known results of thermal equilibrium theory. In fact, upon closer examination one finds that all functions reduce, as they should, to their thermal equilibrium counterparts. It is clear that the long-time, long-space behavior is exhibited in thermal equilibrium in examining the fluctuation spectrum.

Finally, we wish to comment on the various terms which appear with the decay $1/t$. This type of behavior has been found by Green and Piccarelli.[15] Such terms clearly give rise to logarithmic behavior in the next order and thus one should expect $\ln\epsilon$ terms in the expansion. These terms have, in face, been found[16] and form the basis for a subsequent paper.

ACKNOWLEDGMENTS

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APPENDIX

We now show that the result of considering the integration limits to be independent of $\mathbf{x}_{13}(\mathbf{x}_{23})$ for I_2 and I_3 in Sec. III is correct. From (3.17) we have

$$\int_0^t dt'\, S_{-(t-t')}(12) \int d\mathbf{x}_3\, d\mathbf{v}_3\, \Theta(13)$$

$$\times S_{-t'}(123, 23)f_1^{(0)}f_1^{(0)}f_1^{(0)}. \quad (A1)$$

In relative coordinates, we have

$$\Theta(13) = H^{(0)}(12) - H^{(0)}(123, 23)$$

$$+ \mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} - \mathbf{v}_1\cdot\frac{\partial}{\partial \mathbf{x}_{13}}. \quad (A2)$$

[15] M. S. Green and R. A. Piccarelli, Phys. Rev. **132**, 1388 (1963).

[16] R. Goldman and E. A. Frieman, Bull. Am. Phys. Soc. **10**, 531 (1965).

Thus (A1) becomes

$$\int_0^t dt'\, S_{-(t-t')}(12) \int d\mathbf{x}_3\, d\mathbf{v}_3 \times \left[H^{(0)}(12) - H^{(0)}(123, 23) + \mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} - \mathbf{v}_1\cdot\frac{\partial}{\partial \mathbf{x}_{13}}\right] S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)}. \tag{A3}$$

We next note that

$$S_{-(t-t')}(12)\ |\mathbf{x}_{13}| = \left|\mathbf{x}_{13} - \int_{t'}^{t} \mathbf{v}_1(t'')\, dt''\right|, \tag{A4}$$

where $\mathbf{v}_1$ is obtained from the solution of the two-body problem.

We then can write (A3) as

$$\int_0^t dt' \int_{|\mathbf{x}_{13} - \int_{t'}^{t} \mathbf{v}_1(t'')dt''| = 0}^{|\mathbf{x}_{13} - \int_{t'}^{t} \mathbf{v}_1(t'')dt''| = 1} d\mathbf{x}_3\, d\mathbf{v}_3\, S_{-(t-t')}(12) \times [H^{(0)}(12) - H^{(0)}(123, 23)] S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)} + \int_0^t dt' \int_\alpha^\beta d\mathbf{x}_3\, d\mathbf{v}_3\, S_{-(t-t')}(12) \times \left(\mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} - \mathbf{v}_1\cdot\frac{\partial}{\partial \mathbf{x}_{13}}\right) S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)}, \tag{A5}$$

where α and β are the same as the limits of the first integral in (A5). The first integral in (A5) can be written

$$\int_0^t dt' \int_\alpha^\beta d\mathbf{x}_3\, d\mathbf{v}_3 \frac{\partial}{\partial t'} S_{-(t-t')}(12) \times S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)}. \tag{A6}$$

We further rewrite (A6) as

$$\int_0^t dt' \frac{\partial}{\partial t'} \int_\alpha^\beta d\mathbf{x}_3\, d\mathbf{v}_3 \times S_{-(t-t')}(12) S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)} - \int_0^t dt' \frac{\partial}{\partial t'''} \left[\int_{|\mathbf{x}_{13} - \int_{t'''}^{t} \mathbf{v}_1(t'')dt''| = 0}^{|\mathbf{x}_{13} - \int_{t'''}^{t} \mathbf{v}_1(t'')dt''| = 1} d\mathbf{x}_3\, d\mathbf{v}_3 \times S_{-(t-t')}(12) S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)}\right]_{t'''=t'}. \tag{A7}$$

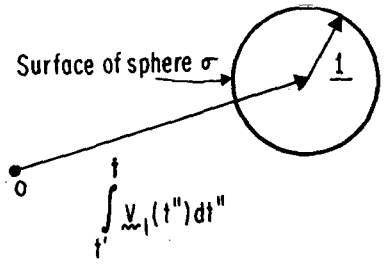

FIG. 9. Sphere of integration for Eq. (A8).

Our object now is to show that the last term in (A5) cancels the second term in (A7) leaving a finite term plus the secularity producing term that we have already obtained in I_2. Thus, upon using Gauss' theorem, the last term in (A5) becomes

$$\int_0^t dt' \int_\sigma S_{-(t-t')}(12) S_{-t'}(123, 23) \times \mathbf{v}_1(t')\cdot d\boldsymbol{\sigma}\, d\mathbf{v}_3\, f_1^{(0)} f_1^{(0)} f_1^{(0)}, \tag{A8}$$

where σ is the surface of the sphere shown in Fig. 9. To treat the second integral in (A7) it is convenient to write the limits in explicit rather than implicit form. Thus we get

$$\mathbf{x}_{13} = \int_{t'''}^{t} \mathbf{v}_1(t'')\, dt'' \tag{A9}$$

for the lower limit and

$$\mathbf{x}_{13} = \mathbf{1}(\sigma) + \int_{t'''}^{t} \mathbf{v}_1(t'')\, dt'' \tag{A10}$$

for the upper limit. We therefore write

$$-\int_0^t dt' \frac{\partial}{\partial t'''} \left[\int_{\mathbf{x}_{13} = \mathbf{1}(\sigma) - \int_{t'''}^{t} \mathbf{v}_1(t'')dt''}^{\mathbf{x}_{13} = -\int_{t'''}^{t} \mathbf{v}_1(t'')dt''} d\mathbf{x}_3\, d\mathbf{v}_3 \times S_{-(t-t')}(12) S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)}\right] = +\int_0^t dt' \int_\sigma S_{-(t-t')}(12) S_{-t'}(123, 23) \times \mathbf{v}_1(t')\cdot d\boldsymbol{\sigma}\, d\mathbf{v}_3\, f_1^{(0)} f_1^{(0)} f_1^{(0)}. \tag{A11}$$

The last result follows from simply carrying out the time derivatives using

$$\frac{\partial}{\partial t'''} = \sum_{i=1}^{3} \frac{\partial}{\partial x_{13_i}} \frac{\partial x_{13_i}}{\partial t'''}. \tag{A12}$$

Thus, (A1) becomes

$$\int_0^t dt' \frac{\partial}{\partial t'} \int_\alpha^\beta d\mathbf{x}_3\, d\mathbf{v}_3 \times S_{-(t-t')}(12) S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)} + \int_0^t dt' \int_\alpha^\beta d\mathbf{x}_3\, d\mathbf{v}_3\, S_{-(t-t')}(12) \times \mathbf{v}_{13}\cdot\frac{\partial}{\partial \mathbf{x}_{13}} S_{-t'}(123, 23) f_1^{(0)} f_1^{(0)} f_1^{(0)}, \tag{A13}$$

which essentially agrees with (3.22) since the $H_r(13)t_\infty$ terms can be treated in a similar fashion to those above and the differences between the H and H_r operators vanish. It is clear that arguments similar to those used above can also be used on (3.30) in examining I_3.

Peratization of the Logarithmically Singular Potential

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The potential of the form $(gr^{-4}\ln^2 r - g^{\frac{1}{2}}r^{-3})\vartheta(r - r_0)$ is shown explicitly to be regularizable by an infinitesimal cutoff. It is also shown that, when a modified sense of the peratization technique is applied to the regulated scattering length, the correct answer is regained.

1. INTRODUCTION

THE technique of peratization is designed to give meaning to a series in which each term is a divergent function of some parameter. It has been applied to the calculation of the scattering length of various repulsive singular potentials.

For a repulsive singular potential $gV(r)$, the scattering length as a function of the coupling constant g has an essential singularity at the origin,[1] and is well defined nearby, since the potential is repulsive. Hence, an attempt to expand the scattering length in a Born series is frustrated by infinite integrals. To overcome this, one introduces a one-parameter family of regular potentials, $V(r, \alpha)$, such that $V(r, 0) = V(r)$. A series for the scattering length in the coupling constant then exists for each value of α; however, as is to be expected, each term diverges as $\alpha \to 0$. If the series can be summed, and the limit $\alpha \to 0$ then be taken, the process of *regularization* is said to have been applied. If the coefficient of a given power of the coupling constant consists of more than one term in α, the prescription of *peratization* can be applied by discarding all but the most singular term, then summing the resulting series, and finally letting $\alpha \to 0$.

Potentials with singularities of pole,[2,3] exponential,[4,5] and logarithmic[6-8] type have been investigated. Regularization succeeds with poles, but there is no possibility of peratization since only one term in α exists in each order of the coupling constant. Calogero[9], pointing out the difficulties in any general argument for regularization, has shown that one can choose $V(r, \alpha)$ complicated enough so that the limit $\alpha \to 0$ does not give the right answer. For straightforward ways of choosing $V(r, \alpha)$, it has been possible to show in each case that the limit does give the right answer. Pais and Wu[10] have shown that the result as *used* by Khuri and Pais[3] and others[4,7] is valid in general for singular potentials, resting on a cutoff intrinsic to the general scattering formalism. (A discussion of regularization is found in the Appendix.) An exponentially singular potential has been solved directly,[4,5] by the intrinsic cutoff method,[4] and by regularization and peratization[5] in a successful manner.

The scattering lengths due to a pair of regularized logarithmic potentials have been expanded in the Born series, and are found to yield nonfinite answers upon peratization,[6] unless all order singularities are sequentially summed.[8] The regularization used in both cases was $V(r, \alpha) = \vartheta(\alpha - r)V(r)$, where $\vartheta = 1$ if $x < 0$, $\vartheta = 0$ if $x > 0$. Since the scattering length (the existence of which is certain) could not be written down explicitly for comparison, the result cannot be clearly interpreted: either the peratization or the regularization (upon which the peratization was built) might have failed. The slightly modified potential $(gr^{-4}\ln^2 r - g^{\frac{1}{2}}r^{-3})\vartheta(r - r_0)$ still has a leading logarithmic singularity in r, but has been solved directly and by the intrinsic cutoff method.[7] We introduce for this potential the same regularization $V(r, \alpha) = \vartheta(\alpha - r)V(r)$, and show explicitly that the regularization is successful. We then apply a peratization argument and show that, as in a previous case,[5] the retention of two leading singularities is necessary to regain the correct answer.

2. SOLUTION

The equation

$$\frac{d^2\psi}{dr^2} = (gr^{-4}\ln^2 r - g^{\frac{1}{2}}r^{-3})\psi \qquad (1)$$

* National Science Foundation Trainee in Physics.
[1] R. J. Jabbur, Phys. Rev. **138**, B1525 (1965).
[2] G. Tiktopoulos and S. B. Treiman, Phys. Rev. **134**, B844 (1964).
[3] N. N. Khuri and A. Pais, Rev. Mod. Phys. **36**, 590 (1964).
[4] H. H. Aly, Riazuddin, and A. H. Zimerman, Nuovo Cimento **35**, 324 (1965).
[5] F. Calogero and M. Cassandro, Nuovo Cimento **37**, 760 (1965).
[6] H. H. Aly, Riazuddin, and A. H. Zimerman, Phys. Rev. **136**, B1174 (1964).
[7] H. H. Aly, Riazuddin, and A. H. Zimerman, J. Math. Phys. **6**, 1115 (1965).
[8] T. T. Wu, Phys. Rev. **136**, B1176 (1964).
[9] F. Calogero, Phys. Rev. **139**, B602 (1965).
[10] A. Pais and T. T. Wu, Phys. Rev. **134**, B1303 (1964).

has the two general solutions $y_1(r) = r \exp [F(r)]$, and $y_2(r) = y_1(r)L(r)$, where

$$F(r) = g^{\frac{1}{2}}r^{-1}(\ln r + 1) \tag{2}$$

and

$$L(r) = \int_{\xi}^{r} x^{-2} \exp (-2F(x))\, dx. \tag{3}$$

The ξ is arbitrary and, in the following, we choose $\xi = r_0$. As usual, we limit our consideration to zero-energy s-wave scattering, so that, for the range $0 \leq r \leq r_0$, Eq. (1) is the Schrödinger equation with the regular solution $\psi(r) = y_1(r)$. For the range $r > r_0$, the Schrödinger equation is $D^2\psi = 0$, with the solution $\psi(r) = br + ba$. By equating the logarithmic derivatives at $r = r_0$, we find a, the scattering length, to be

$$a = g^{\frac{1}{2}} \ln r_0(1 - g^{\frac{1}{2}}r_0^{-1} \ln r_0)^{-1}. \tag{4}$$

3. REGULARIZATION

We introduce the one-parameter family of potentials

$$V(r, \alpha) = \vartheta(\alpha - r)(gr^{-4} \ln^2 r - g^{\frac{1}{2}}r^{-3})\vartheta(r - r_0),$$

so that the Schrödinger equation is

$$\frac{d^2\psi(r, \alpha)}{dr^2} = \begin{cases} 0, & 0 \leq r \leq \alpha, \\ (gr^{-4} \ln^2 r - g^{\frac{1}{2}}r^{-3})\psi(r, \alpha), & \alpha < r \leq r_0, \\ 0, & r_0 < r < \infty, \end{cases} \tag{5}$$

with the solution

$$\psi(r, \alpha) = \begin{cases} cr + d, & 0 \leq r \leq \alpha, \\ A(\alpha)y_1(r) + B(\alpha)y_2(r), & \alpha \leq r \leq r_0, \\ b(\alpha)r + b(\alpha)a(\alpha), & r_0 \leq r < \infty. \end{cases} \tag{6}$$

In order for $\psi(0, \alpha)$ to be zero, we set $d = 0$ and $c = 1$. By joining the solutions at α and at r_0, we find

$$\begin{aligned} B(\alpha) &= -\alpha^2F'(\alpha) \exp [F(\alpha)], \\ A(\alpha) &= \exp [-F(\alpha)] + \alpha^2F'(\alpha) \exp [F(\alpha)]L(\alpha), \end{aligned} \tag{7}$$

and

$$\begin{aligned} a(\alpha) &= \frac{-A(\alpha) \exp [F(r_0)]r_0^2F'(r_0) + B(\alpha) \exp [-F(r_0)]}{A(\alpha) \exp [F(r_0)][1 + r_0F'(r_0)] + B(\alpha) \exp [-F(r_0)]} \\ &= \frac{-A'(\alpha)r_0^2F'(r_0) + B'(\alpha)}{A'(\alpha)[1 + r_0F'(r_0)] + B'(\alpha)}, \end{aligned} \tag{8}$$

where

$$A'(\alpha) = 1 + \alpha^2F'(\alpha) \exp [2F(\alpha)]L(\alpha)$$

and

$$B'(\alpha) = \alpha^2F'(\alpha) \exp [2F(\alpha) - 2F(r_0)].$$

Now $B'(\alpha) \to 0$ exponentially, and, by the theorem of the mean, we find that $\exp [2F(\alpha)]L(\alpha)$ does likewise as $\alpha \to 0$. Then

$$a(0) = \lim_{\alpha \to 0} a(\alpha) = \frac{-r_0^2F'(r_0)}{1 + r_0F'(r_0)} = \frac{g^{\frac{1}{2}} \ln r_0}{1 - g^{\frac{1}{2}}r_0^{-1} \ln r_0}. \tag{9}$$

Thus we see explicitly that regularization has succeeded.

4. PERATIZATION

Having divided through numerator and denominator by $\exp [-F(\alpha)]$, we have gotten a (α) in a closed form, where it has no singular terms remaining for a constant g. The application of peratization is purely pedagogical but possible, since we observe singular terms by expanding. We must expand both numerator and denominator in terms of g, then keep only the most singular (as a function of α) term in each order of g. This does not work, because the terms of interest to us are not singular in α, and they are combined additively in their order in g with singular terms. Exactly, in the denominator, we would discard $g^{\frac{1}{2}}r_0^{-1} \ln r_0$, so that we would obtain

$$a = g^{\frac{1}{2}} \ln r_0. \tag{10}$$

If we retain, as did Calogero and Cassandro,[5] two leading terms, we obtain

$$a(\alpha) = \frac{-A''(\alpha)g^{\frac{1}{2}} \ln r_0 + B''(\alpha)}{A''(\alpha)(1 + r_0^{-1}g^{\frac{1}{2}} \ln r_0) + B''(\alpha)} \tag{11}$$

with

$$A''(\alpha) = 1 + g^{\frac{1}{2}}\alpha^{-1} \ln \alpha \exp (2g^{\frac{1}{2}}\alpha^{-1} \ln \alpha)$$

and

$$B''(\alpha) = g^{\frac{1}{2}} \ln \alpha \exp (2g^{\frac{1}{2}}\alpha^{-1} \ln \alpha),$$

so that $A''(\alpha) \to 1$, $B''(\alpha) \to 0$, and $a(\alpha) \to a$, regaining the correct scattering length.

5. DISCUSSION

We have examined the scattering length of a particular potential with a leading logarithmic singularity, and found that the regularization procedure works. We have also shown why a peratization procedure retaining two leading singularities is needed. The main difference in this potential and the previously investigated logarithmic potentials

(where peratization failed) is that the former is already nonanalytic in g. The Born series for this solvable potential may be investigated to help resolve the conflict.

In conclusion, the first-order peratization (keep only the first leading singularity) has been shown to fail in some cases. A second-order peratization worked in solvable cases.

ACKNOWLEDGMENT

The author is particularly grateful to Professor I. Duck, who initiated this research, for his guidance and for many helpful discussions.

APPENDIX

The regularization argument of Khuri and Pais has given the scattering length $a = \lim_{\alpha\to 0} \lim_{\sigma\to 0} f(\alpha, \sigma)$ [where $f(\alpha, \sigma)$ represents the expression on the right-hand side of their formula 2.17]. Pais and Wu have shown that the scattering length of a singular potential is the limit of a ratio of Jost functions. By substituting the corresponding notations, this ratio reduces to $f(0, \sigma)$, with σ now identified as the intrinsic cutoff. Thus, in general,

$$a = \lim_{\sigma\to 0} \lim_{\alpha\to 0} f(\alpha, \sigma),$$

which computation method we refer to as the intrinsic cutoff method.

Thus, the problem of regularization can be stated as that of finding the necessary and the sufficient conditions for this interchange to be valid. Calogero has given an example for which it is invalid. This may be a fruitful place to look for necessary conditions, but for practical verification one appeals more readily to the original condition for regularization: $a(g, 0) = \lim_{\alpha\to 0} a(g, \alpha)$. Using the latter formulation, we can state stringent sufficient conditions. If $V(g, r, \alpha)$ is analytic in g in a neighborhood of the origin, and continuous in r, α (both positive), then the (zero-energy s-wave) wavefunction behaves likewise.[11] Since the scattering length $a(g, \alpha) = \lim_{\alpha\to\infty} (\psi(g, r, \alpha) - r)$ exists, it is continuous in α, for α positive. Finally, since $(ag, 0)$ exists on physical grounds, $a(g, 0) = \lim_{\alpha\to 0}(ag, \alpha)$.

The regularization $V(g, r, \alpha) = V(g, r + \alpha)$ satisfies the conditions given if the potential $V(g, r)$ is already analytic in g, continuous in r. The conditions are by no means necessary; indeed, the widely used ϑ regularization violates these conditions though it still works in many cases. In particular, the regularized potential considered in the body of this paper does not satisfy any of the conditions, and yet regularization succeeds.

[11] E. A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill Book Company, Inc., New York, 1955), Theorems 7.4 and 8.3, pp. 29–36.

Algebraic Aspects of Regge Recurrences*

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The algebraic structure of Regge recurrences is examined, and its relation to symmetry schemes underlying various models is established. The relationship between the Spectrum Generating Algebras (SGA) and the noncompact subalgebras of the rotational states are discussed for the Coulomb potential, the three-dimensional oscillator, the signature which appears in exchange potentials, as well as the $U(6, 6)$ and the other suggested SGA of hadron physics.

INTRODUCTION

THE classification of hadron states was mainly achieved by group-theoretical means. Originally, the group had a geometrical–kinematical origin (spin and the Lorentz group); then came the "internal" symmetry $U(3)$; and more recently we have witnessed the application of its extensions $U(6)$, $U(6) \times U(6)$ and perhaps $U(6, 6)$. It seems most probable that such extensions are of dynamical origin; one example of this kind is provided by the system of current space-integrals, which has been applied as an algebra of transition[1] operators (TOA) generating[2] the group $U(12)$, in situations exhibiting the dynamical features[3] explicitly. Indeed, it may yet turn out that such dynamical mechanisms as the strong-coupling static model (perhaps in a reciprocal bootstrap) are at the origin of the $U(6) \times U(6)$ system, for instance.

The notion of hadrons as Regge poles,[4] and the related idea of a system of recurrences,[5] represented an earlier attempt at basing a classification upon dynamical concepts. The scheme was first superimposed upon the "internal" order. With the inclusion of spinlike transformations in $U(6)$ and the higher[1] rest-ASA's (Approximate Symmetry Algebras), some understanding of the connections between the two structures is now essential to further progress. Several schemes in which such a synthesis is achieved have recently been suggested[6]; we now analyze the mathematical background of this problem.

The genesis of Regge poles can be traced back to potential theory; its development, however, is entirely inspired by the methods of analysis. To connect them with symmetries, we first have to bring out their algebraic structure. The present work contains a study of some examples which should provide the basis for such an understanding. In the first section, we review the analytical Regge poles structure of the Coulomb potential, the three-dimensional oscillator, and the signature[5] appearing in exchange potentials. We then review in the second section the system[1] of spectrum generating algebras (SGA) corresponding to these examples. We proceed to identify the various noncompact[7] subalgebras whose unitary representations provide the sequence of recurring bound states. The last section is devoted to a discussion of the connections with the hadron ASA's and SGA's. In our algebraic discussion, we do not intend to comment on the analytical continuation in J by itself (this has been discussed recently[8]), neither do we touch on the various implications of Regge poles not related to the classification scheme.

I. REGGE RECURRENCES FOR THE COULOMB POTENTIAL AND THREE-DIMENSIONAL OSCILLATOR

In order to gain additional understanding of the Regge recurrences, we consider two cases for which an exact solution of the Schrödinger equation can be obtained.

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† Also of Israel Atomic Energy Commission, Soreq Nuclear Research Centre, Yavne.

[1] Y. Dothan and Y. Ne'eman, in *Symmetry Groups in Nuclear and Particle Physics*, F. Dyson, Ed. (W. A. Benjamin Company, Inc., New York, 1966), pp. 287 ff.

[2] R. Dashen and M. Gell-Mann, Phys. Letters **17**, 142 (1965).

[3] R. Dashen and M. Gell-Mann, Phys. Letters **17**, 145 (1965); B. W. Lee, Phys. Rev. Letters **14**, 676 (1965); S. L. Adler, *ibid.*, **14** 1051 (1965); W. I. Weisberger, *ibid.*, **14** 1047 (1965).

[4] G. F. Chew and S. C. Frautschi, Phys. Rev. Letters **7**, 394 (1961).

[5] S. C. Frautschi, M. Gell-Mann, and F. Zachariasen, Phys. Rev. **126**, 2204 (1962).

[6] Y. Dothan, M. Gell-Mann, and Y. Ne'eman, Phys. Letters **17**, 148 (1965).

[7] R. Hermann, in *High Energy Physics and Elementary Particles* (International Atomic Energy Agency, Vienna, 1965), p. 625 ff. discusses the Gell-Mann formula.

[8] E. M. Stein and S. Wainger, Arkiv Mat. **5**, 553 (1965).

A. The Coulomb Potential[9,10]

The Schrödinger equation for the lth partial wave leads to an S-matrix, where the bound states of the Coulomb potential are given by the singularities which correspond to the poles of

$$\Gamma\left[l+1-\frac{ie^2}{\hbar^2}\left(\frac{M}{2E}\right)^{\frac{1}{2}}\right].$$

The corresponding Regge trajectories are thus

$$\alpha_n(E) = -n_r + \frac{ie^2}{\hbar}\frac{M}{2E}, \qquad n_r = 1, 2, \cdots, \tag{1}$$

from which we see that the nth Regge pole crosses physical l values at energies

$$E(n) = \frac{-Me^4}{2(n_r + l)^2\hbar^2}, \qquad n_r = 1, 2, \cdots. \tag{2}$$

(The n_r is related to the number of nodes in the wavefunction.)

B. The Three-Dimensional Harmonic Oscillator

The radial Schrödinger equation leads, in this case, to Regge trajectories given by

$$\alpha_n(E) = E/\hbar\omega - 2n_r - \tfrac{3}{2} \quad (n_r = 0, 1, 2, \cdots). \tag{3}$$

Consequently, the nth Regge pole crosses physical l values at

$$E(n) = \hbar\omega(2n_r + l + \tfrac{3}{2}) \quad (n_r = 0, 1, 2, \cdots). \tag{4}$$

C. Exchange Potentials[5]

Corresponding to the Coulomb case, we can consider a potential of the form

$$V = \frac{-2M}{\hbar^2 r}[e^2 + (-1)^l f^2], \tag{5}$$

which has a behavior analogous to exchange forces in the relativistic domain.

Separating the Schrödinger equation into two independent parts, one for even l and one for odd l, leads to two Regge trajectories,

$$\begin{aligned}\alpha_{\text{even}}(E) &= -n_r + i\left(\frac{M}{2E}\right)^{\frac{1}{2}}\frac{(e^2+f^2)}{\hbar},\\ \alpha_{\text{odd}}(E) &= -n_r^{-1} + i\left(\frac{M}{2E}\right)^{\frac{1}{2}}\frac{(e^2-f^2)}{\hbar};\end{aligned} \tag{6}$$

$$(n_r = 1, 2, 3, \cdots)$$

Correspondingly, the Regge poles on the even trajectory cross physical values at energies

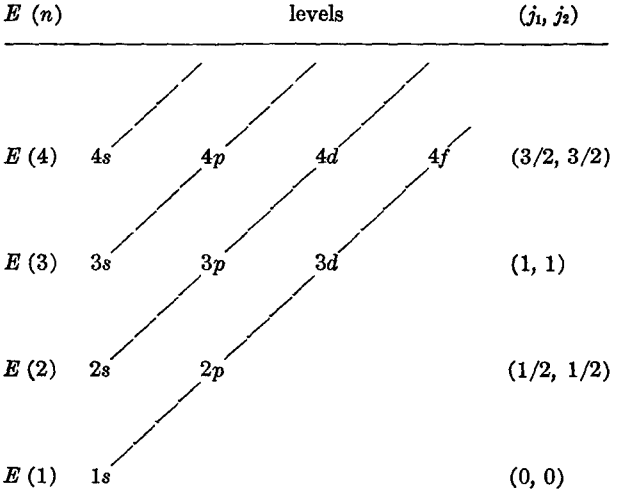
$$E^{(e)}_{(n)} = \frac{-M(e^2+f^2)^2}{2(n_r + l_{\text{even}})^2\hbar^2}, \qquad (l_{\text{even}} = 0, 2, \cdots) \tag{7}$$

and, on the odd trajectory, cross at energies

$$E^{(0)}_{(n)} = \frac{-M(e^2-f^2)^2}{2(n_r + l_{\text{odd}} + 1)^2\hbar^2}, \qquad (l_{\text{odd}} = 1, 3, \cdots). \tag{8}$$

II. THE SGA AND THE ALGEBRAS OF ROTATIONAL STATES (ARS) FOR THE COULOMB POTENTIAL

Let us now view the complete set of energy levels of the Coulomb potential[1] in the following tabulation:



In this tabulation, we have also given the degenerate levels in terms of the $SO(4)$ representations (j_1, j_2), with the Pauli[11] $SU(2)$ quasi-spins

$$\mathbf{j}_1 = \mathbf{L} + \mathbf{A}, \qquad \mathbf{j}_2 = \mathbf{L} - \mathbf{A}, \tag{9}$$

where $\mathbf{L}$ is the orbital angular momentum and $\mathbf{A}$ the quantized Laplace–Lentz operator with an appropriate normalization,

$$\mathbf{A} = H^{-\frac{1}{2}}(\tfrac{1}{2}ze^2m)\{(\mathbf{L}\wedge\mathbf{p}) - (\mathbf{p}\wedge\mathbf{L})\} + \mathbf{r}/r. \tag{10}$$

We note that $\mathbf{A}\cdot\mathbf{L} = 0$, which requires $j_1 = j_2$. The degeneracy ASA is in fact $SO(4) \otimes SO(2)$, where the $SO(2)$ or $U(1)$ stands for the generator $H^{-\frac{1}{2}}$ whose eigenvalues n label the levels.

It has been previously noted[1,12] that the entire spectrum of the Coulomb potential forms one infinite-dimensional reprsentation of the SGA $SO(1, 4)$ with its compact subalgebra $SO(4)$ as an ASA. Alternatively, we can use $SO(2, 4)$ with the above-

[9] P. M. Morse and H. Feshbach, *Methods of Theoretical Physic* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 2, p. 1662.

[10] S. C. Frautschi, *Regge Poles and S-Matrix Theory* (W. A. Benjamin, Inc., New York, 1963), Chap. 10.

[11] W. Pauli, Z. Physik **36**, 336 (1926); V. Fock, *ibid.* **98**, 145 (1935).

[12] The problem has also been studied by Bacry, Barut, Budini and Fronsdal; see A. Salam, *The Role of Symmetry Physics* (Oxford Conference Summary, September 1965).

mentioned compact $SO(4) \otimes SO(2)$ ASA subsystem. If u^i denotes the abstract coordinate in a metric space supporting the Pauli $SO(4)$ ASA, we can construct the[7] noncompact generators of $SO(1, 4)$,

$$N^i = \tfrac{1}{2}i[L^2 + A^2, u^i]. \tag{11a}$$

To get $SO(2, 4)$, we adjoin

$$M^i = \tfrac{1}{2}i[L^2 + A^2, v^i] \tag{11b}$$

with the condition

$$\mathbf{u}\cdot\mathbf{v} = 0. \tag{11c}$$

The Regge trajectories are characterized by their ground-state energies E_s, or by the n-value of the S-state,

$$n = n_s + l.$$

We note that these sequences lie along the dotted lines in our tables and form infinite-dimensional representations $(n_s, 0)$ of the homogeneous Lorentz group[13]

$$l = 0, 1, 2, 3, \cdots,$$

where we have characterized the representations by $(n_s, l_{\min})$. This abstract Lorentz group $SL(2, C)$ is the $SO(3, 1)$ subgroup of the $SO(4, 1)$ SGA, which we get when we reduce the $SO(4)$ ASA to the $SO(3)$ L subgroup. This is typical of the other cases we study, i.e., every representation of the compact subgroup occurs only once.

We now consider the signature-dependent situation. In this case, we require an SGA which chooses either even or odd states. This is the $SL(4, R)$ group whose noncompact generators behave like (1, 1) and are given[1] by

$$N^{ia} = \tfrac{1}{2}i[L^2 + A^2, r^{ia}], \tag{12a}$$

where r^{ia} is a $j_1 = j_2 = 1$ tensor (i and a are the j_1 and j_2 indices, respectively). These generators close with the Pauli $SO(4)$ set $\mathbf{J}_1$ and $\mathbf{J}_2$ upon $SL(4, R)$, provided $j_1 = j_2$ and

$$\begin{aligned} r^{ia}r_{ja} &= \top\ \delta^i_j, \\ r^{ia}r_{ib} &= \perp\ \delta^a_b. \end{aligned} \tag{12b}$$

We can now trace the corresponding subalgebra of the rotational states. Again, we take the L subgroup of $J_1 \otimes J_2$ only; our $SL(4, R)$ is now reduced to $SL(3, R)$, with the noncompact generators

$$R^{mn} = \tfrac{1}{2}i[L^2, r^{mn}], \tag{13}$$

where r^{mn} is the symmetric 2nd-rank tensor in 3-space, with similar orthonormality conditions.

III. THE SGA AND THE ARS FOR THE OSCILLATOR

The energy levels of the 3-dimensional oscillator are:

$E\ (n)$	levels	(n, r, s)
$E(3)$	$3p$ $\quad$ $3d$	(3, 0, 0)
$E\ (2)$	$2s$ $\quad$ $2d$	(2, 0, 0)
$E\ (1)$	$1p$	(1, 0, 0)
$E\ (0)$	$0s$	(0, 0, 0)

In this tabulation, (n, r, s) denote the representations of the $U(3)$ degeneracy ASA, whose generators[14,15] are

$$U^a = \lambda^a_{ij}a^i a^{j\dagger},$$

where λ^a_{ij} is the (i, j)th-matrix element of the λ^a matrices of $U(3)$; a^i and $a^{i\dagger}$ are the usual creation and annihilation operators.

The SGA is $U(1, 3)$, with the[12,14] noncompact generators $(2^{-\frac{1}{2}})(H - \frac{1}{2})^{\frac{1}{2}}a^i$ and $(2^{-\frac{1}{2}})a^{i\dagger}(H - \frac{1}{2})^{\frac{1}{2}}$. The rotational sequences correspond to the reduction of the $U(3)$ ASA to its $SO(3)$ subgroup; the $U(1, 3)$ SGA then yields an $SO(1, 3)$ spectrum generating subalgebra, with representations $(n_s, 0)$ lying along the dotted lines and characterized by even values of n_s.

A signature chooses, in a trajectory, bound states of odd or even levels. The complete SGA is now the[15,16] Lipkin–Goshen $Sp(6, R)$, whose noncompact generators (behaving like $L = 0$ and 2) are

$$N^A = s^A_{ij}(a^{i\dagger}a^{j\dagger} + a^i a^j) \quad \text{and} \quad \frac{1}{i}s^A_{ij}(a^{i\dagger}a^{j\dagger} - a^i a^j),$$

where s^A_{ij} are the (i, j)th symmetric reduction coefficients of 3×3 or $3^* \times 3^*$. The Regge subalgebra is again reached by taking the L subgroup of the $U(3)$ degeneracy ASA; we get an $SL(3, R)$ subgroup

[13] M. A. Naimark, Usp. Mat. Nauk 9, 19 (1954) [English transl.: Am. Math. Soc. Transl. Ser. 2, 6, 379 (1957)].

[14] Y. Ne'eman, in *Tokyo Summer Lectures on Theoretical Physics*, G. Takeda, Ed. (W. A. Benjamin, Inc., New York, 1966), Pt. 2, p. 68.

[15] H. J. Lipkin, *Lie Groups for Pedestrians* (North-Holland Publishing Company, Amsterdam, 1965), p. 69.

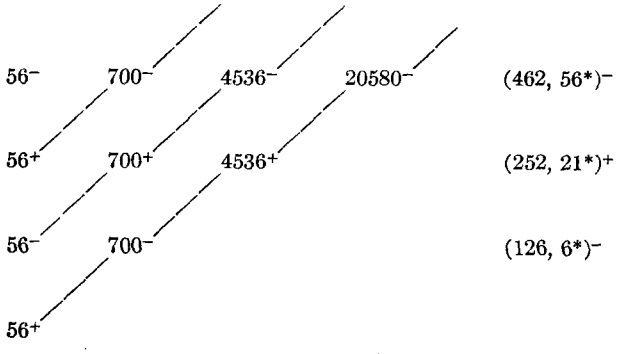
[16] S. Goshen and H. J. Lipkin, Ann. Phys. (N.Y.) 6, 301 (1959).

of $Sp(6, R)$,with the noncompact generators reducing to the $L = 2$ parts of the N^4.

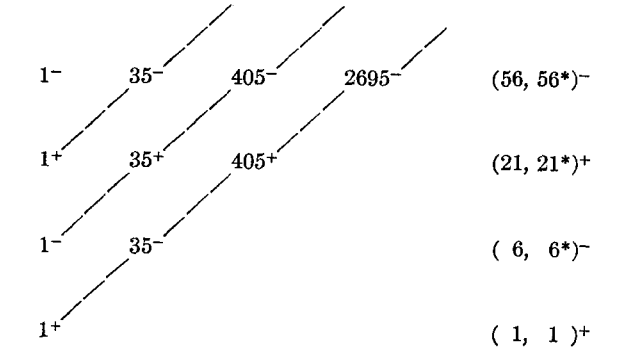
A. The ARS in Hadron Physics : The U(6, 6) Case

Such infinite sequences of rotational levels represent an idealization of the actual state of affairs in hadron physics. Presumably we are faced with finite sequences; however, we can stick to the idealizations provided by the former examples, hoping that they do represent a rough approximation.

The $U(6, 6)$ group, considered in Ref. 5 as either a SGA or a rest-ASA of the hadron system, contains an $SL(2, C)$ Regge subalgebra as in our simple nonrelativistic examples. For the baryon ladder representation



and the mesons representation



the dotted lines follow infinite-dimensional alternating-parity representations of an $SL(6, C)$ subgroup whose compact piece is plain $SU(6)$ and whose noncompact generators behave like s-wave mesons in a 35^-. We note that $U(6, 6)$ also contains another $SL(6, C)$ with even parity noncompact generators behaving like p-wave mesons in a 35^-, i.e., they form a 35^+ as in a strong-coupling static model. These leave out every other row and mark the sequences $56^{\pm}$, $700^{\pm}$, $4536^{\pm}$, $\cdots$ starting at various values of the $n(\beta)_{\min}$ eigenvalues. Similary, for the mesons, we get 1^+, 35^+, 405^+, $\cdots$.

The $SL(6, C)$ rotational sequences, in fact, include two coupled trajectories of different parities. To separate out the subgroup corresponding to $\Delta j = 2$ fixed-parity trajectories, we have to use the $SL(3, R)$ subgroup of the $SL(4, R)$ contained in the double-step SGA when we take the $U(3)$ index 0. Note that, upon reduction to the scalar $U(3)$ content, $U(6, 6)$ reduces to $U(2, 2)$ and we are back at the mathematics for the Coulomb case, with the Dirac β playing the role of the hydrogen n.

B. The SL(12, C) and the SL(3, R)$_q$ Cases

The next possibility studied in Ref. 6 corresponds to the group $SL(12, C)$. Considering that $SL(12, C)$ contains $U(6, 6)$, we note that the required Regge algebras are again present.

The third suggestion assumes an $SL(3, R)$ SGA whose compact subgroup is the quark orbital angular[17] momentum L_q. This is again in complete analogy to our classical examples; in fact, one would extend the method and use first an $SL(2, C)$ SGA, with alternating parities in the representations. These schemes may be superimposed either on the $U(6) \times U(6)$ β-decomposition ASA, on $U(6, 6)$ itself, and even on the entire $SL(12, C)$.

ACKNOWLEDGMENTS

One of the authors (Y.N.) is indebted to R. W. Griffith, R. Peierls, I. Ozsvath, and S. C. Frautschi for several enlightening discussions.

[17] M. Gell-Mann, Phys. Rev. Letters 14, 77 (1965).

Asymptotic Expansions of the Dirac Density Matrix*

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Asymptotic expansions are derived for the density operator

$$\rho_N(x', x) = \sum_{n=1}^{N} \psi_n(x')\psi_n(x)$$

for small and large values of the relative distance $x' - x$ with a WKB expansion for bound-state wavefunctions in a plane, one-dimensional potential. In addition to some previously obtained corrections, the particle-density expansion includes a number of steady and oscillating correction terms to the zero-order Thomas–Fermi density which are related to the more recently derived corrections of Payne and of Kohn and Sham. A convenient and accurate approximation to the density operator for *all* arguments is also obtained from the first two terms of the expansion for large relative distances. The expansions become inadequate in the vicinity of the classical turning point of the highest energy state, as illustrated by numerical comparisons with the exact-density operator for the quadratic potential. A novel method is described for summing a finite series of oscillating terms such as occur in the density operator.

INTRODUCTION

THE expectation value of the normal one-particle operator $\theta(x', x)$ in the group of the N lowest one-particle states approximating an N-particle quantum system can be calculated by integrating the operator sum

$$\Theta_N(x', x) \equiv \sum_{n=1}^{N} \Psi_n^*(x')\theta(x', x)\Psi(x). \qquad (1)$$

Such operator sums can usually be expressed simply as $\theta(x', x)\rho_N(x', x)$ if one has a suitable approximation for the density matrix

$$\rho_N(x', x) = \sum_{n=1}^{N} \Psi_n^*(x')\Psi_n(x). \qquad (2)$$

Asymptotic approximations of the particle density

$$\rho_N(x) \left[\equiv \lim_{x' \to x} \rho_N(x', x) \right]$$

have been studied extensively in connection with the Thomas–Fermi statistical many-particle theory.

In spite of this effort, no reliable systematic approximation method appears to have been developed until recently. Brillouin[1] long ago pointed out that the Thomas–Fermi statistical particle density could be derived from semiclassical wavefunctions in formula (2) in the limit as Planck's constant $\hbar$ vanishes. Recently[2] a formal expansion of $\rho_N(x)$ in powers of $\hbar$ has been developed with several operator and Green's function methods, but the resulting corrections are much smaller than the oscillating deviations from the Thomas–Fermi density which are known from numerical evaluations of $\rho_N(x)$ for simple cases. Stephens and Zalewski[3] have indicated, by an exact expression for $\rho_N(x)$ for the case of the quadratic potential, that the oscillating component of the density is lacking in the previously obtained series in powers of $\hbar$ and that any such expansion for a general potential must be incomplete. What are presumably more convergent expansions of the density have recently been developed[4] by new operator approximations, but the resulting oscillating component of the density seems to give a poor numerical approximation to the exact density for simple potentials.

In the present work a systematic asymptotic expansion for the density matrix was derived from an asymptotic, WKB expansion of the wavefunctions in the density sums, Eq. (2). After the completion of this work, two related works by Payne[5] and by Kohn and Sham[5] came to the attention of the author in which some of the results reported here were obtained by different methods also with the WKB and Airy function approximations. The method used in the present work is novel in the manner of approximating the oscillating sums occurring in Eq. (2). The first terms of the approximation give exact results for the infinitely deep

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

[1] L. Brillouin, Actualités Sci. Ind. No. 160 (1934).

[2] A. S. Kompaneets and E. S. Pavlovskii, Zh. Eksperim. i Teor. Fiz. **31**, 427 (1956) [English transl. Soviet Phys.—JETP **4**, 328 (1957)]; D. A. Kirzhnits, Zh. Eksperim. i Teor. Fiz. **32**, 115 (1957) [English transl.: Soviet Phys.—JETP **5**, 64 (1957)]; S. Golden, Phys. Rev. **107**, 1283 (1957); G. A. Baraff and S. Borowitz, *ibid.* **121**, 1704 (1961).

[3] M. J. Stephens and K. Zalewski, Proc. Roy. Soc. (London) **A270**, 435 (1962).

[4] L. C. R. Alfred, Phys. Rev. **121**, 1275 (1961); W. Macke and P. Rennert, Ann. Physik **7**, 84 (1963).

[5] H. Payne, J. Chem. Phys. **38**, 2016 (1963); W. Kohn and L. J. Sham, Phys. Rev. **137**, A1697 (1965).

square-well potential. The applicability of this expansion to general potentials is illustrated by a high-order comparison of the density matrix expansion with the exact density matrix for the quadratic potential.

DENSITY SUMS WITH WKB-LIKE WAVEFUNCTIONS

The asymptotic expansion of the sums (2) follow from the asymptotic WKB expansion[6,7] of the corresponding wavefunctions which is reviewed here. If a bound-state wavefunction in a plane one-dimensional potential $V(x)$ is written in the real form

$$\Psi_n(x) = \frac{\sin \xi(\epsilon_n, x)}{k^{\frac{1}{2}}(\epsilon_n, x)\mathfrak{N}_n^{\frac{1}{2}}}, \quad \xi(n, x) \equiv \int_{-\infty}^{x} k(\epsilon_n, y)\, dy, \tag{3}$$

then the Schrödinger equation for $\Psi_n(x)$ is equivalent to the following differential equation for $k^2(\epsilon, x)$:

$$k^2(\epsilon, x) = k_0^2(\epsilon, x) + \frac{5}{16}\left[\frac{1}{k^2}\frac{dk^2}{dx}\right]^2 - \frac{1}{4k^2}\frac{d^2k^2}{dx^2}, \tag{4}$$

where $k_0^2(\epsilon, x) \equiv \epsilon - v(x)$, and ϵ and $v(x)$ are defined in terms of $V(x)$, particle energy E, and mass m, such that $\epsilon = 2mE/\hbar^2$ and $v(x) = 2mV(x)/\hbar^2$. The required bound-state eigenvalues ϵ_n in Eq. (3) are determined by

$$\int_{-\infty}^{+\infty} k(\epsilon_n, x)\, dx = n\pi. \tag{5}$$

Plaskett derives an interesting property of the integral of Ψ_n^2 between any two nodes a and b of Ψ_n, namely,

$$\int_a^b \Psi_n^2(x)\, dx = \frac{1}{\mathfrak{N}_n}\int_a^b \frac{dk(\epsilon, x)}{d\epsilon}\, dx. \tag{6}$$

Therefore the normalization constant $\mathfrak{N}_n$, in (3), can be written as

$$\mathfrak{N}_n = \int_{-\infty}^{+\infty} \frac{dk}{d\epsilon}\, dx = \pi\frac{dn}{d\epsilon}. \tag{7}$$

The WKB approximation and higher corrections to it can be generated from Eq. (4) by an iteration starting with $k^2(\epsilon, x) \simeq k_0^2(\epsilon, x)$. In this manner an asymptotic expansion for k^2 in powers of $k_0^{-2}(\epsilon, x)$ is developed,

$$k^2(\epsilon, x) = k_0^2 + \frac{v''}{4k_0^2} + \frac{5v'^2 - v^{iv}}{16k_0^4} - \frac{4v''^2 + 28v'v''' - v^{vi}}{64k_0^6} + \cdots \tag{8}$$

[6] J. S. Plaskett, Proc. Phys. Soc. (London) **A66**, 178 (1953).
[7] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 178.

in terms of the space derivatives of the potential $v^{(n)}(x)$. The phase function in (3) for the eigenstate n is then expanded,

$$\xi(n, x) = \frac{\pi}{4} + \int_{p(\epsilon)}^{x} k_0(\epsilon, x)\, dx + \cdots, \tag{9}$$

where

$$(n - \tfrac{1}{2})\pi = \tfrac{1}{2}\oint_C k_0\, dx\left(1 - \frac{v'^2}{32k_0^6} + \cdots\right).$$

The contour C in the complex x plane encloses a region including both of the classical turning points[8] $p(\epsilon)$, where $\epsilon = v(p)$, but none of the singularities of $v(x)$ (if it is possible to find such a contour). The WKB expansion (8) is asymptotic for large values of $k_0(\epsilon, x)$ which, according to Eq. (9), for typical potentials is equivalent to large values of n. Several possible ways of grouping terms in such an expansion as Eq. (8) are possible but we simply group them in inverse powers of k_0^2. The resulting expansions can be easily rearranged to correspond to the particular manner in which one wishes to approach the limit of large k_0.

The density matrix (2), derived from the wavefunctions (3), is

$$\pi\rho_N(x', x) = \sum_{n=1}^{N}\frac{d\epsilon}{dn}\frac{[\cos\xi_{n-}(x', x) - \cos\xi_{n+}(x', x)]}{2[k(\epsilon_n, x)k(\epsilon_n, x')]^{\frac{1}{2}}}, \tag{10}$$

where

$$\xi_{n\pm}(x', x) \equiv \xi(n, x') \pm \xi(n, x).$$

The particle density is the diagonal part of (10),

$$\pi\rho_N(x) = \sum_{n=1}^{N}\frac{d\epsilon}{dn}\frac{[1 - \cos 2\xi(n, x)]}{2k(\epsilon_n, x)} \equiv \sum_{n=1}^{N} g(n)(1 - \cos 2\xi). \tag{11}$$

The Euler–Maclaurin (E–M) formula[9] is then usually applied to replace a sum like the first term on the right of Eq. (11) by an integral with additional correction terms,

$$\sum_{n=1}^{N} g(n) = \int_{\frac{1}{2}}^{N+\frac{1}{2}} dn\, g(n) + \sum_{s=1}\frac{B_{2s}(\frac{1}{2})}{(2s)!}\left|\frac{d^{(2s-1)}g(n)}{dn^{2s-1}}\right|_{\frac{1}{2}}^{N+\frac{1}{2}}. \tag{12}$$

$B_s(\frac{1}{2})$ are the values of the Bernoulli polynomials $B_s(x)$ at $x = \frac{1}{2}$. If one attempts a WKB approxi-

[8] J. L. Dunham, Phys, Rev. 41, 713 (1932).
[9] L. M. Milne-Thomson, *Calculus of Finite Differences* (Macmillan and Company, Ltd., London, 1933), Chap. 7.5; K. Jordan, *Calculus of Finite Differences* (Chelsea Publishing Company, New York, 1950), Chap. 3.

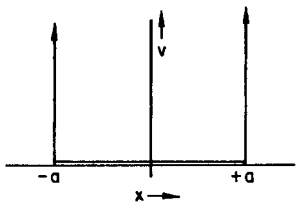

FIG. 1. Potential well case.

mation to (12) using the first terms in Eqs. (8) and (9), a Thomas–Fermi-like density is obtained as the first term from the integral

$$\pi\rho_N(x) \simeq k_0(\epsilon_{N+\frac{1}{2}}, x) \equiv \pi\rho_N^{\mathrm{TF}}(x). \tag{13}$$

It is, however, not possible to deduce any further terms from this procedure, for two reasons. First, the lower limits in the correction terms of the E–M formula (12) cannot be approximated with the expansion terms in Eq. (8). Because k_0 becomes very small near the lower limit, the series of terms in Eq. (8) and similar terms which are needed in formula (12) cannot be unambiguously evaluated. Secondly, the cosine terms in the summation of Eq. (11) should not be ignored. However, the E–M formula for this sum does not give a reliable approximation because of the oscillating nature of the terms.

An elementary example clarifies this last point and is also useful in the following sections. It is the case of particles bound in an infinite square well as shown in Fig. 1. According to (8), k is identical to k_0 and the eigenvalue condition (5) is $k = \epsilon^{\frac{1}{2}} = n\pi/2a$. The eigenfunctions (3) are

$$\Psi_n(x) = (1/a^{\frac{1}{2}}) \sin (n\pi/2a)(x + a). \tag{14}$$

Then the density matrix is

$$\rho_N(x', x) = \frac{1}{2a} \sum_{n=1}^{N} \left[\cos \frac{n\pi}{2a} (x - x') - \cos \frac{n\pi}{2a} (x + x' + 2a) \right],$$
$$\rho_N(x) = \frac{1}{2a} \sum_{n=1}^{N} \left[1 - \cos \frac{n\pi}{a} (x + a) \right]. \tag{15}$$

One cannot expect to obtain a good approximation to the sums on the right side of Eqs. (15) by using only the first few terms of the E–M formula. To an extent depending on the arguments x and x', successive terms in the sums of (15) differ by irregular and large amounts, whereas the usefulness of the E–M formula depends on the smallness and regularity of the differences (or equivalently, on the smallness of higher derivatives of the terms with respect to n). However, the trigonometric sums in Eqs. (15) can be summed using elementary identities (see next section) to give

$$\rho_N(x', x) = \frac{1}{4a} \left\{ \frac{\sin [(N + \frac{1}{2})(\pi/2a)(x' - x)]}{\sin (\pi/4a)(x' - x)} + \frac{(-1)^{N+1} \cos [(N + \frac{1}{2})(\pi/2a)(x + x')]}{\cos (\pi/4a)(x + x')} \right\}, \tag{16}$$

$$\rho_N(x) = \frac{1}{4a} \left[2N + 1 + \frac{(-1)^{N+1} \cos (N + \frac{1}{2})(\pi x/a)}{\cos (\pi x/2a)} \right].$$

The closure relation for the complete set of states (14) follows from Eq. (16) in the limit $N \to \infty$,

$$\rho_{N\to\infty}(x', x) \to (2\pi/4a)\ \delta[(\pi/2a)(x' - x)] = \delta(x' - x). \tag{17}$$

The summation problem in the density matrix (10) for a general smooth and monotonic potential is assumed to be like that in Eq. (15) to the following extent. The ξ_n arguments of the cosine terms do not necessarily differ from one value of n to the next by an amount much less than 1, but the amount of variation is a slowly varying function of n. More specifically, if we rewrite (10) as a sum of terms like

$$\mathrm{Re}\,[g(n)e^{if(n)}], \tag{18}$$

it is reasonable to assume that all the derivatives of both $g(n)$ and df/dn are bounded and $\ll 1$. In that case the sums in (10) can be evaluated in a manner similar to that used in deriving (16) from (15), as is shown in the next section.

METHOD OF SUMMING A FINITE SERIES OF OSCILLATING TERMS

Consider the sum $\sum_{n=1}^{N} e^{inx}$, which is related to the trigonometric sum in Eq. (15). Since it is actually the sum of a geometric series, it can be rewritten and immediately summed,

$$\frac{1}{e^{ix} - 1} \sum_{n=1}^{N} (e^{i(n+1)x} - e^{inx}) = \frac{e^{i(N+1)x} - e^{ix}}{e^{ix} - 1}.$$

If in place of nx there is a function $f(n)$ whose derivative with respect to n is slowly varying, then the sum of terms of the type (18) should be similarly rewritten as follows with the forward difference operator Δ:

$$\sum_{n=1}^{N} g(n)e^{if(n)} = \sum_{n=1}^{N} g(n) \frac{e^{if(n+1)} - e^{if(n)}}{e^{i[f(n+1)-f(n)]} - 1}$$
$$= \sum_{n=1}^{N} \Delta \left[\frac{g(n)e^{if(n)}}{e^{i\Delta f(n)} - 1} \right] - \sum_{n=1}^{N} e^{if(n+1)} \Delta \left[\frac{g(n)}{e^{i\Delta f(n)} - 1} \right].$$

Therefore the following exact reduction is achieved:

$$\sum_{n=1}^{N} g(n)e^{if(n)} = \frac{g(n)e^{if(n)}}{e^{i\,\Delta f(n)} - 1}\Bigg|_{1}^{N+1} - \sum_{n=1}^{N} \Delta\left[\frac{g(n)}{e^{i\,\Delta f(n)} - 1}\right] e^{if(n+1)}. \tag{19}$$

First of all, the second term according to our assumptions is intrinsically smaller than the first, which is therefore the first approximation to the sum. Secondly, the second term of (19) is itself of the same form as the sum on the left side and in turn can be similarly approximated. By iteration of this procedure one obtains an expansion in the form of $e^{if(n)}G(n)$, where $G(n)$ is a solution of a difference equation containing slowly varying functions of n.

To derive a systematic expansion of the sum in a more economical manner, we start over again with the ansatz

$$\sum_{n=1}^{N} g(n)e^{if(n)} = \left| e^{if(n)}G(n) \right|_{n=\frac{1}{2}}^{n=N+\frac{1}{2}}. \tag{20}$$

With the centered mean and difference operators[9] defined by

$$\mu\phi(n) = \tfrac{1}{2}[\phi(n + \tfrac{1}{2}) + \phi(n - \tfrac{1}{2})],$$
$$\delta\phi(n) = \phi(n + \tfrac{1}{2}) - \phi(n - \tfrac{1}{2}),$$

Eq. (20) may be rewritten as

$$\delta[e^{if(n)}G(n)] = g(n)e^{if(n)}. \tag{21}$$

Since $\delta(AB) = \delta A\mu B + \mu A\delta B$, Eq. (21) can be expanded and rearranged to obtain the following basic difference equation for $G(n)$:

$$G(n) = \frac{e^{if(n)}g(n)}{\delta[e^{if(n)}]} - \frac{\mu}{\delta}[e^{if(n)}]\,\delta G(n) - (\mu - 1)[G(n)]. \tag{22}$$

We seek a simple approximate solution of Eq. (22) which can be used in Eq. (20) to provide a convenient approximation to the sums. With standard trigonometric formulas the following defined quantities can be re-expressed as:

$$G_0(n) \equiv \frac{g(n)}{e^{-if(n)}\,\delta[e^{if(n)}]} = \frac{g(n)e^{-\frac{1}{2}i\,\delta_{\frac{1}{2}}^2[f(n)]}}{2i\sin(\frac{1}{2}\delta f)},$$
$$\frac{\mu}{\delta}[e^{if(n)}] \equiv \frac{\mu(e^{if})}{\delta(e^{if})} = \frac{1}{2i}\cot(\tfrac{1}{2}\delta f), \tag{23}$$

where $\delta_{\frac{1}{2}}^2$ is the second-order centered difference operator calculated for an interval of $\frac{1}{2}$ in n. Since μ satisfies the operator identity $\mu = (1 + \frac{1}{4}\delta^2)^{\frac{1}{2}}$, the last two terms of Eq. (22) are by hypothesis dominated by the first term on the right, $G_0(n)$. Therefore an approximate solution of Eq. (22) can be generated by iteration starting with $G \simeq G_0$, i.e., using $G_{\nu-1}(n)$ on the right side of Eq. (22) to evaluate $G_\nu(n)$, to the νth order of accuracy, on the left. Through terms of second-order one obtains

$$G(n) = G_0(n) - \frac{\cot(\frac{1}{2}\delta f)}{2i}\,\delta G_0 - \tfrac{1}{4}\{\cot(\tfrac{1}{2}\delta f)\,\delta[\cot(\tfrac{1}{2}\delta f)]\,\delta G_0 + [\cot^2(\tfrac{1}{2}\delta f) + \tfrac{1}{2}]\,\delta^2 G_0\} + \cdots. \tag{24}$$

In most of what follows it is sufficient to keep only the leading terms through first order in Eq. (24). The following approximation can be derived from Eq. (23):

$$\frac{\delta G_0}{G_0} \simeq \frac{\delta g}{g} - \frac{\delta^2 f}{2}\cot(\tfrac{1}{2}\delta f).$$

If this is substituted into Eq. (24) the cosine sums in Eqs. (10) and (11), when evaluated through first order, are

$$\sum_{n=1}^{N} g(n)\cos f(n) = \mathrm{Re}\sum_{n=1}^{N} g(n)e^{if(n)} = \left|\frac{g}{2\sin(\frac{1}{2}\delta f)}\{\sin f + \tfrac{1}{2}[(\delta g/g)\cot(\tfrac{1}{2}\delta f) - \tfrac{1}{2}\delta^2 f \times \cot^2(\tfrac{1}{2}\delta f) - \delta_{\frac{1}{2}}^2 f]\cos f + \cdots\}\right|_{\frac{1}{2}}^{N+\frac{1}{2}}. \tag{25}$$

The difference operators in (25) may simply be replaced by differentiation with respect to n to two higher orders of accuracy, and this, in fact, is the main reason for using centered differences in every step of the above derivation.

In many simple cases the first term alone in Eq. (25) is an excellent approximation to the desired sums. For example, the leading terms in powers of $1/N$ of the oscillating sum $\sum_n^N n^\nu e^{inx}$ are given by $G_0(n)$ except for small values of N when $\nu < 0$. This is because such a series can be expressed as the νth derivative with respect to n of the sum $\sum e^{inx}$, which as previously noted can be exactly evaluated from $G_0(n)$. Another related example is the sum of an alternating series

$$\sum_{N_1}^{N_2}(-1)^n g(n) = \sum_{N_1}^{N_2} g(n)e^{in\pi} \simeq \tfrac{1}{2}[(-1)^{N_2}g(N_2 + \tfrac{1}{2}) + (-1)^{N_1}g(N_1 - \tfrac{1}{2})]$$

using $G_0(n)$ for $G(n)$. If, on the other hand, the alternating sum is done, for N_1 an odd and N_2 an even number, by grouping pairs of terms and evaluating the resulting conventional sum by the E–M formula, the same leading term is obtained (see Jordan, Ref. 9). The expansion obtained in this section for oscillating sums can also be described as a generalization of this method of evaluating a sum of alternating terms. The calculations in the next section show the usefulness of these mathematical approximations for cases in which $f(n)$ is not simply linear in n.

Note that in obtaining the particle density we must consider the case $f(n) \to 0$ for all n. In this limit the iterative solution for G shown in Eq. (24) does not usually converge. For Eqs. (24) and (25) to be useful it is usually necessary that

$$(d^2f/dn^2)(df/dn)^{-2} < 1. \tag{26}$$

However, in the case $f(n) = nx$, condition (26) is satisfied for all x. In most cases, as $f(n) \to 0$ the condition is not satisfied, and the appropriate way to approximate the sum (20) is with the E–M formula [see Eq. (12)]. The latter approximation can also be obtained from Eq. (22) by a different iteration procedure starting with the assumption that the first two terms on the right in Eq. (22) are the dominant ones.

APPLICATION TO THE DENSITY MATRIX

The density sums must be evaluated in a somewhat indirect way because of difficulties like those previously mentioned in connection with the lower limits of the summation in Eq. (25). However, if we use the closure property of a complete set of wavefunctions, the density matrix (2) can be written

$$\begin{aligned}\rho_N(x', x) &= \lim_{M\to\infty}\left[\sum_{n=1}^{M}\Psi_n^*(x')\Psi_n(x) - \sum_{n=N+1}^{M}\Psi_n^*(x')\Psi_n(x)\right] \\ &= \delta(x' - x) - \lim_{M\to\infty}\sum_{n=N+1}^{M}\Psi_n^*(x')\Psi_n(x).\end{aligned} \tag{27}$$

We can then apply the techniques of the last section to the second term on the right side of (27). To do this most simply we enclose the system in a large box; that is, modify the potential by the addition of an infinite potential wall at a large distance a so that as the energy ϵ_n becomes very large and positive, Ψ_n approaches the simple plane-wave form (14). Then according to Eq. (10)

$$\begin{aligned}&\rho_N(x', x) - \delta(x', x) \\ &= \lim_{M\to\infty}\sum_{N+1}^{M}\frac{d\epsilon}{dn}\frac{[\cos\xi_{n-}(x', x) - \cos\xi_{n+}(x', x)]}{2\pi[k_n(x')k_n(x)]^{\frac{1}{2}}} \\ &= -\frac{1}{\pi}\lim_{M\to\infty}\operatorname{Re}\,[e^{i\xi_{n-}}G_-(n) - e^{i\xi_{n+}}G_+(n)]_{n=N+\frac{1}{2}}^{n=M+\frac{1}{2}},\end{aligned} \tag{28}$$

where $G_\pm$ are G functions defined by Eq. (24) for

$$f(n) \equiv \xi_{n\pm}(x) = \int_{-\infty}^{x'} k(\epsilon_n, y)\,dy \pm \int_{-\infty}^{x} k(\epsilon_n, y)\,dy$$

and

$$g(n) \equiv \tfrac{1}{2}(d\epsilon/dn)[k(\epsilon_n, x')k(\epsilon_n, x)]^{-\frac{1}{2}}.$$

The quantum number M at the upper limit of Eq. (28) now refers to the high-energy continuum states, which fill the entire box. With the use of the asymptotic wavefunctions (14) for large values of M, the bracket in Eq. (28) can be easily evaluated at the upper limit, since the higher-order corrections to $G_0(n)$ in Eq. (24) become arbitrarily small. The contribution is given by Eq. (16) at $N = M$ which in the limit $M \to \infty$ becomes a δ function according to Eq. (17). In this manner, cancellation of the δ function on the left is accomplished independent of the value of the distance a, so long as it is much larger than the spatial extent of the highest, or Nth, occupied state. With the iterative solution for $G(n)$, Eq. (24), we may therefore write the density matrix for $x' \neq x$ as

$$\begin{aligned}\pi\rho_N(x', x) = [&G_{R-}(n)\cos\xi_{n-} + G_{I+}(n)\sin\xi_{n+} \\ &- G_{R+}(n)\cos\xi_{n+} - G_{I-}(n)\sin\xi_{n-}]_{n=N+\frac{1}{2}},\end{aligned} \tag{29}$$

where G_R and G_I are the real and imaginary parts of G, respectively.

Valid asymptotic expansions for the density matrix can now be obtained by introducing the asymptotic, WKB expansions, Eqs. (8) and (9), into Eq. (28). Then the terms whose smallness justifies the expansion for $G(n)$ in Eq. (24) are given to lowest order by

$$\begin{aligned}&\frac{\delta g}{g} \simeq \frac{\epsilon_0''}{\epsilon_0'} - \frac{\epsilon_0'}{4}[k_0^{-2}(\epsilon, x') + k_0^{-2}(\epsilon, x)], \\ &\delta^2 f_\pm \simeq \frac{d^2}{dn^2}(\xi_{0\pm}) \simeq \epsilon_0'\chi_{0\pm}(x', x) - \frac{\epsilon_0'}{2}\left(\frac{\chi_2}{k_0^2}\right)_\pm(x', x),\end{aligned} \tag{30}$$

where the quantities subscripted with + and − are obtained in the usual manner from

$$\xi_0(x) \equiv \int_p^x k_0(\epsilon, y)\, dy,$$

$$\chi_0(x) \equiv \frac{d\xi_0}{dx} = \frac{1}{2}\int_p^x \frac{dy}{k_0(\epsilon, y)},$$

$$\chi_2(x)/k_0^2(\epsilon, x) \equiv -2\frac{d\chi_0}{d\epsilon} = \lim_{\eta\to 0}\left\{\frac{1}{2}\int_{p+\eta}^x dy/k_0^3(\epsilon, y) - \frac{[-v'(p)]^{\frac{1}{2}}}{\eta^{\frac{1}{2}}}\right\}. \tag{31}$$

In Eqs. (30) the difference operators are replaced by differentiation with respect to n, indicated by primes, and the function $\epsilon_0(n)$ is defined by the second of Eqs. (9) in lowest order. The limiting process in $\chi_2(x)$ of (31) is required because of the divergence of the integrand in $\chi_0(x)$ near the classical turning point $p(\epsilon)$. According to Eq. (9), ϵ_0''/ϵ_0' contains an integral of the same type as in χ_2/k_0^2, and therefore both can be assumed to become $\ll 1$, something like k_0^{-2}, as $k_0 \to \infty$. This assumption seems to apply to most typical potentials with which one is concerned. Therefore, in first approximation, according to Eq. (23) only G_{0I} contributes in Eq. (29) to the density matrix; and

$$\pi\rho_N(x', x) \simeq \tfrac{1}{4}\left\{\frac{\epsilon_0'}{[k_0(\epsilon x')k_0(\epsilon x)]^{\frac{1}{2}}}\left[\frac{\sin\xi_{0-}(x', x)}{\sin(\frac{1}{2}\xi_{0-}')} - \frac{\cos\xi_{0+}(x', x)}{\sin(\frac{1}{2}\xi_{0+}')}\right]\right\}_{n=N+\frac{1}{2}}. \tag{32}$$

The first correction terms to (32) which contain the quantities (31) are shown in Table I as explained below, and higher-order terms can be generated using analogous arguments by inclusion of successively higher-order terms in Eqs. (8) and (24).

The above derivation can be modified to obtain an expansion for the particle density in spite of the previously mentioned difficulties, by taking the limit $\xi_{0-}(x', x) \to 0$ as $x' \to x$. When the WKB expansion for k^{-1} derived from Eq. (8),

$$k^{-1} = k_0^{-1}\left[1 - \frac{v''}{8k_0^4} - \frac{5v'^2 - v^{iv}}{32k_0^6} + \frac{16v''^2 + 28v'v''' - v^{vi}}{128k_0^8} + \cdots\right] \equiv k_0^{-1}\sum_{\nu=0} a_\nu k_0^{-2\nu} \tag{33}$$

is substituted in the E–M formula for the sum of the first terms on the right of Eq. (28), the result is, for $\xi_{n-} \to 0$,

$$\pi\sum_{n=N+1}^{M} g(n) = \left|\sum_{\nu=0}\frac{a_\nu k_0^{1-2\nu}}{1-2\nu} + \sum_{s=1}\frac{B_{2s}(\frac{1}{2})}{(2s)!}\frac{d^{2s-1}g}{dn^{2s-1}}\right|_{M+\frac{1}{2}}^{N+\frac{1}{2}} \equiv |\phi_n(x)|_{M+\frac{1}{2}}^{N+\frac{1}{2}}. \tag{34}$$

It is evident that under conditions similar to those discussed in connection with Eqs. (30), the right side of Eq. (34) defines an asymptotic expansion of the left side. For the plane-wave states at $n = M + \frac{1}{2}$, all terms in Eq. (34) proportional to derivatives of $g(n)$ vanish [see Eq. (15)]. An interesting equality for $\phi_n(x)$ follows to order k_0^{-4} from Eq. (33):

$$\phi_n(x) \simeq k_0(\epsilon_n, x) \simeq \lim_{x'\to x}\{\mathrm{Re}\,[e^{i\xi_{n-}}G_{0-}(n)]\} \tag{35}$$

when the leading minus term in the density matrix, Eq. (28), is evaluated with $k^2 \simeq k_0^2$ [see Eq. (25)]. Recalling that $G_-(M + \frac{1}{2}) \to G_{0-}(M + \frac{1}{2})$ for *all* values of x' and x as $M \to \infty$ we see that $\phi_n(x)$ can therefore replace the G_- terms in Eq. (29) and that the δ-function subtraction in Eq. (28) is still justified. The asymptotic expansion for the particle density is therefore finally given by

$$\pi\rho_N(x) = [\phi_n(x) - G_R(n, x)\cos 2\xi_n(x) + G_I(n, x)\sin 2\xi_n(x)]_{n=N+\frac{1}{2}}, \tag{36}$$

where

$$G(n, x) \equiv \lim_{x'\to x} G_+(n, x', x),$$

$\phi_n(x)$ is defined by Eq. (34), and $\xi_n(x)$ by Eq. (9).

A second interesting result of Eq. (35) is that if

TABLE I. First several terms in asymptotic expansion of the particle density $\pi\rho_N(x)/k_0(\epsilon_{N+\frac{1}{2}}, x)$ [Eq. (36)]. See text for definition and explanation of entries.

$\epsilon_0^{(n)} \to$ / k_0^{-2n}	const	ϵ_0'	ϵ_0''
Const	1	0	0
k_0^{-2}	0	$\dfrac{-\epsilon_0'\cos 2\xi_0}{4k_0^2\sin(\epsilon_0'\chi_0)}$	$\dfrac{-\epsilon_0''}{48k_0^3}\left\{1 - \dfrac{3\{2\cot(\epsilon_0'\chi_0) - \epsilon_0'\chi_0[2\cot^2(\epsilon_0'\chi_0)+1]\}\sin 2\xi_0}{\sin(\epsilon_0'\chi_0)}\right\}$
k_0^{-4}	$v''/24k_0^4$	$\dfrac{\epsilon_0'^2}{96k_0^4}\left\{1 - \dfrac{3\{2\cot(\epsilon_0'\chi_0) - \epsilon_0'\chi_0[2\cot^2(\epsilon_0'\chi_0)+1]\}\sin 2\xi_0}{\sin(\epsilon_0'\chi_0)}\right\}$	$\dfrac{-\epsilon_0''}{48k_0^3}\left\{1 + \dfrac{3(-1)^N\{2\tan(\epsilon_0'\chi_0) + \epsilon_0'\chi_0[2\tan^2(\epsilon_0'\chi_0)+1]\}\sin 2\xi_0}{\cos(\epsilon_0'\chi_0)}\right\}$
k_0^{-6}	$\dfrac{5v'^2 - v^{iv}}{160k_0^5}$	$\dfrac{\epsilon_0'^2}{96k_0^4}\left\{1 + \dfrac{3(-1)^N\{2\tan(\epsilon_0'\chi_0) + \epsilon_0'\chi_2[2\tan^2(\epsilon_0'\chi_0)+1]\}\sin 2\xi_0}{\cos(\epsilon_0'\chi_0)}\right\}$	$\dfrac{(-1)^{N+1}\epsilon_0'\cos 2\xi_0}{4k_0^2\cos(\epsilon_0'\chi_0)}$

$G_0(n)$ is a satisfactory approximation to $G(n)$ for large $x' - x$, Eq. (35) suggests that it may be used for *all* x' and x, or that Eq. (32) gives a satisfactory approximation to the density matrix for all spatial arguments. The particle density obtained in this approximation from Eq. (32) in the limit $x' \to x$ is

$$\pi\rho_N(x) = k_0(N+\tfrac{1}{2}, x)\left[1 - \frac{\epsilon_0' \cos 2\xi_0(x)}{4k_0^2(\epsilon, x)\sin(\epsilon_0'\chi_0)}\right]_{n=N+\frac{1}{2}}$$
$$\equiv \rho_N^{TF}(x) + \rho_N^{(1)}(x). \quad (37)$$

The E–M expansion used in deriving Eq. (36) can be readily generalized to cover a region of very small $x' - x$. Then the region not covered by either the asymptotic expansion (29) or (36) is, from Eq. (26), the region where $d^2f/dn^2 \sim (df/dn)^2$, which according to a WKB estimate corresponds to $x' - x \sim k_0^{-1}(N + \frac{1}{2}, x)$.

We can see the variety of types of asymptotic terms that contribute to the density matrix by examining the particle-density expansion Eq. (36). Table I lists the correction terms relative to the leading Thomas–Fermi term of unity, obtained from Eq. (36) through first-order terms of Eq. (24). All terms are understood to be evaluated at $n = N + \frac{1}{2}$ and the definitions in Eq. (31) are used. With respect to the squares above and to the left of the heavy line in the table, column two lists, in descending powers of k_0^2, the terms from the integral in the E–M formula for $\phi(n)$, the first term on the right side of Eq. (34). These terms describe the asymptotic series which had previously been obtained by formal methods.[2] In the third and fourth columns there are additional terms of oscillating and slowly varying character which are listed according to the highest derivative of $\epsilon_0(n)$ that they contain. The latter arise from the Bernoulli corrections in Eq. (34) and are of the same order of magnitude as the terms in the first column, while the former are greater in magnitude by a factor of k_0^2. The density-matrix expansion can be written to the same order from Table I as the difference of two terms each having the form of the oscillating terms in the table. Terms with quantities having a + subscript are to be subtracted from those having quantities with − subscripts where the subscripted quantities are defined by the substitutions [see Eq. (31)],

$$2\xi_0(x) \to \begin{cases}\xi_{0-}(x', x) - \tfrac{1}{2}\pi, \\ \xi_{0+}(x', x),\end{cases}$$

$$\frac{\chi_\nu(x)}{k_0^2} \to \begin{cases}\tfrac{1}{2}(\chi_\nu/k_0^2)_-(x', x), \\ \tfrac{1}{2}(\chi_\nu/k_0^2)_+(x', x),\end{cases} \quad \text{for } \nu = 0, 2.$$

All powers of $k_0(x)$ are to be evenly divided between the arguments x' and x.

COMPARISON WITH PARTICLE DENSITY FOR A QUADRATIC POTENTIAL

The quadratic potential provides a convenient example for numerical comparison, since closed expressions exist for the exact particle sums. If the potential $V(x)$ is written as $\frac{1}{2}Kx^2$, the energy parameters ϵ_n and the corresponding normalized wavefunctions, $\Psi_n(x)$, are[10]

$$\epsilon_n = (2n-1)\alpha^2, \quad n = 1, 2, \cdots, \quad \alpha^2 = (mK/\hbar^2)^{\frac{1}{2}},$$
$$\Psi_n(x) = \alpha^{\frac{1}{2}}U_n(\xi) = \frac{\alpha^{\frac{1}{2}}e^{-\xi^2/2}H_{n-1}(\xi)}{[\pi^{\frac{1}{2}}2^{n-1}(n-1)!]^{\frac{1}{2}}}, \quad \xi \equiv \alpha x. \quad (38)$$

The Christoffel–Darboux sum relation[11] for the Hermite polynomials $H_n(\xi)$ can be applied directly to the density matrix to obtain

$$\frac{\rho_N(x', x)}{\alpha} = \left(\frac{N}{2}\right)^{\frac{1}{2}} \frac{U_{N+1}(\xi')U_N(\xi) - U_N(\xi')U_{N+1}(\xi)}{\xi' - \xi}. \quad (39)$$

With the standard differential and difference relations for Hermite polynomials, the particle density obtained from (39) can be expressed in either of two forms

$$\frac{\rho_N(x)}{\alpha} = \begin{cases}NU_N^2(\xi) - [N(N-1)]^{\frac{1}{2}}U_{N+1}(\xi)U_{N-1}(\xi), \\ NU_{N+1}^2(\xi) - [N(N+1)]^{\frac{1}{2}}U_{N+2}(\xi)U_N(\xi).\end{cases} \quad (40)$$

A numerical comparison of Eqs. (39) and (40) is made with the approximate formulas of the last

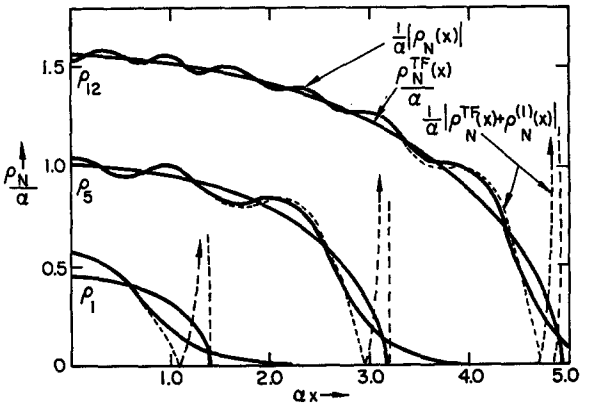

FIG. 2. Comparison of particle density $\rho_N(x)$ for quadratic potential with T–F density and with Eq. (37) for $N = 1$, 5, and 12.

[10] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), Chap. 4.

[11] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (Dover Publications, New York, 1965), Chap. 22.

section in Figs. 2 through 5 for several values of N. In Fig. 2 the exact particle density is compared with the zero-order Thomas–Fermi density and the first corrected density given, respectively, by the first and the combined terms of Eq. (37). In these calculations, we have used an alternative form for the density corrections that is convenient for a one-dimensional potential which is symmetrical about the origin. In this form the phase integrals ξ_0, χ_0, and χ_2 are integrated from the origin to x instead of from a classical turning point [see Eq. (36)]. In Table I, these alternative forms are listed to the right and below the heavy line and can be identified with the corresponding terms in the upper left part of the table by the first coefficients.

The agreement in Fig. 2 is excellent except within a phase of about 1 rad away from the classical turning point, where the Thomas–Fermi density vanishes. Because they are too small to judge in Fig. 2, the differences between Eqs. (37) and (40) are plotted in Figs. 3 and 4. In Fig. 3, the x dependence of the difference is compared with the next correction terms in the fourth row of Table I for $N = 5$ and 12. Since $\epsilon_0'^2/\alpha^4 = 2v''/\alpha^4 = 4$ and $\epsilon_0'' = 0$, these corrections are simply

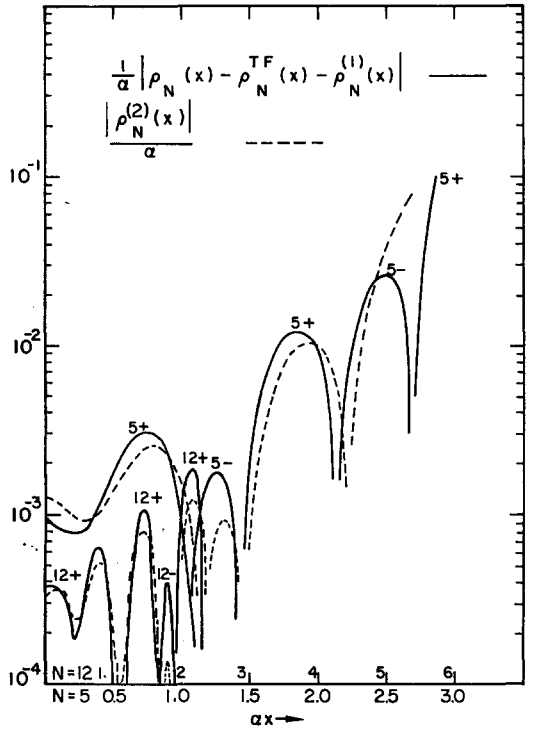

FIG. 3. Comparison of the x distribution of errors in the approximate particle density given by Eq. (37) with the second-order correction, Eq. (42), for the quadratic potential for $N = 5$ and 12. The traces are identified by the value of N and the sign of the error.

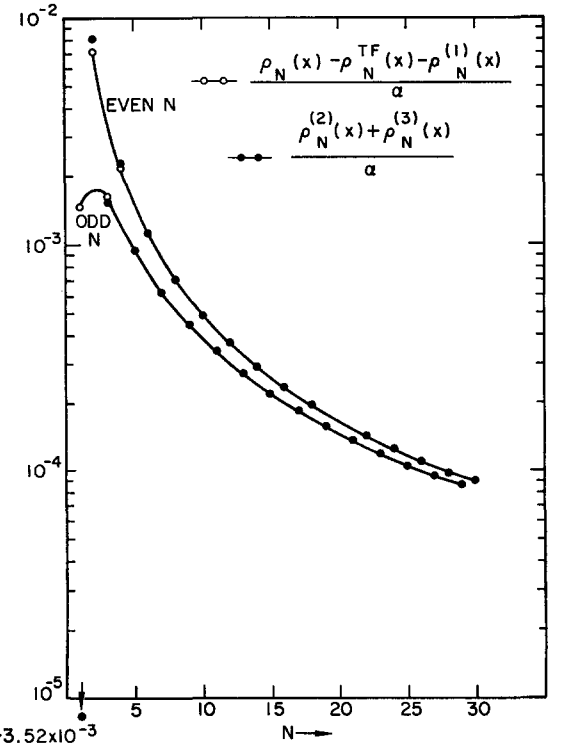

FIG. 4. Comparison of the N-dependence of the errors in Eq. (37) at the origin with the second- and third-order corrections, Eq. (43).

$$\rho_N^{(2)} = \left|\frac{1}{8k_0^3} + (-1)^N \times \frac{[\tan 2\chi_0 + \chi_2(2\tan^2 2\chi_0 + 1)]\sin 2\xi_0}{4k_0^3 \cos 2\chi_0}\right|_{x=N+\frac{1}{2}}. \quad (41)$$

As is evident in the case of $N = 5$, a substantial portion of the error contained in Eq. (37) is accounted for by Eq. (41) except near the boundary. $N = 5$ is apparently not large enough for the asymptotic correction (41) to be useful within the last cycle of oscillation. Near the center, however, the correction for $N = 12$ appears to be improving.

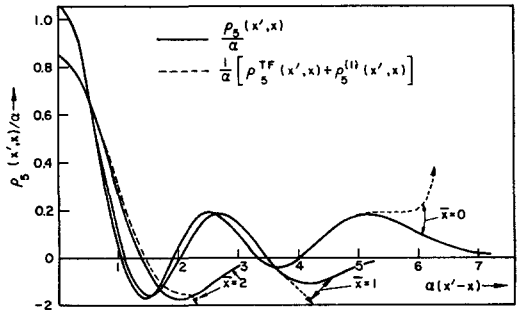

FIG. 5. Comparison of the dependence of $\rho_N(x', x)$, Eq. (32), on $x' - x$ for several values of $\bar{x} \equiv x + \frac{1}{2}x'$ with the exact density matrix for the quadratic potential.

This is shown more clearly in Fig. 4 where the *next two* higher-order correction terms to (37) are calculated at $x = 0$ as a function of N and compared with $\rho_N(0) - \rho_N^{(1)}(0)$. The number of terms contributing in this order to the particle-density expansion is much less than for nonzero x:

$$\rho_N^{(2)}(0) + \rho_N^{(3)}(0) = \frac{1}{8\pi}\left[\frac{1}{(2N)^{3/2}} + \frac{5(-1)^N}{2(2N)^{5/2}}\right]. \quad (42)$$

Except for $N = 1$ the corrections (42) appear to be useful at the origin. In Fig. 5 the suggested approximation, Eq. (32), for the entire density matrix for $N = 5$ compares similarly with Eq. (39) at several values of $\frac{1}{2}(x + x')$.

It is to be emphasized that next-higher-order corrections to an approximation consisting of the first several terms of the density expansion do not necessarily improve the approximation, because of the asymptotic nature of this expansion. However, they should be useful in estimating the order of magnitude of the error made in the approximation.

The first expansions of the particle density mentioned in the Introduction are seen to be inadequate. The operator expansion method[2] gives rise only to terms in the first column of Table I, in which the first correction to the leading term is seen to be of order k_0^{-4}. The omission of the remaining terms, which contain the derivatives $\epsilon_0(n)$, is apparently the result of a poorly converging expansion, involving local derivatives of the potential. Since $\epsilon_0(n)$ and its derivatives are determined by an integral condition in Eq. (9), therefore its effects on $\rho_N(x)$ could not be accurately included unless the expansion converged in good approximation over the whole range of the wavefunctions. In later work both Alfred and Macke and Rennert[4] have partially remedied this defect, but their results for the density are difficult to evaluate numerically. More seriously, however, the asymptotic form of their oscillating component for large k_0 vanishes as k_0^{-1} instead of as k_0^{-2}. In the most recent work[5] the derived particle density is apparently equivalent to Eq. (37) in the classical region of the Nth state, although Eq. (37) is the simpler to evaluate. Higher-order corrections were not investigated by these authors. However, in their work, formulas for the particle density are developed that can also be approximated in and outside the region of the classical turning point. In addition, Kohn and Sham apply their approximate Green's function method to a number of additional quantum problems of interest.

Approximations such as (32) and (37) to the density matrix have many attractive properties, at least for theoretical calculations in plane symmetry. In the first place they do not require integrations over n as does the E–M approximation, but rather contain only quantities appearing in the wavefunction of the highest occupied state or their derivatives. In addition, the evaluation of the expectation values of one-particle operators from sums like Eq. (1) generally involves only one or two integrations. Most importantly, Eqs. (32) and (37) are written as functionals of an arbitrary potential $v(x)$. This permits the approximations to be used readily in a Hartree–Fock model for systems of interacting particles. In such calculations the value of $\epsilon_0'(n)$ necessary to evaluate the effects of the oscillating component in the density matrix can be consistently calculated with the zero-order or Thomas–Fermi particle density together with Eq. (9). It remains to be seen how much these advantages can be exploited in more realistic spherical systems to which Hartree–Fock theory is usually applied.

The Solution of the Nonrelativistic Quantum Scattering Problem without Exchange

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The method of "*amplitude density functions*" is a new formalism which allows a scattering problem to be broken up into problems with weaker interaction potentials. These simpler problems may be solved separately and be "added" together to give the total solution. A numerical method is discussed which takes advantage of this property. The formulas are given for the use of this method in the solution of the one-dimensional atom–molecule collision and the e^+–H collision. A numerical example is discussed.

1. INTRODUCTION

In this paper we discuss the solution of the nonrelativistic quantum mechanical scattering problem. We limit our discussion to the problem of nonrearrangement collisions.

The problem is cast in the form of an integral equation whose solution gives all of the information sought in a scattering problem. This method allows a scattering problem to be broken down into a number of scattering problems with weaker interactions which may be solved independently and be "added" together. We discuss in detail a numerical method of solution which is well-adapted to high-speed digital computers.

Two examples are discussed. The simplest example we consider is the colinear collision of an atom with a diatomic molecule. This problem has been much discussed in the past.[1] As a second example, we give the pertinent equations for the solution of the positron–hydrogen-atom scattering problem.[2]

[1] K. Takayanagi, Progr. Theoret. Phys. (Kyoto) Suppl. **25**, 1 (1963). This is a review article in which this problem is discussed with extensive references to earlier work. Some notable recent papers not included in this review are C. E. Treanor, J. Chem. Phys. **43**, 532 (1965); T. E. Sharp and D. Rapp, J. Chem. Phys. **43**, 1233 (1965); F. H. Mies, J. Chem. Phys. **42**, 2709 (1965), *ibid.* **41**, 903 (1964), *ibid.* **40**, 532 (1964); H. K. Shin, *ibid.* **41**, 2864 (1964); D. Rapp, *ibid.* **40**, 2813 (1964); D. Rapp, in *Atomic Collision Process*, M. R. C. McDowell, Ed., (North-Holland Publishing Company, Amsterdam, 1964), p. 1096.

[2] P. G. Burke and Kenneth Smith, Rev. Mod. Phys. **34**, 458 (1962). This is a review article in which this problem is discussed with references to earlier work. Some recent works not discussed in the review are P. G. Burke, H. M. Schey, and K. Smith, Phys. Rev. **129**, 1258 (1963); Y. Hahn, T. F. O'Malley, and L. Spruch, in *Atomic Collision Processes*, M. R. C. McDowell, Ed., (North-Holland Publishing Company, Amsterdam, 1964), p. 312; W. J. Cody, J. Lawson, Sir H. Massey, and K. Smith, Proc. Roy. Soc. (London) **278A**, 479 (1964); R. J. Drachman, Phys. Rev. **138**, A1582 (1965); R. P. McEachran and P. A. Fraser, Proc. Phys. Soc. (London) **86**, 369 (1965); Y. Hahn and L. Spruch, Phys. Rev. **140**, A18 (1965); C. J. Kleinman, Y. Hahn and L. Spruch, *ibid.* **140**, A413 (1965).

2. THE AMPLITUDE DENSITY FUNCTION

For scattering problems in which no rearrangement is involved, the Schrödinger equation may be written as

$$[H^1(r) + H^2(r, \mathbf{x}) + V(r, \mathbf{x}) - E]\Psi = 0. \quad (1)$$

Here H^1 depends only on one variable, which is related to the separation between the systems, and H^2 contains all of the rest of the coördinates. The interaction potential $V(r, \mathbf{x})$ is such that it vanishes[3] faster than $1/r$ for large r. For large r the solutions of Eq. (1) have the forms

$$\psi^{i+} = \phi_i(\mathbf{x})n_i(r) \quad (2)$$

and

$$\psi^{i-} = \phi_i(\mathbf{x})m_i(r), \quad (3)$$

where ϕ_i is an eigenfunction of

$$H^2(r, \mathbf{x})\phi_i(\mathbf{x}) = E_i^2(r)\phi_i(\mathbf{x}), \quad (4)$$

and n_i and m_i are independent solutions to the equation

$$[H^1(r) + E_i^2(r) - E]R = 0. \quad (5)$$

The ψ^{i+} are referred to as outgoing waves and ψ^{i-} as incoming waves. The Schrödinger equation, (1), may be written in the form of an integral equation,[4]

$$\Psi(r, \mathbf{x}) = \Phi(r, \mathbf{x}) - \iint g^1G(r, \mathbf{x}; r', \mathbf{x}')V(r', \mathbf{x}')\Psi(r', \mathbf{x}')\, d\mathbf{x}'\, dr', \quad (6)$$

[3] This is not a serious restriction, since potentials which die off as the reciprocal of the separation may be included in H^1. For example, if one is considering the scattering of a positron from a singly charged positive He^+ ion, he may take H^1 to be the radial Hamiltonian for a positron–proton scattering and H^2 to consist of the H-atom Hamiltonian and the angular part of the coulomb scattering problem. Then V is the remainder of the positron He nucleus repulsion and the positron–electron attraction.

[4] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), pp. 828–833.

where $\Phi(r, \mathbf{x})$ is the initial incoming wave, g is the determinant of the metric tensor, and $G(r, \mathbf{x}; r', \mathbf{x}')$ is a Green's function given by

$$G(r, \mathbf{x}; r', \mathbf{x}') = \sum_i c_i \phi_i^*(\mathbf{x}) \phi_i(\mathbf{x}) n_i(r_>) m_i(r_<). \quad (7)$$

The constants c_i are normalizing constants. The ϕ_i are the eigenfunctions of Eq. (4). In general, they may include a continuum in which case the sum in Eq. (7) must be understood to indicate a sum over discrete states and an integral over the continuum. The notation $r_<$ indicates the lesser of r and r', and $r_>$ is the greater of these two variables.

Let us define a function which we refer to as an "*amplitude density function,*"

$$F_n(r) = \int g^{\frac{1}{2}} \phi_n^*(\mathbf{x}) V(r, \mathbf{x}) \Psi(r, \mathbf{x}) \, d\mathbf{x}, \quad (8)$$

where the asterisk indicates complex conjugation. This function has certain interesting and useful properties. It vanishes on any interval of the r axis for which $V(r, \mathbf{x})$ vanishes for all values of $\mathbf{x}$. It also vanishes for those values of r for which Ψ vanishes.

Equation (6) may be written

$$\Psi(r, \mathbf{x}) = \Phi(r, \mathbf{x}) - \int \sum_i c_i \phi_i(\mathbf{x}) n_i(r_>) m_i(r_<) F_i(r') \, dr'. \quad (9)$$

As r approaches infinity, V approaches zero and therefore so does F_i. In this limit $r' < r$ in the integral of Eq. (9) and it follows that the asymptotic form of the wavefunction is

$$\Psi(r, \mathbf{x}) = \Phi(r, \mathbf{x}) - \sum_i c_i \phi_i(\mathbf{x}) n_i(r) \times \int m_i(r') F_i(r') \, dr' \quad (10)$$

$$= \Phi(r, \mathbf{x}) - \sum_i R_i \phi_i(\mathbf{x}) n_i(r),$$

where

$$R_i = \int c_i m_i(r) F_i(r) \, dr. \quad (11)$$

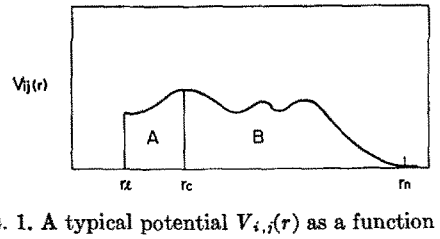

FIG. 1. A typical potential $V_{i,j}(r)$ as a function of r.

The second term on the right of Eq. (10) is the scattered wave. The R_i completely define the asymptotic solution to the problem. They may be easily computed when we know the "*amplitude densities,*" F.

We may obtain an integral equation for the $F_i(r)$ by substituting Eq. (9) into Eq. (8) to obtain

$$F_n(r) = \tilde{V}_n(r) - \int \sum_i V_{ni}(r) c_i m_i(r_<) n_i(r_>) F_i(r') \, dr', \quad (12)$$

where

$$V_{ni}(r) = \int g^{\frac{1}{2}} \phi_n^*(\mathbf{x}) V(r, \mathbf{x}) \phi_i(\mathbf{x}) \, d\mathbf{x} \quad (13)$$

and $\tilde{V}_n(r)$ is defined similarly with Φ in place of ϕ_i.

The problem consists of solving this one-dimensional infinite system of coupled linear integral Eqs. (12). Since $F_n(r)$ vanish in any region where the potential vanishes, it is possible to break up the potential into two or more parts and solve the problem for each part independently. Then the total solution can be obtained as a linear combination of complete sets of these partial solutions. This solution by parts is discussed in the following section.

3. SOLVING THE INTEGRAL EQUATION BY PARTS

Let us assume that the $V_{i,j}(r)$ are nonzero only over a finite interval $[r_l, r_h]$ for all i and j. Figure 1 is a plot of a typical potential $V_{i,j}(r)$. Let us arbitrarily break all of the $V_{i,j}(r)$ into two parts $V_{i,j}^A(r)$ and $V_{i,j}^B(r)$ such that,

$$V_{i,j}^A(r) = 0, \quad r > r_c, \quad (14)$$

$$V_{i,j}^B(r) = 0, \quad r \leq r_c, \quad (15)$$

and

$$V_{i,j}(r) = V_{i,j}^A(r) + V_{i,j}^B(r), \quad (16)$$

where A is the set of points r in the interval $[r_l, r_c)$ and B is the set $[r_c, r_h]$. Let us define a complete set of functions $F_n^{Ai+}(r)$ as the solutions to the equations,

$$F_n^{Ai+}(r) = V_{n,i}^A(r) n_i(r) - \int \sum_j V_{n,j}^A(r) c_i m_i(r_<) n_i(r_>) F_i^{Ai+}(r') \, dr'. \quad (17)$$

The $V_{n,i}^A(r) n_i(r)$ corresponds to a particular incident wave. We label F with the superscript A and $i+$ to indicate that this is the amplitude density for the potential V^A when the incident wave is an outgoing wave with the system in state i. We may define F_n^{Ai-} with an equation similar to

Eq. (17) but with m_i in place of n_i in the first term on the right of Eq. (17). This gives us a complete set of F_n^A functions. We may expand any F_n function for scattering from the potential V^A in terms of these F_n^{Ai+} and F_n^{Ai-}. We may define a similar set for the potential V^B.

A set of $F_n^{i+}(r)$ for the complete potential may now be obtained as a linear combination of those for V^A and V^B in the form,

$$F_n^{i+}(r) = F_n^{Ai+}(r) + F_n^{Bi+}(r) + \sum_j [a_j^{i+}F_n^{Aj-}(r) + b_j^{i+}F_n^{Bj+}(r)]. \quad (18)$$

This may be easily verified by direct substitution of this expression into Eq. (12), and using the property of the *"amplitude density"*, such that, when $r \in A$, $F_l^{Bk}(r)$ is zero and, when $r \in B$, $F_l^{Ak}(r)$ is zero. Upon performing this substitution and letting $r \in A$, one obtains

$$a_j^{i+} = -\sum_l b_l^{i+}R_j^{Bl+} - R_j^{Bi+}, \quad (19)$$

and letting $r \in B$ and using Eq. (19) to eliminate a_j^{i+},

$$b_j^{i+} = \sum_l b_l^{i+} \sum_k R_k^{Bl+}R_j^{Ak-} + \sum_k R_k^{Bi+}R_j^{Ak-} - T_j^{Ai+}. \quad (20)$$

Similarly,

$$a_j^{i-} = -\sum_l b_l^{i-}R_j^{Bl+} - T_j^{Bi-} \quad (21)$$

and

$$b_j^{i-} = \sum_l b_l^{i-} \sum_k R_k^{Bl+}R_j^{Ak-} + \sum_k T_k^{Bi-}R_j^{Ak-} - R_j^{Ai-}. \quad (22)$$

Here

$$R_j^{i+} = \int c_i n_i(r)F_j^{i+}(r)\,dr, \quad (23)$$

$$R_j^{i-} = \int c_i m_i(r)F_j^{i-}(r)\,dr, \quad (24)$$

$$T_j^{i+} = \int c_i m_i(r)F_j^{i+}(r)\,dr, \quad (25)$$

and

$$T_j^{i-} = \int c_i n_i(r)F_j^{i-}(r)\,dr. \quad (26)$$

The physical interpretation of these quantities is very simple. In a one-dimensional scattering problem, one may consider m_i to be a wave moving from right to left and n_i to be a wave moving in the opposite direction. In a three-dimensional problem, this must be modified a bit. If r is the radial distance to a scattering center, then assuming that $V_{i,j}(r)$ is nonzero only over an interval of r is to assume that $V(r, \mathbf{x})$ is nonvanishing on a spherical shell. $m_i(r)$ can then be thought of as an incoming spherical wave and $n_i(r)$ as an outgoing spherical wave.

The R_i^{Bl+} is a reflection coefficient for waves in state l coming from the left being reflected in the state i by $V(B)$, or, in the three-dimensional case, it may be thought of as the reflection coefficient for an outgoing wave originating inside of the spherical shell in state l being reflected back in the state i by the shell B.

The T_i^{Bl+} is a transmission coefficient for a wave in state l traveling to the right (or outgoing) being transmitted through the barrier $V(B)$ in state i.

The coefficient a_j^{i+} is the amplitude of all waves in state j impinging on $V(A)$ from the right (or outside) and b_j^{i+} is the amplitude of all waves in state j impinging on $V(B)$ from the left (or inside). Thus, the a's account for all waves striking $V(A)$ from $V(B)$ and the b's account for the waves striking $V(B)$ from $V(A)$. The superscript on the a and b indicate that these quantities depend on the initial wave. Thus Eq. (21) tells us that the waves in state j striking $V(A)$ from the right are those initially in state i reflected from $V(B)$ in state j plus all waves striking $V(B)$ from the left and reflected back in state j. Equation (22) says that state-i waves striking $V(B)$ from the left are state-i waves transmitted by $V(A)$ in state-j plus the state-i wave reflected in all states and reflected back in state j plus all waves in any state which were reflected from $V(B)$ and re-reflected from $V(A)$ in state j. The system of equations, (21) and (22) contain implicitly the multiple reflections between $V(A)$ and $V(B)$ of all orders.

The total reflection coefficient R_i^{i+} is obtained by substituting Eq. (18) into Eq. (23) to give

$$R_j^{i+} = R_j^{Ai+} + R_j^{Bi+} + \sum_l (a_l^{i+}T_j^{Al-} + b_l^{i+}R_j^{Bl+}). \quad (27)$$

This equation says that the scattered wave moving to the left is the sum of that scattered by $V(A)$ and $V(B)$ from the initial wave plus all transmitted waves striking $V(A)$ from the right, and all reflected waves striking $V(B)$ from the left. The reflection coefficient R_i^{i-} is computed from an equation similar to Eq. (27), but with the + signs replaced by − signs on the first two terms on the right and on a and b in the sum. Also, the T_j^{Al-} in the sum must be replaced by R_j^{Al-}, and R_j^{Bl+} must be replaced

by T_j^{Bi+}. The transmission coefficients, T_j^i, are computed by similar equations.

Thus, if we can solve the problem for each of the fragmentary potentials, then we may add the solutions together to obtain a total solution. The sum in Eq. (27) is an infinite sum, however, the a_j^{i+} corresponding to high virtual excitations is small, and we can terminate the sum at some large value of j. Then the system of equations, (22), becomes a finite system which may be solved by matrix inversion methods. If the region in which $V(B)$ is nonzero is made narrow enough, the iterated Born approximation for $F_n^{Bi+}(r)$ converges.[5] By breaking $V_{i,j}(r)$ into small enough regions, we could solve them each by the iterated Born approximation and then combine the results to obtain the final solution.

4. A NUMERICAL METHOD

The method of "*amplitude density functions*" is especially amenable to solution by numerical methods. A well-known approximation used in solving integral equations is to replace the integral in the equation by a quadrature sum. Then a linear integral equation is transformed into a matrix equation which may, in principle, be solved by matrix-inversion techniques. Thus we might replace Eq. (12) by the discrete system of equations,

$$F_n^{k+}(r_i) = V_{n,k}(r_i)n_k(r_i) - \sum_p \sum_j W_p V_{n,j}(r_i)c_j m_j(r_<)n_j(r_>)F_j^{k+}(r_p), \quad (28)$$

where W_p and r_p are the weights and points, respectively, of a quadrature formula. Probably the best quadrature formula to use here is the repeated trapezoid rule (see note added in proof). It has been shown that, for integrating functions with discontinuous first derivatives, the repeated trapezoid rule has the smallest maximum error.[6] We have used both the trapezoid rule and Simpson's rule on a test problem for which we know the answer, and both methods give essentially the same result. The trapezoid rule does seem to be slightly better in the examples we have tried when the step size is large, but Simpson's was better for small step size.

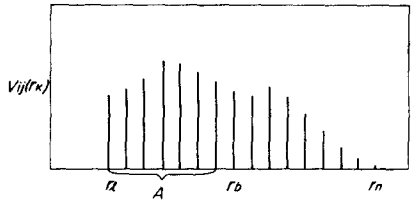

FIG. 2. A typical discrete potential $V_{i,j}$.

The sum over j in Eq. (28), of course, is infinite and, before there is any hope of solving such a system, it is necessary to truncate this sum at some reasonably high value. If, for example, we truncate the j sum at 10 and carry 50 points in the numerical integration, we might hope to get a reasonably accurate solution to the integral equation. Such a system contains 500 unknowns. The inversion of a matrix of this size is no small task and, for the modest accuracy which we would obtain with this number of quadrature points, this method is completely impractical. Equation (28) may be solved by a much simpler method, similar to that of the last section. This equation has the same property as its continuous analog, Eq. (12), of being soluble by parts.

If we assume that we have solved Eq. (28) for a subset of points in the integral sum,[7] we may add the next point by a method similar to that of the last section. Let A be a set of points for which the solution of Eq. (28) is known. That is to say, we have solved this equation in which the sum over p has been arbitrarily truncated before including the point r_b in Fig. 2. Figure 2 represents a typical $V_{i,j}$ in the discrete representation of Eq. (28). Then we call $F_n^{Ak+}(r_i)$ the solution of Eq. (28) with the sum over p terminated with the point r_{b-1}. The region B is taken to consist of only one point r_b, thus F_n^{Bk+} is given by

$$F_n^{Bk+} = V_{n,k}(r_b)n_k(r_b) - \sum_j W_b V_{n,j}(r_b)c_j m_j(r_b)n_j(r_b)F_j^{Bk+}. \quad (29)$$

We would have to solve a similar system of equations for F_n^{Bk-}. Here we can achieve a considerable simplification by solving, instead of two systems, the single system

$$A_n^{bk} = V_{n,k}(r_b) - \sum_j W_b V_{n,j}(r_b)c_j m_j(r_b)n_j(r_b)A_j^{bk}. \quad (30)$$

Then

$$F_n^{Bk+} = A_n^{bk}n_k(r_b) \quad (31)$$

and

$$F_n^{Bk-} = A_n^{bk}m_k(r_b). \quad (32)$$

Equation (30) is very simply solved, since it requires the equivalent of the inversion of a matrix of an

[5] W. Kohn, Rev. Mod. Phys. 26, 292 (1954).
[6] D. Secrest, J. SIAM Numer. Anal. 2, 52 (1965).

[7] We note that, if only a subset of points in the integral sum are retained, the sum no longer necessarily approximates an integral. Thus, the intermediate problems are not approximations to the continuous intermediate problem.

order depending only on the number of states j retained in the sum. If we retain N states then the matrix of coefficients is of order N and the matrix of free terms, $V_{n,k}(r_b)$, is of order N. Thus the solution is equivalent to the inversion of an $N \times N$ matrix and gives the $N \times N$ solution matrix, A_n^{bk}.

The transmission and reflection coefficients T^B and R^B are given by

$$T_j^{Bi+} = W_b c_j m_j(r_b) A_j^{bi} n_i(r_b), \tag{33}$$

$$T_j^{Bi-} = W_b c_j n_j(r_b) A_j^{bi} m_i(r_b), \tag{34}$$

$$R_j^{Bi+} = W_b c_j n_j(r_b) A_j^{bi} n_i(r_b), \tag{35}$$

and

$$R_j^{Bi-} = W_b c_j m_j(r_b) A_j^{bi} m_i(r_b). \tag{36}$$

The coefficients a_j^i and b_j^i can now be determined by Eqs. (20), (19), (22), and (21). The b_j^i coefficients are obtained from Eqs. (20) and (22) by the inversion of an $N \times N$ matrix. The a_j^i are readily computed once the b_j^i are known. The total reflection coefficient for the set of points $A + b$ is obtained from Eq. (27). The R_j^i obtained in this way may now be labeled R_j^{Ai} and we may proceed to add the next point. Thus, at each point, it is necessary to solve the two $N \times N$ systems, Eqs. (30) and (20). This is the equivalent in computational effort of inverting two $N \times N$ matrices. The intermediate R_j^i are not in general approximations to the corresponding continuous problem, since the truncated integral sum may not approximate the integral. The final R_j^i is exactly the quantity one would obtain if he solved Eq. (28) and integrated the F_j^i using the quadrature sum to obtain the R_j^i. The computational effort, however, is much reduced. We are not limited mechanically, in the number of points used in the numerical quadrature as we would be if the integral equation in discrete form, Eq. (28), were solved directly. Furthermore, if we double the number of quadrature points used, we double the computation time. If, on the other hand, we were solving Eq. (28) directly, doubling the number of quadrature points increases the computation time by a factor of 8. That is to say, the solution time depends linearly on the number of integration points used in the method of *"amplitude density functions"*, whereas it depends on the cube of the number of points used when the integral equation is solved by the direct inversion of the matrix, Eq. (28). We do not actually solve Eq. (28), but we determine the R_j^i and the T_j^i directly. Since these are the quantities of physical interest, it is never necessary to compute the F_j^i.

The first point is, of course, a special case. When A consists of only the first point, we may compute the R_j^{Ai} and the T_j^{Ai} by Eqs. (30), and (33)–(36).

To illustrate the usefulness of this method, we derive the equations for a few simple examples in the next two sections and discuss a numerical example.

5. THE COLLISION OF AN ATOM WITH A DIATOMIC MOLECULE

The simplest inelastic scattering problem which can be considered is that of a structureless particle colliding with a molecule with one degree of freedom. Such a simple system is difficult to find in nature. Two models which have been considered in the literature over the past few years do exhibit these properties.[1,8] One model is the collision of an atom, considered to be structureless, with a diatomic molecule constrained in such a way that all three nuclei lie in a straight line. The two bound atoms of the molecule interact with a particular potential and the scattered atom interacts with the molecule with another potential. The simplest case of scattering of this type is encountered when no reaction is permitted to take place, as in the low-energy collision of an inert-gas atom with a diatomic molecule. It can easily be shown that this problem is equivalent to the collision of a free particle with a particle bound to an equilibrium position. Figure 3 is a schematic diagram of this problem. Another problem of the same degree of complexity is the collision of an atom with a homonuclear diatomic molecule in which the atom approaches the center of mass of the molecule at an angle of 90° with the internuclear axis. The coördinates for this example are shown in Fig. 4. The Hamiltonian for each of these problems in dimensionless coördinates is

$$H = -\frac{1}{m}\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V_M(y) + V(x, y), \tag{37}$$

where m is a ratio of reduced masses, $V_M(y)$ is

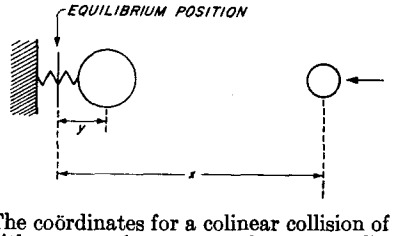

FIG. 3. The coördinates for a colinear collision of a diatomic molecule with an atom in a center-of-mass coördinate system.

[8] I. Korobkin and Z. I. Slawsky, J. Chem. Phys. **37**, 226 (1962).

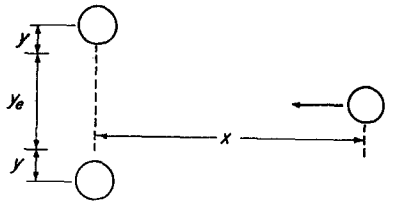

FIG. 4. The coördinates for the collision of an atom with the center of mass of a homonuclear diatomic molecule for which the internuclear axis is constrained to remain at an angle of 90° with respect to the direction of collision.

the internal potential energy of the molecule, and $V(x, y)$ is the interaction potential.

First we must solve the Schrödinger equation for internal structure which, in this case, depends only on the y coördinate. For illustrative purposes, we assume that the molecular potential is represented sufficiently accurately by a harmonic oscillator potential. The Schrödinger equation for the molecule is then

$$-\frac{\partial^2}{\partial y^2}\phi_n + y^2\phi_n = E_n\phi_n. \tag{38}$$

We can write down the solution to this problem immediately,

$$\phi_n = H_n, \tag{39}$$

the Hermite functions, and

$$E_n = 2n + 1. \tag{40}$$

The free waves are

$$n_n(x) = e^{ip_n x} \tag{41}$$

and

$$m_n(x) = e^{-ip_n x}. \tag{42}$$

Here, p_n is given by

$$p_n = [m(E - 2n - 1)]^{\frac{1}{2}}. \tag{43}$$

The Green's function is given by

$$G(x, y; x', y') = -\sum_{n=0}^{\infty} mH_n(y')H_n(y)e^{ip_n|x'-x|}/2ip_n. \tag{44}$$

If we wish to solve the scattering problem for which the oscillator is initially in the state I, and the scattered particle is approaching from the right, the initial wave is

$$\Phi = H_I(y)e^{-ip_I x}. \tag{45}$$

The integral equation we wish to solve is Eq. (6), where, in this case, $g^{\frac{1}{2}}$ is 1, dx is dy and dr is dx. Which of the two problems, Fig. 3 or Fig. 4, we are discussing depends only on the form of the potential $V(x, y)$.

We determine the $V_{i,j}(x)$ according to Eq. (13). These integrals must be computed numerically unless $V(x, y)$ is a very simple function. After the integrals in Eq. (13) have been evaluated at a few representative points, we get some idea how many excited states of the oscillator must be retained. The integral over x' in Eq. (12) extends from $-\infty$ to ∞. However, the potential $V_{i,j}(x')$ is negligible over part of this range and Ψ may be zero over part of the range so that F_i^j is of significant size only over a finite range. Thus, the sum in Eq. (28) may be taken over only a finite number of points. At each point in the sum over p we must solve the system of equations, (30), for all n and k. Here c_i is $-m/(2ip_i)$. The integration weight W_p depends on what integration formula we are using. The R_i^{Bk} and T_i^{Bk} can then be determined by Eqs. (33)–(36).

The total R_n^k and T_n^k at each step are computed by formulas similar to Eq. (27). The R_n^{k-} computed on the last step are the sought solutions to the problem. *We notice that, for this problem, it is never necessary to compute R_n^{k+} or T_n^{k+} at any point in the calculation, since they are never needed.* Similarly, a_i^{i+} and b_i^{i+} are not needed in this problem, since, only the $-$ superscript is of interest. It is necessary, however, to compute R_n^{Bk} and T_n^{Bk} with both $+$ and $-$ superscripts. The total T_n^{k-} computed on the last step is the transmission coefficient. This is of interest in the problem diagrammed in Fig. 4 for which the particle approaches at an angle of 90° to the molecule axis. For the colinear collision, Fig. 3, T_n^{k-} should be zero and need not be computed, although it takes little extra work to carry it through the computation as a check.

In order to test the feasibility of this method, we have computed the solution to a problem for which a solution is known by other methods. Very few problems of this sort have been solved. The solution to the colinear scattering problem [see Fig. (3)] by Shuler and Zwanzig[9] was chosen as an example for comparison purposes. The problem was solved by Shuler and Zwanzig for a rigid-sphere interaction between the atom and the molecule. The potential $V(x, y)$ was taken zero for x greater than y and infinite for x less than or equal to y. This is not an ideal example on which to test the method described here, as we are unable to handle infinite potentials. Therefore, we chose to solve

[9] K. E. Shuler and R. Zwanzig, J. Chem. Phys. **33**, 1778 (1960).

the problem similar to this, but for which the infinite step is replaced by a large finite one. Taking the zero-point energy of the harmonic oscillator as the unit of energy, we chose a step 25 units high. That is, $V(x, y)$ is zero for x greater than y and 25 for x less than or equal to y. A few calculations were carrried out with a step of 100 energy units but no significant change in the results was detected. The potentials $V_{i,j}(x)$ have a finite extension in the positive x direction [i.e., $V_{i,j}(x)$ goes to zero sufficiently rapidly as x approaches infinity], but the extent is infinite in the negative x direction. Since $F_i^{Ak}(x)$ is not computed, it was necessary to compute T_i^{Ak-} in order to determine how far the integration should be carried in the minus x direction. Simpson's rule was used as the quadrature formula in the integral equation, and also for the computation of the $V_{i,j}(x)$. It was found that if two closed channels were carried in the Green's function for this problem the solution was correct to two decimal places. The addition of more excited states effected the answer only in the third decimal place. Since we used various values of total energy E in the range 3 to 10 energy units (the zero point energy of the oscillator being the unit of energy) there were never more than five open channels so it was not necessary to carry more than seven oscillator states in the calculation. Thus, in the solution of the problem, it was necessary to solve two 7×7 systems of equations at each point. Each system had a 7×7 matrix of free terms (or constants) so the work involved was the same as that for the inversion of two 7×7 matrices. The agreement with the results of Shuler and Zwanzig was very good. We agree perfectly at low energies insofar as their results can be read from the graphs in their paper.[9] In order to see how good the agreement was, we repeated their calculation. At the high-energy end of the graph there is a slight discrepancy, which is probably due to the fact that we are using a finite barrier of 25 units while in the Shuler and Zwanzig problem the barrier is infinite. It was found necessary at times to carry 20 oscillator states when using the method of Shuler and Zwanzig to obtain a good result, while by the method of this paper, it was never necessary to carry more than 7 states. Shuler and Zwanzig have expanded the wavefunction as a finite sum of eigenfunctions of the Hamiltonian, $e^{ip_n x}H_n(y)$, in the asymptotic region. They have determined the coefficients such that the wavefunction approximately satisfies the boundary condition at $x = y$. On the other hand, the solution obtained by the present method is equivalent to exapnding the wavefunction as

$$\Psi = \sum_{i=0}^{N} f_i(x)H_i(y). \tag{46}$$

The $f_i(x)$ are determined to satisfy the condition

$$\int_{-\infty}^{\infty} H_n(y)(H - E)\Psi \, dy = 0, \tag{47}$$

where H is the total Hamiltonian for the problem.

This method is not restricted to the form of the potential $V(x, y)$ as is the method of Shuler and Zwanzig. We may solve problems with equal ease for any potential. We are presently computing results for various interaction potentials spanning the range from very soft to very hard. We are also studying the effects of interaction potentials with an attractive well.

6. HYDROGEN-ATOM–POSITRON SCATTERING

In order to illustrate the use of this method for a more complicated and physically realistic problem, we write down the equations involved in H-atom–positron scattering. The Schrödinger equation for this problem in reduced coördinates may be written,

$$\left[\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right) + \left(-\frac{1}{r^2}\sin\theta\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{r^2}\sin^2\theta\frac{\partial^2}{\partial\phi^2} + \left\{-\nabla_e^2 - \frac{2}{r_e}\right\}\right) + 2\left(\frac{1}{r} - \frac{1}{r_{12}}\right) - E\right]\Psi = 0, \tag{48}$$

to correspond with Eq. (1). Here the unsubscripted variables refer to the coördinates of the positron, the subscript e refers to the coördinates of the electron and r_{12} is the distance between the positron and the electron. The vector $\mathbf{x}$ in Eq. (1) has the components θ, ϕ, r_e, θ_e, and ϕ_e in this example. We might take

$$\phi_i(\mathbf{x}) = \Psi^H_{n_e l_e m_e}(\mathbf{r}_e)\, Y_l^m(\theta, \varphi), \tag{49}$$

where $\Psi^H_{n_e l_e m_e}$ are the hydrogen-atom eigenfunctions and Y_l^m are normalized spherical harmonics. Thus, the subscript i refers to the five quantum numbers, n_e, l_e, m_e, m, and l. We take for m and n,

$$m_{ln_e}(r) = j_l(k_{n_e}r) \tag{50}$$

and

$$n_{ln_e}(r) = h_l^{(1)}(k_{n_e}r), \tag{51}$$

where j_l is the spherical Bessel function of the first

kind,[10] and $h_l^{(1)}$ is the spherical Hankel function.[10] In the following, we drop the superscript (1), and write this function $h_l(k_{n_e}r)$. The wave number k_{n_e} is given by

$$k_{n_e} = \left(\frac{1}{n_e^2} + E\right)^{\frac{1}{2}}. \tag{52}$$

For low-energy positrons, k_{n_e} becomes pure imaginary, when n_e is large. We must take the positive imaginary value of k_{n_e} in order that both $j_l(k_{n_e}r)$ and $h_l(k_{n_e}r)$ behave properly. With this choice of sign, h_l is a decaying exponential for large r.

The initial wave Φ in Eq. (6) is given by the well-known expansion of a plane wave in spherical Bessel functions,[11]

$$\Phi = \Psi_I^H(\mathbf{r}_e) \sum_{l=0}^{\infty} [4\pi(2l+1)]^{\frac{1}{2}} i^l Y_l^0(\theta) j_l(k_I r). \tag{53}$$

The subscript I refers to the three quantum numbers of the initial state of the atom. The definition we have used here for the spherical harmonic is

$$Y_l^0(\theta) = \left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}} P_l(\cos\theta), \tag{54}$$

where P_l is a Legendre polynomial. The c_i of Eq. (7) is given by

$$c_i = ik_{n_e}. \tag{55}$$

The V_{ij} are given by Eq. (13) with

$$g^{\frac{1}{2}}\, d\mathbf{x} = r^2 r_e^2 \sin\theta \sin\theta_e\, dr\, dr_e\, d\theta\, d\theta_e\, d\varphi\, d\varphi_e. \tag{56}$$

As is obvious from Eq. (48),

$$V(r, \mathbf{x}) = 2\left(\frac{1}{r} - \frac{1}{r_{12}}\right). \tag{57}$$

The V_{ij} can be computed analytically for any particular set of subscripts.

At this point we might remark that $V_{i,i'}$ (where i represents 5 indices) is zero if i and i' correspond to different states of total azimuthal angular momentum. Thus all $F_i^{i'}(r)$ with different azimuthal angular momentum than that of the initial state occurs only in homogeneous integral equations and are, therefore, zero. For this reason the fivefold sum in G in the integral of Eq. (6) reduces to a fourfold sum, m' being related to m_e' by the relation

$$m' + m_e' = m_I, \tag{58}$$

where m_I is the initial azimuthal angular momentum of the system. Furthermore, the $V_{i,i'}$ for which i and i' are states of different parity are zero. This eliminates approximately half of the terms in the sum in Eq. (30). This equation contains terms of even parity only, when i is of even parity; and odd parity only, when i is of odd parity.

In order to solve this system, we must truncate the sum over l' and n_e' in the integral of Eq. (12). The n_e' sum contains an integral over the continuum. The continuum contributes virtual positronium states whose neglect would of course be a rather bad approximation.[12] We hope in the future to investigate the magnitude of this error by including selected continuum states.

The system of equations which must be solved at each point is given by Eq. (30) with $c_i = ik_{n_e}$. The sum over j is a fourfold sum. Proceeding as described in Sec. 4, we obtain the reflection and transmission coefficients R_n^k and T_n^k. The computation of the b_i^j and a_i^j then follow as before by use of Eqs. (20), (19), (22), and (21). The total reflection matrix is then given by Eq. (27).

The reflection matrix we are interested in is a linear combination of the ones we have just computed. From Eq. (53) we obtain

$$R_i^I = \sum_{l'=0}^{\infty} i^{l'} [4\pi(2l'+1)]^{\frac{1}{2}} R_i^{i'-}, \tag{59}$$

where i' represents the five indices l', $m(=0)$, n_I, l_I, and m_I, and i refers to five indices l, m, n_e, l_e, and m_e. It is not necessary to terminate this sum, since it always contains only a finite number of nonzero terms. When $l' > l_e + l_I + l$, the corresponding $V_{i,i'}$ is zero and thus $R^{i'-}$ is zero, and the sum in Eq. (59) terminates.

We are presently engaged in solving these equations for the positron–hydrogen scattering problem. We investigate the rapidity of convergence of this method by solving the system retaining different numbers of terms in the Green's function sum. This method as described here is not well adapted in its present form to electron–hydrogen atom scattering because of the importance of the continuum in that case. We discuss this in detail in a future paper.

7. CONCLUSIONS

The method of "*amplitude density functions*" allows us to solve quickly and easily a large class of scattering problems which were formerly solvable only

[10] H. A. Antosiewicz, in *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds., (National Bureau of Standards, AMS 55, 1964), p. 437.

[11] Ref. 4, p. 1574.

[12] H. S. W. Massey and A. H. A. Moussa, Proc. Phys. Soc. (London) **71**, 38 (1958); W. J. Cody, J. Lawson, Sir H. Massey, and K. Smith, Proc. Roy. Soc. (London) **278A**, 479 (1964); R. P. McEachran and P. A. Fraser, Proc. Phys. Soc. (London) **86**, 369 (1965).

by a great computational effort. The scattering of a particle from a rigid rotor, the scattering of two rigid rotors, the scattering of an atom from a rotating vibrator, or the scattering of two rotating vibrators are a few of the problems for which this method is ideally suited. The large matrices which arise in the usual methods of numerically inverting integral equations are avoided. This results from the fact that we compute the asymptotic form of the wavefunction directly without needing to store great quantities of intermediate results. This method has the added advantage of being simpler and less time consuming than the usual methods.

Quite often, for problems of this type, one solves, instead of the integral equation, the corresponding system of coupled differential equations. This method is also plagued with the requirement of large amounts of storage space for intermediate information, though not quite to the same degree as in the integral equation method. When one solves the differential equations, he must resort to some procedure to get the proper starting conditions. The method of "*amplitude density functions*" has the advantage of being a direct method, requiring very little intermediate storage.

Note added in proof: It has been found that for an actual computation, one can derive a special quadrature formula for functions with discontinuous first derivatives of this particular type. The use of such a formula may reduce the required number of quadrature points by a factor of as much as 20. See, for example, Don Secrest and B. Robert Johnson, J. Chem. Phys. **45**, 4556 (1966).

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Properties of a Causal Green's Function for the Bethe–Salpeter Equation*

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The following properties of the free, but off-mass-shell, Bethe–Salpeter causal Green's function, for two spinless bosons whose masses may differ, are investigated: (a) its symmetries, (b) its expression in terms of the common higher transcendental functions, and (c) its forms in the asymptotic region and near the origin. An energy–spectral integral representation is also obtained.

1. INTRODUCTION

FOR two spinless bosons, the configuration-space Bethe–Salpeter[1] equation in the ladder approximation may be cast into the form[2]

$$\chi(x) = \lambda \int G(x - x')V(x')\chi(x')[dx']$$

for a bound system where x is the relative coordinate of the two particles; or with the inhomogeneous term $e^{ip\cdot x}$ added to the right member when the scattering situation is being described.[3] Whatever the potential function V, the "Green's function" $G(x - x')$ is common to all such equations. It seems desirable, therefore, to examine the properties of G in the expectation that we are able to deduce, among other things, properties of the wavefunction χ that are independent of V.

Previous investigations have considered the Green's function only for the cases of equal-mass bosons (see Schwartz and Zemack of Ref. 1). Wick[2] obtained asymptotic exponential factors for bound systems. This analysis was performed for what has become known as the "rotated" equation—where the relative-time and relative-energy coordinates have been analytically continued to their respective imaginary axes and four-dimensional Euclidean configuration and momentum-spaces produced. More recently, Swift and Lee[3] developed an energy–spectral representation for the nonrotated Green's function, and also investigated its asymptotic properties for all real nonnegative energies. Ciafaloni and Menotti[4] have treated the equal-mass case in detail.

Here we consider the general function with unequal masses. In Sec. 2 we define the Green's function, demonstrate its symmetries, and write down a convenient parametrization. The energy–spectral representation is developed in Sec. 3. In Secs. 4 and 5 we consider the rotated Green's function and Wick's hyperspherical representation. Special cases which admit exact expression of the (rotated) Green's function in terms of the common higher transcendental functions without integrals are examined in Secs. 6–8. The general cases are studied in Secs. 9–11. Finally, in Sec. 12 the case where both bosons have zero mass is briefly investigated. In the Appendix we derive a Laplace transformation which has proved to be a useful tool in determining the properties of the Green's function in the asymptotic region.

2. THE GREEN'S FUNCTION AND ITS SYMMETRIES

We consider a system where there are two interacting scalar bosons of masses m_a, m_b and 4-momenta p_a, p_b respectively.[5] We denote the total 4-momentum of the system by P. Then if μ_a, μ_b are given (for m_a, m_b not both zero[6]) by

$$\mu_a = m_a/(m_a + m_b), \quad \mu_b = m_b/(m_a + m_b), \tag{2.1}$$

we define the relative 4-momentum p by the equations

$$p_a = \mu_a P + p, \quad p_b = \mu_b P - p, \tag{2.2}$$

or

$$p = \tfrac{1}{2}[p_a - p_b - P(\mu_a - \mu_b)]. \tag{2.3}$$

If x is the relative coordinate canonically conjugate to p, we define the "causal Green's function" by

$$g(m_a, m_b, P; x) = \lim_{\substack{\xi\to 0\\ \eta\to 0}} \frac{1}{(2\pi)^4} \times \int \frac{e^{ip\cdot x}[dp]}{(p_a^2 + m_a^2 - i\xi)(p_b^2 + m_b^2 - i\eta)}, \tag{2.4}$$

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[1] H. A. Bethe and E. E. Salpeter, Phys. Rev. **84**, 1232 (1951); M. Gell-Mann and F. E. Low, *ibid.* **84**, 350 (1951); C. Schwartz and C. Zemach, *ibid.* **141**, 1454 (1966). The latter paper recently investigated the unequal mass case for scattering, the results of which agree with ours in Sec. 2 below.
[2] G. C. Wick, Phys. Rev. **96**, 1124 (1954).
[3] A. R. Swift and B. W. Lee, J. Math. Phys. **5**, 908 (1964).
[4] M. Ciafaloni and P. Menotti, Phys. Rev. **140**, B929 (1965).
[5] We take $\hbar = c = 1$. The relative 4-momentum $p = (p_0, \mathbf{p})$ and $p^2 = \mathbf{p}^2 - p_0^2$. Similarly we have the scalar product $p\cdot x = \mathbf{p}\cdot\mathbf{x} - p_0x_0$.
[6] For $m_a = m_b = 0$ see Sec. 12.

where $[dp] = d^3\mathbf{p}\cdot dp_0$, and the integration is over the whole of p-space. ξ, η are small and positive, and the limits are taken after the integration has been performed. We usually omit writing the ξ, η terms and their corresponding limit symbol explicitly. We sometimes omit the arguments of the Green's function where no confusion arises, or change the arguments—e.g., replacing x by x_0, $\mathbf{x}$ or by some corresponding spherical polar coordinates.

g is clearly invariant under all homogeneous Lorentz transformations including reflections, and also under scale transformations where all momenta change proportionally and the coordinates change in inverse proportion.

In the center-of-mass system, where $P = (E, \mathbf{O})$ and E is the total energy of the interacting system, we have from (2.2) and (2.4)

$$p_a = (\mu_a E + p_0, \mathbf{p}), \quad p_b = (\mu_b E - p_0, -\mathbf{p}), \tag{2.5}$$

$$g(m_a, m_b, E; x) = \frac{1}{(2\pi)^4}\int \frac{e^{ip\cdot x}[dp]}{[\mathbf{p}^2-(\mu_a E+p_0)^2+m_a^2][\mathbf{p}^2-(\mu_b E-p_0)^2+m_b^2]}. \tag{2.6}$$

This is clearly still invariant under spatial rotations and reflections, in the internal (x) space, but

$$g(m_a, m_b, E; \mathbf{x}, -x_0) = g(m_b, m_a, E; \mathbf{x}, x_0) \tag{2.7}$$

$$= g(m_a, m_b, -E; \mathbf{x}, x_0), \tag{2.8}$$

so that the time-reflection symmetry is more complicated.

Following Wick[2] we take $\frac{1}{2}(m_a + m_b)$ as the unit of mass, and

$$m_a = 1 + \Delta, \quad m_b = 1 - \Delta \tag{2.9}$$

so that $-1 \leq \Delta \leq 1$. From (2.7) we see that there is no loss of generality if we restrict the range of Δ to $0 \leq \Delta \leq 1$.

We introduce the following parameters:

$$\epsilon = E/(m_a + m_b) = \tfrac{1}{2}E, \tag{2.10}$$

$$\epsilon_a = (\mathbf{p}^2 + m_a^2)^{\frac{1}{2}} = [\mathbf{p}^2 + (1 + \Delta)^2]^{\frac{1}{2}}, \quad \epsilon_b = (\mathbf{p}^2 + m_b^2)^{\frac{1}{2}} = [\mathbf{p}^2 + (1 - \Delta)^2]^{\frac{1}{2}}, \tag{2.11}$$

$$\epsilon_a^0 = \mu_a E = (1 + \Delta)\epsilon, \quad \epsilon_b^0 = \mu_b E = (1 - \Delta)\epsilon. \tag{2.12}$$

In place of (2.6) we may now write

$$g(\Delta, \epsilon; x) = (2\pi)^{-4}\int d^3\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{x}} I(\Delta, \epsilon; \mathbf{p}; x_0), \tag{2.13}$$

where

$$I(\Delta, \epsilon; \mathbf{p}; x_0) = \int_{-\infty}^{\infty} \frac{e^{-ip_0 x_0}\, dp_0}{[(p_0 + \epsilon_a^0)^2 - \epsilon_a^2][(p_0 - \epsilon_b^0)^2 - \epsilon_b^2]}. \tag{2.14}$$

3. ENERGY-SPECTRAL REPRESENTATION

The poles of the integrand of I[in (2.14)] lie at

$$p_0 = -\epsilon_a^0 \pm \epsilon_a \mp i\xi', \quad p_0 = \epsilon_b^0 \pm \epsilon_b \mp i\eta', \tag{3.1}$$

where ξ', η' are small and positive. Call the poles A, B, C, and D, respectively. For $x_0 > 0$ we complete the contour for the p_0-integration for I with a large semicircle in the lower half-plane. This contributes nothing so that I is determined by the residues at poles A and C. Noting that $\epsilon = \frac{1}{2}(\epsilon_a^0 + \epsilon_b^0)$, we find

$$I_+ = \frac{\pi i}{2\epsilon + \epsilon_b - \epsilon_a}\left[\frac{e^{-i(\epsilon_a-\epsilon_a^0)x_0}}{\epsilon_a(\epsilon_a + \epsilon_b - 2\epsilon)} - \frac{e^{-i(\epsilon_b+\epsilon_b^0)x_0}}{\epsilon_b(\epsilon_a + \epsilon_b + 2\epsilon)}\right], \tag{3.2}$$

where the subscript $(+)$ is to indicate $x_0 > 0$. Thus I_+ depends only on $\mathbf{p}^2$ and not on the direction of $\mathbf{p}$. We redefine p to be $|\mathbf{p}|$ and perform the angular integrations in (2.13) to obtain

$$g_+ = \frac{1}{4\pi^2 r}\int_0^{\infty} p \sin(pr) I_+\, dp, \tag{3.3}$$

where $r = |\mathbf{x}|$. If we define

$$\epsilon' = \tfrac{1}{2}(\epsilon_a + \epsilon_b), \tag{3.4}$$

we have $\epsilon_a - \epsilon_b = (\epsilon_a^2 - \epsilon_b^2)/2\epsilon' = 2\Delta/\epsilon'$. Also using $\epsilon_a d\epsilon_a = \epsilon_b d\epsilon_b = pdp$, we find $d\epsilon' = \epsilon' pdp/\epsilon_a\epsilon_b$, which gives $d\epsilon'/dp > 0$. Combining these results with (3.2), (3.3) we obtain

$$g_+ = \frac{i}{(4\pi)^2 r}\int_1^{\infty} \frac{d\epsilon' \sin(pr)}{\epsilon\epsilon' - \Delta} \times \left[\frac{\epsilon_b e^{-i(\epsilon_a-\epsilon_a^0)x_0}}{\epsilon' - \epsilon} - \frac{\epsilon_a e^{-i(\epsilon_b+\epsilon_b^0)x_0}}{\epsilon' + \epsilon}\right]. \tag{3.5}$$

Here p must be expressed in terms of ϵ', viz.,

$$p = \{[1 - (\Delta^2/\epsilon'^2)](\epsilon'^2 - 1)\}^{\frac{1}{2}}. \tag{3.6}$$

If the integrand in (3.5) is rewritten so as to be completely expressed in terms of ϵ, ϵ', and Δ, and recast slightly, we obtain

$$g_+ = \frac{i}{2(2\pi)^2 r}\int_1^{\infty} \frac{d\epsilon'}{\epsilon'} \frac{\sin(pr)}{\epsilon'^2 - \epsilon^2} e^{ix_0(\Delta\epsilon-\epsilon')} \times \left\{\epsilon' \cos\left[x_0\left(\epsilon - \frac{\Delta}{\epsilon'}\right)\right] + i\left[\left(\epsilon'^2 - \frac{\Delta\epsilon}{\epsilon'}\right)\left(\epsilon - \frac{\Delta}{\epsilon'}\right)^{-1}\right]\sin\left[x_0\left(\epsilon - \frac{\Delta}{\epsilon'}\right)\right]\right\}. \tag{3.7}$$

We use (2.7), or, in terms of Δ and ϵ

$$g(\Delta, \epsilon; \mathbf{x}, -x_0) = g(-\Delta, \epsilon; \mathbf{x}, x_0) \tag{3.8}$$

together with (3.7) to obtain the corresponding expression g_- for x_0 negative. Finally we have the the result, true for all real x_0,

$$\begin{aligned} g(\Delta, \epsilon; x) = \frac{i}{(4\pi)^2 r} \int_1^\infty \frac{d\epsilon'^2}{\epsilon'^2 - \epsilon^2} \sin(pr) e^{-i(\epsilon' - \nu\Delta\epsilon)|x_0|} \\ \times \left\{ \frac{1}{\epsilon'} \cos\left[|x_0| \left(\epsilon - \nu \frac{\Delta}{\epsilon'} \right) \right] \right. \\ + i \left[\left(1 - \nu \frac{\Delta\epsilon}{\epsilon'^3} \right) \left(\epsilon - \nu \frac{\Delta}{\epsilon'} \right)^{-1} \right] \\ \left. \times \sin\left[|x_0| \left(\epsilon - \nu \frac{\Delta}{\epsilon'} \right) \right] \right\}, \end{aligned} \tag{3.9}$$

where $\nu = \nu(x_0) = 1, 0, -1$ according as $x_0 >, =, < 0$, respectively. It is easily seen that this reduces to Swift and Lee's Eq. (A5)[3] in the case $\Delta = 0$ (apart from a factor 2). Unlike the $\Delta = 0$ case, the integrand of (3.9) for $\Delta \neq 0$ is no longer an even function of ϵ and there is an additional cut in the ϵ^2 complex plane along the negative real axis. The discontinuity across it is a complicated function which is not very revealing and it seems better to consider g as a function in the ϵ complex plane. There the cuts run from $-\infty$ to -1 and from 1 to ∞. The discontinuity is readily found:

$$\begin{aligned} \text{disc } g(\Delta, \epsilon; x) = -\frac{1}{8\pi r |\epsilon|} \\ \times \sin\left\{ \left[\left(1 - \frac{\Delta^2}{\epsilon^2} \right)(\epsilon^2 - 1) \right]^{\frac{1}{2}} r \right\} e^{ix_0\Delta[\epsilon - (1/\epsilon)]}. \end{aligned} \tag{3.10}$$

4. ROTATED GREEN'S FUNCTION

Wick[2] has shown how for bound systems the wave equations may be rotated in the complex p_0 and x_0 planes, the result being a description in terms of real p_4 and real $x_4 (p_4 = ip_0, x_4 = ix_0)$ which form the fourth coordinates in Euclidean four-dimensional spaces.

The appropriate Green's function is

$$\begin{aligned} G(m_a, m_b, P; x) \\ = \frac{1}{(2\pi)^4} \int \frac{e^{ip\cdot x}[dp]'}{(p_a^2 + m_a^2)(p_b^2 + m_b^2)}, \end{aligned} \tag{4.1}$$

where[7] $[dp]' = d^3\mathbf{p}dp_4$ and $p\cdot x = \mathbf{p}\cdot\mathbf{x} + p_4x_4$. The Wick rotation does not affect the total 4-momentum P which thus has components $P = (\mathbf{P}, iP_0)$ with P_0, the total energy, still being real.

In the center-of-mass system we have, instead of (2.5),

$$p_a = (\mathbf{p}, i\mu_a E + p_4), \quad p_b = (-\mathbf{p}, i\mu_b E - p_4); \tag{4.2}$$

introducing the same parameters as in Sec. 2 we find in place of (2.13), (2.14),

$$G(\Delta, \epsilon; x) = (2\pi)^{-4} \int d^3\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{x}} I_1(\Delta, \epsilon; \mathbf{p}; x_4), \tag{4.3}$$

where

$$\begin{aligned} I_1(\Delta, \epsilon; \mathbf{p}; x_4) \\ = \int_{-\infty}^{\infty} \frac{e^{ip_4x_4}\, dp_4}{[(p_4 + i\epsilon_a^0)^2 + \epsilon_a^2][(p_4 - i\epsilon_b^0)^2 + \epsilon_b^2]}. \end{aligned} \tag{4.4}$$

For bound states we have, since $\epsilon < 1$,

$$\begin{aligned} \epsilon_a - \epsilon_a^0 = [p^2 + (1 + \Delta)^2]^{\frac{1}{2}} - (1 + \Delta)\epsilon \\ \geq (1 + \Delta)(1 - \epsilon) > 0, \end{aligned}$$

and similarly $\epsilon_b - \epsilon_b^0 > 0$. Thus the poles of the integrand of I_1, namely,

$$p_4 = i(-\epsilon_a^0 \pm \epsilon_a), \quad p_4 = i(\epsilon_b^0 \pm \epsilon_b), \tag{4.5}$$

which we call respectively A', B', C', D', are such that A', C' lie above the real p_4 axis for all $\mathbf{p}$ and B', D' lie below the real p_4 axis for all $\mathbf{p}$.

For $x_4 > 0$ we complete the contour in the integration for I_1 [Eq. (4.4)] with a semicircle of large radius in the upper half p_4-plane. Thus the integral is determined by the residues of poles A' and C'. Noting that we have from (3.1)

$$A' = iA, \quad B' = iB, \quad C' = iC, \quad D' = iD, \tag{4.6}$$

it is easily seen that

$$I_+(\Delta, \epsilon; \mathbf{p}; x_0) = iI_{1+}(\Delta, \epsilon; \mathbf{p}; ix_0). \tag{4.7}$$

Again, since changing the sign of x_0 (or x_4) is the same as changing the sign of Δ [cf. (3.8)], we have by substituting $-\Delta$ for Δ in (4.7)

$$I_-(\Delta, \epsilon; \mathbf{p}; x_0) = iI_{1-}(\Delta, \epsilon; \mathbf{p}; ix_0). \tag{4.8}$$

(4.7) and (4.8) then combine with (4.3) and (2.13) to give

$$g(\Delta, \epsilon; \mathbf{x}, x_0) = iG(\Delta, \epsilon; \mathbf{x}, e^{\frac{1}{2}i\pi}x_0). \tag{4.9}$$

If definition (4.1) for G is adhered to when $\epsilon > 1$ we cannot deduce (4.9). The reason is that, if $\epsilon > 1$, poles A' and D' for certain ranges of $\mathbf{p}$ lie on the other side of the real p_4 axis from where they do when $\epsilon < 1$. We are really interested in the analytical properties of the function that reduces for

[7] To preserve the numerical sequence of the indices the time coordinate is put last in the Euclidean spaces; i.e., we write $x = (\mathbf{x}, x_4)$, $p = (\mathbf{p}, p_4)$.

bound states to the right-hand member of Eq. (4.1). Therefore we abandon definition (4.1) and define G by Eq. (4.9). In this way we have the analytical continuation of the function which agrees with (4.1) when $\epsilon < 1$.

5. WICK'S HYPERSPHERICAL REPRESENTATION

Wick[8] derived for $\epsilon < 1$ the equation[9]

$$G(\Delta, \epsilon; x) = (4\pi)^{-2} e^{\epsilon \Delta x_4} \int_{-1}^{1} dy\, e^{y \epsilon x_4} K_0(|x|\, U^{\frac{1}{2}}), \quad (5.1)$$

where U is a quadratic function of y. Rewriting this in terms of four-dimensional spherical polar coordinates (R, θ, ϕ, ψ) it becomes

$$G(\Delta, \epsilon; R, \theta) = (4\pi)^{-2} e^{\epsilon \Delta R \cos\theta} \int_{-1}^{1} dy\, e^{y \epsilon R \cos\theta} K_0(R U^{\frac{1}{2}}) \quad (5.2)$$

with

$$U = [\epsilon y + (\Delta/\epsilon)]^2 - q^2 \quad (5.3)$$

and

$$q^2 = [1 - (\Delta^2/\epsilon^2)](\epsilon^2 - 1). \quad (5.4)$$

From (3.6) we see that q is the value of p when $\epsilon' = \epsilon$. For convenience we define ξ_a, ξ_b to be the values of ϵ_a, ϵ_b, respectively, when $\epsilon' = \epsilon$; i.e., from (2.11)

$$\xi_a = \epsilon + \Delta/\epsilon, \quad \xi_b = \epsilon - \Delta/\epsilon. \quad (5.5)$$

Then if we put $u = \epsilon y + \Delta/\epsilon$ in (5.2) we obtain, when $\epsilon \neq 0$,

$$G(\Delta, \epsilon; R, \theta) = \frac{1}{(4\pi)^2 \epsilon} e^{\Delta[\epsilon - (1/\epsilon)] R \cos\theta} \times \int_{-\xi_b}^{\xi_a} du\, e^{uR\cos\theta} K_0[R(u^2 - q^2)^{\frac{1}{2}}]. \quad (5.6)$$

When $\epsilon = 0$, U is linear in y, and when $\epsilon = 1$ or Δ, U is a perfect square. These special cases admit a representation of the corresponding Green's function in terms of the common higher transcendental functions without integrals appearing. They also divide the range of ϵ into segments and in the different segments the general Green's function has different behavior characteristics. In the next three sections we therefore examine the special cases in detail, before turning to the more general cases in Secs. 9–11.

[8] See Ref. 2, Appendix, pp. 1133–1134.

[9] The notation used throughout for the various higher transcendental functions is that of *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds., (Dover Publications, Inc., New York, 1965).

Particular emphasis is placed in all the following work on determining the form of G near the origin, and in the asymptotic region. We respectively denote these forms by the suffixes O and A, i.e.,

$$G_0(\Delta, \epsilon; R, \theta) = G(\Delta, \epsilon; R, \theta), \quad R \to 0,$$

$$G_A(\Delta, \epsilon; R, \theta) = G(\Delta, \epsilon; R, \theta), \quad R \to \infty.$$

The angular argument could be omitted from G_0, since near $R = 0$ the integral in (5.6) is dominated by the singularity of the K_0 function at $R = 0$, and the largest term involving θ comes from the second term in the series expansion of $e^{uR\cos\theta}$ combined with the logarithmic contribution from K_0—i.e., it is of order $R \ln R$ which vanishes as $R \to 0$. In the following we have evaluated only the terms which are nonvanishing as $R \to 0$, namely, $O(\ln R)$ and $O(R^0)$.

6. $\epsilon = 0$

In this case where the total mass of the system vanishes we have complete four-dimensional symmetry since (5.2) becomes

$$G(\Delta, 0; R) = (4\pi)^{-2} \int_{-1}^{1} dy\, K_0[R(1 + 2y\,\Delta + \Delta^2)^{\frac{1}{2}}]. \quad (6.1)$$

For nonvanishing Δ, if we put z for the argument of the K_0 function, this becomes[10]

$$(\Delta \neq 0) G(\Delta, 0; R) = (4\pi)^{-2} \Delta^{-1} R^{-2} \int_{R(1-\Delta)}^{R(1+\Delta)} dz\, z K_0(z) \quad (6.2)$$

$$= (4\pi)^{-2} \Delta^{-1} R^{-1} \{(1 - \Delta) K_1[R(1 - \Delta)] - (1 + \Delta) K_1[R(1 + \Delta)]\}. \quad (6.3)$$

For $\Delta = 0$, we have directly from (6.1)

$$G(0, 0; R) = 2(4\pi)^{-2} K_0(R). \quad (6.4)$$

For $\Delta = 1$, (6.3) takes the simpler form

$$G(1, 0; R) = (4\pi)^{-2} R^{-2} [1 - 2R K_1(2R)]. \quad (6.5)$$

It is perhaps interesting to notice that the general result (6.3) can be expressed in terms of the form for $\Delta = 1$, viz.,

$$G(\Delta, 0; R) = (4\Delta)^{-1} \{(1 + \Delta)^2 G[1, 0, \tfrac{1}{2}(1 + \Delta)R] - (1 - \Delta)^2 G[1, 0, \tfrac{1}{2}(1 - \Delta)R]\}. \quad (6.6)$$

[10] See Ref. 9, p. 484, Eq. (11.2.27).

Near the origin it is easily shown that G takes the form[11]

$$G_0(\Delta, 0; R) = (4\pi)^{-2}\{-2 \ln R + 2(\ln 2 - \gamma) + 1 + [(1 - \Delta)^2/2\Delta] \ln (1 - \Delta) - [(1 + \Delta)^2/2\Delta] \ln (1 + \Delta)\} + O(R \ln R). \quad (6.7)$$

This reduces, for $\Delta = 0, 1$, to

$$G_0(0, 0; R) = (4\pi)^{-2}[-2 \ln R + 2(\ln 2 - \gamma)] + O(R \ln R), \quad (6.8)$$

$$G_0(1, 0; R) = (4\pi)^{-2}[-2 \ln R + 1 - 2\gamma] + O(R \ln R). \quad (6.9)$$

These forms may also be derived directly from (6.4) and (6.5). In the asymptotic region we use the known asymptotic forms of K_0 and K_1[12] to find

$$G_A(\Delta, 0; R) = (4\pi)^{-2}R^{-\frac{3}{2}}\Delta^{-1}[\tfrac{1}{2}\pi(1 - \Delta)]^{\frac{1}{2}} \times e^{-R(1-\Delta)}[1 + O(R^{-1})], \quad (\Delta \neq 0, 1) \quad (6.10)$$

$$G_A(0, 0; R) = (4\pi)^{-2}R^{-\frac{1}{2}}(2\pi)^{\frac{1}{2}}e^{-R}[1 + O(R^{-1})], \quad (6.11)$$

$$G_A(1, 0; R) = (4\pi)^{-2}R^{-2}[1 + O(R^{\frac{1}{2}}e^{-2R})]. \quad (6.12)$$

A comparison of (6.10) and (6.11) emphasises that the equal-mass ($\Delta = 0$) asymptotic behavior is no guide to the behavior when the masses differ. Nor, by comparing (6.10) and (6.12), does the general case readily give the behavior when the mass of one of the interacting particles vanishes. On the other hand, the behavior near the origin for the general case does approach the $\Delta = 0$ and $\Delta = 1$ forms smoothly.

7. $\varepsilon = 1$

Here the total energy is the sum of the particle proper masses so they are just free.

If we substitute $z = R(y + \Delta)$ in (5.2) for this case we find

$$G(\Delta, 1; R, \theta) = (4\pi)^{-2}R^{-1}\left[\int_0^{R(1+\Delta)} dz\, e^{z\cos\theta} \times K_0(z) + \int_0^{R(1-\Delta)} dz\, e^{-z\cos\theta}K_0(z)\right]. \quad (7.1)$$

The integrals which appear are generalized Schwartz functions and Luke[13] writes down series expansions. For instance,

$$\int_0^R dz\, e^{-z\cos\theta}K_0(z) = 2e^{-R\cos\theta}\sum_{k=0}^{\infty} U_k(\cos\theta)\{-[\gamma + \ln(\tfrac{1}{2}R)]I_{k+1}(R) + \sum_{m=0}^{\infty}(\tfrac{1}{2}R)^{2m+k+1}[\psi(m + k + 2) - \psi(1)]/m!\,(m + k + 1)!\} \quad (7.2a)$$

$$= 2e^{-R\cos\theta}\sum_{k=0}^{\infty} U_k(\cos\theta)[\psi(k + 1) - \ln(\tfrac{1}{2}R)] \times I_{k+1}(R) + 2e^{-R\cos\theta}\sum_{k=0}^{\infty} U_k(\cos\theta) \times \frac{(\frac{1}{2}R)^{k+1}}{k!}\sum_{m=0}^{\infty}\frac{(-\frac{1}{2}R)^m I_m(R)}{m!\,(m + k + 1)^2}, \quad (7.2b)$$

where $U_k(\cos\theta) = \sin(k + 1)\theta/\sin\theta$, $\psi(1) = -\gamma$, and

$$\psi(m) = -\gamma + \sum_{k=1}^{m-1} k^{-1}$$

when $m \geq 2$.

For the special angles $\theta = 0, \frac{1}{2}\pi, \pi$, the solutions are much simpler. Combining (7.1) with the formula[14]

$$\int_0^R dz\, e^{\pm z}K_0(z) = e^{\pm R}R[K_0(R) \pm K_1(R)] \mp 1 \quad (7.3)$$

we find

$$G(\Delta, 1; R, 0) = (4\pi)^{-2}e^{\Delta R}\{e^R(1 + \Delta)[K_0(R_1) + K_1(R_1)] + e^{-R}(1 - \Delta)[K_0(R_2) - K_1(R_2)]\}, \quad (7.4)$$

where R_1, R_2 are, respectively, $R(1 \pm \Delta)$. For $\theta = \pi$ we use $G(\Delta, 1; R, \pi) = G(-\Delta, 1; R, 0)$ with (7.4). For $\theta = \frac{1}{2}\pi$ we combine (7.1) with the formula[15]

$$\int_0^R dz\, K_0(z) = RK_0(R) + \tfrac{1}{2}\pi R[\mathfrak{L}_0(R)K_1(R) + \mathfrak{L}_1(R)K_0(R)], \quad (7.5)$$

where $\mathfrak{L}_0$, $\mathfrak{L}_1$ are modified Struve functions, and obtain

$$G(\Delta, 1; R, \tfrac{1}{2}\pi) = (4\pi)^{-2}\{(1 + \Delta)K_0(R_1) + (1 - \Delta)K_0(R_2) + \tfrac{1}{2}\pi(1 + \Delta)[\mathfrak{L}_0(R_1)K_1(R_1) + \mathfrak{L}_1(R_1)K_0(R_1)] + \tfrac{1}{2}\pi(1 - \Delta)[\mathfrak{L}_0(R_2)K_1(R_2) + \mathfrak{L}_1(R_2)K_0(R_2)]\}. \quad (7.6)$$

[11] γ is Euler's constant, 0.57721 ....
[12] See Ref. 9, p. 378, Eq. (9.7.2).
[13] Y. L. Luke, *Integrals of Bessel Functions* (McGraw-Hill Book Company, Inc., New York, 1962), pp. 239–243.
[14] See Ref. 9, p. 484, Eq. (11.3.15).
[15] See Ref. 9, p. 480, Eq. (11.1.8).

When $\Delta = 0$ and $\Delta = 1$ we have expressions which are much simpler than the right-hand members of (7.1), (7.4), (7.6), but we do not write them down since they may be easily derived by direct substitution or by going to the appropriate limit.

As for the case $\epsilon = 0$, we are able in the present case to express the Green's function for general Δ in terms of that for $\Delta = 1$, namely,

$$G(\Delta, 1; R, \theta) = \tfrac{1}{2}(1 + \Delta)G(1, 1; \tfrac{1}{2}R_1, \theta) + \tfrac{1}{2}(1 - \Delta)G(1, 1; \tfrac{1}{2}R_2, \pi - \theta). \quad (7.7)$$

It is readily shown that, near the origin, (7.1) reduces to

$$G_0(\Delta, 1; R, \theta) = (4\pi)^{-2}[-2 \ln R + 2(1 + \ln 2 - \gamma) - (1 + \Delta) \ln (1 + \Delta) - (1 - \Delta) \ln (1 - \Delta)] + O(R \ln R). \quad (7.8)$$

Asymptotic Form

First we note the following formula[16]:

$$\int_0^\infty dz\, e^{-z \cos\theta} K_0(z) = \frac{\theta}{\sin\theta} \qquad (\theta \neq \pi). \quad (7.9)$$

Next we have, as $R \to \infty$ and for $\theta \neq \pi$,

$$\int_R^\infty dz\, e^{-z \cos\theta} K_0(z) = a^{-1}\left(\frac{\pi}{2R}\right)^{\frac{1}{2}} e^{-aR} F(R, a), \quad (7.10)$$

where $a = 1 + \cos\theta$, and

$$F(R, a) \sim 1 - R^{-1}(4 + a)/8a + O(R^{-2}). \quad (7.11)$$

In fact, F may be calculated to as many terms as we wish by substituting the asymptotic form of $K_0(z)$ into the left member of (7.10), integrating by terms, and substituting the asymptotic form of each of the resulting incomplete gamma functions.

If we now express the integrals in (7.1) as $\int_0^{R_1} = (\int_0^\infty - \int_{R_1}^\infty)$ and $\int_0^{R_2} = (\int_0^\infty - \int_{R_2}^\infty)$ we find, using (7.9), (7.10)

$$G_A(\Delta, 1; R, \theta) = \frac{1}{(4\pi)^2 R}\left[\frac{\pi}{\sin\theta} - \left(\frac{\pi}{2R_1}\right)^{\frac{1}{2}} \frac{e^{-(1-\cos\theta)R_1}}{1 - \cos\theta} F(R_1, 1 - \cos\theta) - \left(\frac{\pi}{2R_2}\right)^{\frac{1}{2}} \frac{e^{-(1+\cos\theta)R_2}}{1 + \cos\theta} F(R_2, 1 + \cos\theta)\right] \quad (7.12)$$

for $\Delta \neq 1$ and $\theta \neq 0, \pi$. The second term is greater than, or less than the third term according as θ is less than or greater than $\cos^{-1}\Delta$. Thus

$$G_A(\Delta, 1; R, \theta) \sim (16\pi R \sin\theta)^{-1} \qquad (\Delta \neq 1, \theta \neq 0, \pi). \quad (7.13)$$

For $\theta = 0, \pi$ we use (7.4) and obtain

$$G_A(\Delta, 1; R, 0) \sim [1/(4\pi)^2][2\pi(1 + \Delta)/R]^{\frac{1}{2}} \times [1 + O(R^{-1})] \qquad (\Delta \neq 1) \quad (7.14)$$

with $G_A(\Delta, 1; R, \pi) = G_A(-\Delta, 1; R, 0)$.

For $\Delta = 1$ the second integral in (7.1) vanishes, and from a similar analysis to that above we find

$$G_A(1, 1; R, \theta) = \frac{1}{(4\pi)^2 R}\left[\frac{\pi - \theta}{\sin\theta} - \left(\frac{\pi}{4R}\right)^{\frac{1}{2}} \times \frac{e^{-(1-\cos\theta)2R}}{1 - \cos\theta} F(2R, 1 - \cos\theta)\right] \sim (\pi - \theta)/(4\pi)^2 R \sin\theta \qquad (\theta \neq 0). \quad (7.15)$$

We use (7.4) for the case $\theta = 0$ and obtain

$$G_A(1, 1; R, 0) \sim \frac{1}{(4\pi)^2}\left\{-\frac{1}{R} + 2\left(\frac{\pi}{R}\right)^{\frac{1}{2}}[1 + O(R^{-1})]\right\}. \quad (7.16)$$

For all Δ the dominant asymptotic term for $\theta \neq 0, \pi$ is a function only of $r = R \sin\theta$, the three-dimensional spatial distance from the origin. It is also independent of Δ except for the case $\Delta = 1$.

For the pure time directions $\theta = 0, \pi$, we have $G_A \sim R^{-\frac{1}{2}}$ in place of $G_A \sim R^{-1}$ for all other angles. ($\Delta = 1, \theta = \pi$ is an exception.) Another feature of the pure time directions is that the remaining terms in the asymptotic expansion vanish much more slowly with respect to the dominant term than is the case for the other directions.

8. $\epsilon = \Delta$

As Cutkosky[17] has pointed out, if bound states with $\epsilon < \Delta$ exist, the particle a of mass m_a is unstable to the decay $a \to (ab) + \bar{b}$, where b is the particle of mass m_b, and $\bar{b}$ is its antiparticle. The case $\epsilon = \Delta$ is therefore in some ways analogous to the case $\epsilon = 1$ and this is reflected in certain similarities of the forms for the Green's function.

With the substitution $z = R(1 + \Delta y)$, Eq. (5.2) becomes

$$G(\Delta, \Delta; R, \theta) = (4\pi)^{-2}\Delta^{-1}R^{-1}e^{-(1-\Delta)zR\cos\theta} \times \int_{R(1-\Delta)}^{R(1+\Delta)} dz\, e^{z\cos\theta} K_0(z). \quad (8.1)$$

The integral here, as for the $\epsilon = 1$ case, may be

[16] *Tables of Integral Transforms*, A. Erdélyi, Ed. (McGraw-Hill Book Company, Inc., New York, 1954), Vol. II, p. 131, Eq. (22).

[17] R. E. Cutkosky, Phys. Rev. 96, 1135 (1954).

expressed as a pair of generalized Schwartz functions. For the special angles $\theta = 0, \pi, \frac{1}{2}\pi$, the Green's function simplifies to the following forms:

$$G(\Delta, \Delta; R, 0) = (4\pi)^{-2}\,\Delta^{-1}R^{-1} \times e^{\Delta^2 R}\{e^{\Delta R}R_1[K_0(R_1) + K_1(R_1)] - e^{-\Delta R}R_2[K_0(R_2) + K_1(R_2)]\}, \quad (8.2)$$

$$G(\Delta, \Delta; R, \pi) = (4\pi)^{-2}\,\Delta^{-1}R^{-1} \times e^{-\Delta^2 R}\{e^{-\Delta R}R_1[K_0(R_1) + K_1(R_1)] - e^{\Delta R}R_2[K_0(R_2) + K_1(R_2)]\}, \quad (8.3)$$

$$G(\Delta, \Delta; R, \tfrac{1}{2}\pi) = (4\pi)^{-2}\,\Delta^{-1}R^{-1}\{R_1K_0(R_1) - R_2K_0(R_2) + \tfrac{1}{2}\pi R_1[\mathfrak{L}_0(R_1)K_1(R_1) + \mathfrak{L}_1(R_1)K_0(R_1)] - \tfrac{1}{2}\pi R_2[\mathfrak{L}_0(R_2)K_1(R_2) + \mathfrak{L}_1(R_2)K_0(R_2)]\}. \quad (8.4)$$

The analog of (7.7) is

$$G(\Delta, \Delta; R, \theta) = \Delta^{-1}e^{-(1-\Delta^2)R\cos\theta} \times [G(1, 1; \tfrac{1}{2}R_1, \theta) - G(1, 1; \tfrac{1}{2}R_2, \theta)]. \quad (8.5)$$

It is easily shown that near the origin we have

$$G_0(\Delta, \Delta; R, \theta) = (4\pi)^{-2}\{-2\ln R + 2(1 + \ln 2 - \gamma) + \Delta^{-1}\ln[(1 - \Delta)/(1 + \Delta)] - \ln(1 - \Delta^2)\} + O(R\ln R). \quad (8.6)$$

The asymptotic form for $\theta \neq 0$ is

$$G_A(\Delta, \Delta; R, \theta) = \frac{e^{-R(1-\Delta)(1+\Delta\cos\theta)}}{(4\pi)^2\,\Delta R(1 - \cos\theta)} \times \left(\frac{\pi}{2R_2}\right)^{\frac{1}{2}}F(R_2, 1 - \cos\theta), \quad (8.7)$$

where F is defined in (7.10), (7.11). When $\theta = 0$ we have instead

$$G_A(\Delta, \Delta; R, 0) = (4\pi)^{-2}\,\Delta^{-1}e^{-R(1-\Delta^2)}(2\pi/R)^{\frac{1}{2}} \times [(1 + \Delta)^{\frac{1}{2}} - (1 - \Delta)^{\frac{1}{2}}][1 + O(R^{-1})], \quad (8.8)$$

i.e.,

$$G_A(\Delta, \Delta; R, \theta) \sim e^{-R(1-\Delta)(1+\Delta\cos\theta)}R^{-\frac{1}{2}}\ (\theta \neq 0), \qquad G_A(\Delta, \Delta; R, 0) \sim e^{-R(1-\Delta^2)}R^{-\frac{1}{2}}. \quad (8.9)$$

Here the special character of the pure time direction is apparent only for $\theta = 0$ (x_4 positive).

9. $0 < \epsilon < \Delta$

First, we note from the definition (5.5) that ξ_b is negative, zero, or positive according as ϵ is less than, equal to, or greater than $\Delta^{\frac{1}{2}}$, respectively, so that for the range of ϵ we are considering in this section ξ_b is negative. Second, $\xi_b^2 = q^2 + (1 - \Delta)^2 \geq q^2$, and q^2 is positive from (5.4). Therefore $-\xi_b > q(=|q|)$ for $\Delta \neq 1$. Again ξ_a is clearly positive from its definition, and [from $\xi_a^2 = q^2 + (1 + \Delta)^2$] is greater than q. Thus the argument of K_0 in (5.6) is real and positive for the complete range of u over which the integration is performed, and we may determine the asymptotic form for G directly, by substituting the asymptotic form for K_0 and integrating. Thus

$$G_A(\Delta, \epsilon; R, \theta) \sim \frac{e^{\Delta[\epsilon-(1/\epsilon)]R\cos\theta}}{(4\pi)^2\epsilon}\left(\frac{\pi}{2R}\right)^{\frac{1}{2}} \times \int_{-\xi_b}^{\xi_a} du\,\frac{e^{-R[(u^2-q^2)^{\frac{1}{2}}-u\cos\theta]}}{(u^2 - q^2)^{\frac{1}{4}}} \times \left[1 - \frac{1}{8R(u^2 - q^2)^{\frac{1}{2}}} + \cdots\right] \quad (\Delta \neq 1). \quad (9.1)$$

Now

$$(d/du)\{e^{-R[(u^2-q^2)^{\frac{1}{2}}-u\cos\theta]}\} = \mathrm{Re}^{-R[(u^2-q^2)^{\frac{1}{2}}-u\cos\theta]}[\cos\theta - u/(u^2 - q^2)^{\frac{1}{2}}]. \quad (9.2)$$

Since, for positive q^2 as we have here, the factor $[\cos\theta - u/(u^2 - q^2)^{\frac{1}{2}}]$ cannot vanish for real θ for any value of u in the range of integration, we may integrate by parts in (9.1) to obtain

$$\int_{-\xi_b}^{\xi_a} du\,\frac{e^{-R[(u^2-q^2)^{\frac{1}{2}}-u\cos\theta]}}{(u^2 - q^2)^{\frac{1}{4}}}\{1 - \cdots\} = \left\{\frac{e^{-R[(u^2-q^2)^{\frac{1}{2}}-u\cos\theta]}}{R[\cos\theta - u(u^2 - q^2)^{-\frac{1}{2}}](u^2 - q^2)^{\frac{1}{2}}}\right\}_{-\xi_b}^{\xi_a} \times [1 + O(R^{-1})] = -R^{-1}(f_+ + f_-), \quad (9.3)$$

where

$$f_+ = f(\Delta, \epsilon; R, \theta) = -\frac{(1 + \Delta)^{\frac{1}{2}}e^{-R[1+\Delta-(\epsilon+\Delta/\epsilon)\cos\theta]}}{(1 + \Delta)\cos\theta - (\epsilon + \Delta/\epsilon)}[1 + O(R^{-1})] \quad (9.4)$$

and $f_- = f(-\Delta, \epsilon; R, \pi - \theta)$. The dominant contribution comes from the term in (9.3) with the greater exponent. From (9.4) $f_\pm \propto \exp(-Rg_\pm)$ with

$$g_\pm = 1 \pm \Delta \mp (\epsilon \pm \Delta/\epsilon)\cos\theta. \quad (9.5)$$

We note that

$$g_+ - g_- = 2(\Delta - \epsilon\cos\theta). \quad (9.6)$$

f_+ or f_- dominates according as $\cos\theta$ is greater or less than Δ/ϵ. In the present case $\Delta/\epsilon > 1$ so that f_- is the dominant expression for all θ and we have

$$G_A(\Delta, \epsilon; R, \theta) \sim -\frac{e^{-R(1-\Delta)(1+\epsilon\cos\theta)}}{(4\pi)^2\epsilon R}\left[\frac{\pi(1-\Delta)}{2R}\right]^{\frac{1}{2}} \times \frac{1}{(1-\Delta)\cos\theta + (\epsilon - \Delta/\epsilon)} \times [1 + O(R^{-1})] \quad (\Delta \neq 1). \quad (9.7)$$

When $\Delta = 1$, $\xi_b = -q$ and the relevant integral from (5.6) may be expressed as

$$\left(\int_q^\infty - \int_{\xi_a}^\infty\right) du\, e^{uR\cos\theta} K_0[R(u^2 - q^2)^{\frac{1}{2}}] \equiv S^+ - S_1, \quad (9.8)$$

say, except for the case $\theta = 0$ when S^+ and S_1 do not exist separately. Putting $z = R(u - q)$ and using (A23), we have asymptotically

$$S_A^+ \sim q^{-1}R^{-2}e^{qR\cos\theta}[1 + O(R^{-1})]. \quad (9.9)$$

Now $S_1 = R^{-1}(\pi/2R)^{\frac{1}{2}}f_+$ so that S^+ dominates for all θ and we may write from (5.6)

$$G_A(1, \epsilon; R, \theta) \sim (4\pi)^{-2}R^{-2}(1-\epsilon^2)^{-1}, \quad \theta \neq 0 \quad (9.10)$$

One finds with some straightforward calculation that near the origin the Green's function takes the form

$$G_0(\Delta, \epsilon; R, \theta) = (4\pi)^{-2}\Big\{-2\ln R + 2(1 + \ln 2 - \gamma) + \frac{1}{\epsilon}\left(\epsilon + \frac{\Delta}{\epsilon}\right)\ln(1+\Delta) - \frac{1}{\epsilon}\left(\epsilon - \frac{\Delta}{\epsilon}\right)\ln(1-\Delta) - \frac{1}{\epsilon}[(\Delta^2 - \epsilon^2)(1-\epsilon^2)]^{\frac{1}{2}} \times \ln\left[\frac{(1-\epsilon^2)^{\frac{1}{2}} - (\Delta^2-\epsilon^2)^{\frac{1}{2}}}{(1-\epsilon^2)^{\frac{1}{2}} + (\Delta^2-\epsilon^2)^{\frac{1}{2}}}\right]\Big\} + O(R\ln R) \quad (9.11)$$

which for $\Delta = 1$ simplifies to

$$G_0(1, \epsilon; R, \theta) = (4\pi)^{-2}[-2\ln R + 2(1-\gamma) + \epsilon^{-2}(1-\epsilon^2)\ln(1-\epsilon^2)] + O(R\ln R). \quad (9.12)$$

10. $\Delta < \epsilon < 1$

This is the most interesting case physically because it describes a bound state which is not associated with an intrinsic instability of the more massive particle as was the case for $\epsilon < \Delta$.

The first thing we notice is that, from (5.4), q^2 is negative for the entire range of ϵ, so that there are no singularities arising from the K_0 function in the integrand in (5.6).

Next, looking at (9.2) we see that care must be taken in attempting to integrate by parts, since with q^2 negative, for each θ in the range 0 to π there is a unique value of u for which the factor $[\cos\theta - u/(u^2 - q^2)^{\frac{1}{2}}]$ vanishes. $u/(u^2 - q^2)^{\frac{1}{2}}$ is an increasing function of u, so that as θ increases from 0 to π, the value of u for which the factor vanishes decreases from ∞ to $-\infty$. The value of u lies within the range of integration in (5.6), viz., ξ_a to $-\xi_b$, only for θ lying between θ_1 and θ_2 where

$$\cos\theta_1 = \xi_a/(1+\Delta), \quad \cos\theta_2 = -\xi_b/(1-\Delta). \quad (10.1)$$

We note for later reference

$$\sin\theta_1 = |q|/(1+\Delta), \quad \sin\theta_2 = |q|/(1-\Delta). \quad (10.2)$$

Thus for $0 \leq \theta < \theta_1$ and $\theta_2 < \theta \leq \pi$, which we call region I and region III, respectively, we may integrate by parts in exactly the same way as we did for the case $\epsilon < \Delta$.

Now

$$\cos\theta_1 - \Delta/\epsilon = (\epsilon^2 - \Delta^2)/\epsilon(1+\Delta) > 0,$$

and

$$\cos\theta_2 - \Delta/\epsilon = (\Delta^2 - \epsilon^2)/\epsilon(1-\Delta) < 0,$$

so that by (9.6), f_+ provides the dominant contribution for region I and f_- provides the dominant contribution for region III. The corresponding asymptotic forms are

Region I: $0 \leq \theta < \theta_1$.

$$G_A(\Delta, \epsilon; R, \theta) \sim \frac{e^{-R(1+\Delta)(1-\epsilon\cos\theta)}}{(4\pi)^2\epsilon R}\left[\frac{\pi(1+\Delta)}{2R}\right]^{\frac{1}{2}} \times \frac{1}{(1+\Delta)\cos\theta - [\epsilon + (\Delta/\epsilon)]}[1 + O(R^{-1})]. \quad (10.3)$$

Region III: $\theta_2 < \theta \leq \pi$.

$$G_A(\Delta, \epsilon; R, \theta) \sim -\frac{e^{-R(1-\Delta)(1+\epsilon\cos\theta)}}{(4\pi)^2\epsilon R}\left[\frac{\pi(1-\Delta)}{2R}\right]^{\frac{1}{2}} \times \frac{1}{(1-\Delta)\cos\theta + [\epsilon - (\Delta/\epsilon)]}[1 + O(R^{-1})]. \quad (10.4)$$

For $\theta_1 \leq \theta \leq \theta_2$ (Region II) we must use a different approach. With the exclusion of $\theta = 0, \pi$ we may write the integral from $-\xi_b$ to ξ_a in the right-hand side of (5.6) as

$$S_0 - S_1 - S_2 \equiv \left(\int_{-\infty}^\infty - \int_{\xi_a}^\infty - \int_{-\infty}^{-\xi_b}\right) du\, e^{uR\cos\theta} \times K_0[R(u^2 - q^2)^{\frac{1}{2}}]. \quad (10.5)$$

S_0 exists for $\theta \neq 0, \pi$ and is evaluated in (A20) upon substituting uR for y, and $-q^2R^2$ for a^2. Both S_1 and S_2 exist since S_0 exists and the integrand is everywhere positive. We call S_0 the "complementary

integral." Since the critical factor $[\cos\theta - u/(u^2 - q^2)^{\frac{1}{2}}]$ does not vanish in the ranges of integration of S_1, S_2, we may evaluate them asymptotically by the same partial-integration method that was used in Sec. 9. We find

$$S_1 = R^{-1}(\pi/2R)^{\frac{1}{2}} f_+, \quad S_2 = R^{-1}(\pi/2R)^{\frac{1}{2}} f_-, \tag{10.6}$$

giving the complete asymptotic behavior as

Region II: $\theta_1 \leq \theta \leq \theta_2$.

$$G_A(\Delta, \epsilon; R, \theta) = \frac{e^{\Delta[\epsilon - (1/\epsilon)]R\cos\theta}}{(4\pi)^2 \epsilon R} \times \left[\frac{\pi e^{-|q|R\sin\theta}}{\sin\theta} - \left(\frac{\pi}{2R}\right)^{\frac{1}{2}}(f_+ + f_-)\right]. \tag{10.7}$$

To find the dominant contributions we must compare the exponential behavior of the terms. Using (9.5), (10.1), (10.2) we have

$$g_+ - |q|\sin\theta = (1 + \Delta)[1 - \cos(\theta - \theta_1)], \tag{10.8}$$

which is positive unless $\theta = \theta_1$. Similarly

$$g_- - |q|\sin\theta = (1 - \Delta)[1 - \cos(\theta_2 - \theta)], \tag{10.9}$$

which is positive unless $\theta = \theta_2$. Thus the complementary integral term dominates except at the extremities θ_1, θ_2. For the next most important contribution we notice that since $\theta_1 < \theta_0 < \theta_2$, where $\theta_0 = \cos^{-1}(\Delta/\epsilon)$, there is a region $(\theta_1 \leq \theta < \theta_0)$ where f_+ dominates and a region $(\theta_0 < \theta \leq \theta_2)$ where f_- dominates, and the exponential factors are equal for $\theta = \theta_0$.

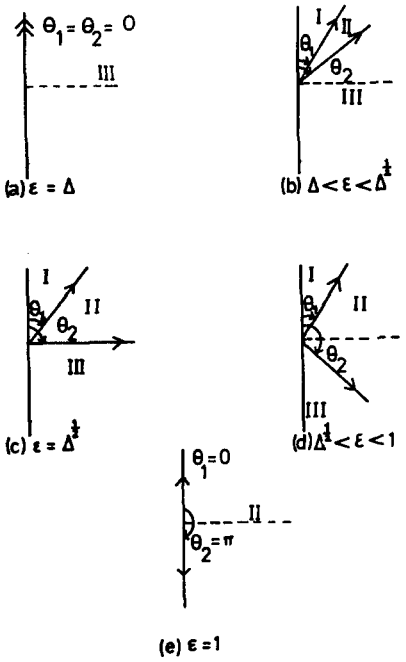

FIG. 1. Representation in an (R,θ) plane of the four-dimensional regions I, II, III for various ϵ; $\Delta \leq \epsilon \leq 1$.

If we keep only the complementary integral term we may write

$$G_A(\Delta, \epsilon; R, \theta) \sim (\exp\{-[(1 - \epsilon^2)(1 - \Delta^2)]^{\frac{1}{2}}R \times \cos[\theta - \tfrac{1}{2}(\theta_1 + \theta_2)]\})(16\pi\epsilon R\sin\theta)^{-1}. \tag{10.10}$$

We now examine how the angles θ_1, θ_2 change with ϵ. Firstly, note that

$$\frac{d\theta_2}{d\epsilon} = \frac{1}{(1 - \Delta)}\left(1 + \frac{\Delta}{\epsilon^2}\right)\left(\frac{1}{\sin\theta_2}\right) > 0 \tag{10.11}$$

and secondly from (10.2)

$$\sin\theta_1/\sin\theta_2 = (1 - \Delta)/(1 + \Delta), \tag{10.12}$$

which is positive, ≤ 1, and independent of ϵ.

When $\epsilon = \Delta$, (10.1) gives $\theta_1 = \theta_2 = 0$ and region III fills the whole (four-dimensional) solid angle. See Fig. 1(a). As ϵ increases from Δ towards $\Delta^{\frac{1}{2}}$, θ_2 increases from 0 towards $\frac{1}{2}\pi$. From (10.12) we see that θ_1 also increases but is always less than θ_2. See Fig. 1(b). At $\epsilon = \Delta^{\frac{1}{2}}$, $\theta_2 = \frac{1}{2}\pi$. Thus $\sin\theta_2$ has its maximum value and (10.12) implies that θ_1 has therefore reached a maximum value. This maximum value is $\theta_{1\max} = \frac{1}{2}\pi - 2\tan^{-1}\Delta^{\frac{1}{2}} = \frac{1}{2}\pi - 2\tan^{-1}\epsilon$. See Fig. 1(c). As ϵ increases from $\Delta^{\frac{1}{2}}$ towards 1, θ_1 decreases from $\theta_{1\max}$ towards zero. See Fig. 1(d). At $\epsilon = 1$, $\theta_1 = 0$ and $\theta_2 = \pi$ and region II fills the whole solid angle. See Fig. 1(e).

The following points are perhaps worthy of comment:

(i) For $\Delta = 0$ we have only the $[(0 =)\Delta^{\frac{1}{2}} \leq \epsilon \leq 1]$-type behavior. As $\epsilon \to 0$, θ_1 and $\theta_2 \to \frac{1}{2}\pi$ and region II disappears. Type-I and type-III behavior are symmetrical about the space axis for all ϵ, viz., $G_A \propto \exp[-R(1 - \epsilon\,|\cos\theta|)]$ which is Wick's result.[8]

(ii) If we compare (10.4) with (9.7) we see that the $\epsilon < \Delta$ case gives type-III behavior for the whole solid angle for all ϵ.

(iii) When $\theta = \frac{1}{2}\pi$, the integrand in (5.6) is an even function of u. If also $\epsilon = \Delta^{\frac{1}{2}}$, then in (10.5), $S_2 = \frac{1}{2}S_0$ since $\xi_b = 0$, and (10.7) becomes

$$G_A(\Delta, \Delta^{\frac{1}{2}}, R, \tfrac{1}{2}\pi) = \frac{e^{\Delta[\epsilon - (1/\epsilon)]R\cos\theta}}{(4\pi)^2\epsilon R} \times \left[\frac{\pi e^{-|q|R\sin\theta}}{2\sin\theta} - \left(\frac{\pi}{2R}\right)^{\frac{1}{2}} f_+\right]. \tag{10.13}$$

(iv) Whereas in regions I and III the ratio of the neglected terms in the asymptotic expansion to the leading term is $\sim R^{-1}$, in region II the ratio is $\sim \exp[-Rh(\theta)]$. Thus in region II the complementary integral term on its own provides a very

accurate approximation to the Green's function.

The form of the Green's function near the origin is obtainable by a straightforward calculation and is

$$G_0(\Delta,\epsilon;R,\theta)=(4\pi)^{-2}\Big[-2\ln R+2(1+\ln 2-\gamma)-\frac{1}{\epsilon}\Big(\epsilon+\frac{\Delta}{\epsilon}\Big)\ln(1+\Delta)-\frac{1}{\epsilon}\Big(\epsilon-\frac{\Delta}{\epsilon}\Big)\times\ln(1-\Delta)-\frac{|q|}{\epsilon}(\theta_2-\theta_1)\Big]+O(R\ln R). \quad (10.14)$$

11. $\epsilon > 1$

Here q^2 is positive, and except for the case $\Delta = 1$, ξ_a and ξ_b are both positive and greater than q, so the argument of K_0 in (5.6) vanishes and becomes purely imaginary in the integration range. To evaluate the integral we therefore use the same complementary integral procedure (for $\theta \neq 0, \pi$) as in the previous section.

We again write

$$S_0 - S_1 - S_2 \equiv \Big(\int_{-\infty}^{\infty} - \int_{\xi_a}^{\infty} - \int_{-\infty}^{-\xi_b}\Big)\,du \times e^{uR\cos\theta}K_0[R(u^2-q^2)^{\frac{1}{2}}] \quad (11.1)$$

and from (A21)

$$S_0 = (\pi/R\sin\theta)e^{iqR\sin\theta}. \quad (11.2)$$

Integrals over the ranges $-\infty$ to $-q$, and q to ∞ exist and are closely related to the one defined in Eq. (A1). Since the integrand is real and nonnegative through these ranges, the integrals S_1, S_2 therefore exist, and the splitting exhibited in (11.1) is allowed. The critical factor $[\cos\theta - u/(u^2-q^2)^{\frac{1}{2}}]$ does not vanish for real θ for any $|u| \geq q$ so we may use the partial integration method to find the asymptotic forms of S_1, S_2. As before,

$$S_1 = R^{-1}(\pi/2R)^{\frac{1}{2}}f_+, \quad S_2 = R^{-1}(\pi/2R)^{\frac{1}{2}}f_-. \quad (11.3)$$

The complete asymptotic behavior is thus[18]

$$G_A(\Delta,\epsilon;R,\theta)=\frac{e^{\Delta[\epsilon-(1/\epsilon)]R\cos\theta}}{(4\pi)^2\epsilon R}\times\Big[\frac{\pi e^{iqR\sin\theta}}{\sin\theta}-\Big(\frac{\pi}{2R}\Big)^{\frac{1}{2}}(f_+ + f_-)\Big]. \quad (11.4)$$

We now determine the dominant contributions. First define

$$\theta_3 = \cos^{-1}[(1+\Delta)/\xi_a], \quad \theta_4 = \cos^{-1}[(1-\Delta)/(-\xi_b)], \quad \psi_1 = \cos^{-1}(\epsilon^{-1}), \quad \psi_2 = \cos^{-1}(-\epsilon^{-1}) = \pi - \psi_1. \quad (11.5), (11.6)$$

Then, for all $\epsilon > 1$,

$$0 < \theta_3 \leq \psi_1 < \tfrac{1}{2}\pi \leq \theta_4 \leq \psi_2 < \pi. \quad (11.7)$$

The first inequality follows from $\xi_a = [(1+\Delta)^2 + q^2]^{\frac{1}{2}} > 1 + \Delta$, the second from $\cos\theta_3 - \cos\psi_1 = \Delta(\epsilon - \epsilon^{-1})/(\epsilon^2 + \Delta) \geq 0$, and the fifth from $\cos\theta_4 - \cos\psi_2 = \Delta(\epsilon - \epsilon^{-1})/(\epsilon^2 - \Delta) \geq 0$, while the others are obvious.

Now, the magnitude of the exponential factor from the complementary integral term is proportional to e^0. Therefore f_+ dominates for $\theta < \theta_3$ and f_- dominates for $\theta > \theta_4$. For $\theta_3 < \theta < \theta_4$ the complementary integral term dominates. We denote the regions I, III, II, respectively, by analogy with what was done in Sec. 9.

When we include the factor $\exp[\Delta(\epsilon - \epsilon^{-1})R\cos\theta]$ in (11.4), the total exponent for the complementary integral term is positive or negative according as θ is less than or greater than $\frac{1}{2}\pi$. The total exponent for the f_+ term is positive or negative according as θ is less than or greater than ψ_1, and for the f_- term is positive or negative according as θ is greater than or less than ψ_2. The asymptotic forms for regions I and III are thus again given by Eqs. (10.3) and (10.4), and for region II by omitting the $f_\pm$ terms in Eq. (11.4)

At $\epsilon = 1$, $\theta_3 = \psi_1 = 0$, and $\theta_4 = \psi_2 = \pi$, region II fills the whole solid angle. See Fig. 2(a). As ϵ increases θ_3 increases but θ_4, ψ_2 decrease. The dominant exponent is positive except for the solid angle $\frac{1}{2}\pi < \theta < \psi_2$, which includes parts of regions II and III. See Fig. 2(b). As $\epsilon \to \infty$, θ_3, θ_4, ψ_2 all ap-

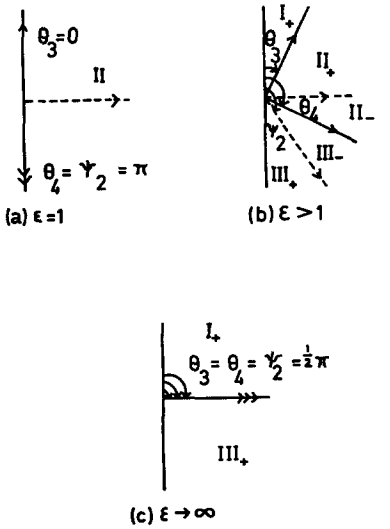

FIG. 2. Representation in an (R,θ) plane of the four-dimensional regions I, II, III for various ϵ; $1 \leq \epsilon$, $\Delta \neq 1$. The subscripts (+ or −) are the sign of the exponent of the dominant term in the Green's function.

[18] Cf. Ref. 4, Eq. (A9) (a) for case $\Delta = 0$.

proach $\frac{1}{2}\pi$, and in the limit, region I fills $(0, \frac{1}{2}\pi)$, region III fills $(\frac{1}{2}\pi, \pi)$ and region II has vanished. See Fig. 2(c).

In place of (10.12) we have from $\tan\theta_3 = p/(1+\Delta)$, $\tan\theta_4 = -p/(1-\Delta)$ that the ratio $\tan\theta_3/\tan\theta_4$ is independent of ϵ.

When $\Delta = 1$, $\xi_b = q = \epsilon - \epsilon^{-1}$ and the relevant integral in (5.6) is best expressed (for $\theta \neq 0$) as

$$S^- - S_1 \equiv \left\{\int_{-q}^{\infty} - \int_{\xi_a}^{\infty}\right\} du\, e^{uR\cos\theta} \times K_0[R(u^2-q^2)^{\frac{1}{2}}]. \quad (11.8)$$

Putting $z = R(u+q)$, and using (A1) with $-q = e^{-i\pi}q$, we obtain

$$S^- = \frac{\pi}{R\sin\theta}e^{iqR\sin\theta} - \frac{i}{2R\sin\theta}[e^{iqR\sin\theta} \times E_1(qRe^{i\theta}) - e^{iqR\sin\theta}E_1(qRe^{-i\theta}]. \quad (11.9)$$

The complete asymptotic behavior of the Green's function is thus

$$G_A(1,\epsilon;R,\theta) = \frac{e^{[\epsilon-(1/\epsilon)]R\cos\theta}}{(4\pi)^2\epsilon R}\left\{\frac{\pi e^{iqR\sin\theta}}{\sin\theta} - \left(\frac{\pi}{2R}\right)^{\frac{1}{2}}f_+ - \frac{i}{2\sin\theta}[e^{iqR\sin\theta}E_1(qRe^{i\theta}) - e^{-iqR\sin\theta}E_1(qRe^{-i\theta})]\right\} \quad (11.10)$$

[cf. Eq. (11.4)]. For all $\theta > \theta_3$ an accurate asymptotic form is given by omitting the f_+ term in this expression, and the leading contributions to the remaining expression may be obtained from Eqs. (A25)–(A27). The behavior in the three regions for this case is therefore:

Region I: Eq. (10.3).

Region II:

$$G_A(1,\epsilon;R,\theta) \sim \frac{\pi e^{[\epsilon-(1/\epsilon)]Re^{i\theta}}}{(4\pi)^2\epsilon R\sin\theta} + O(\epsilon^0). \quad (11.11)$$

Region III:

$$G_A(1,\epsilon;R,\theta) \sim -\frac{1}{(4\pi)^2R^2(\epsilon^2-1)}[1+O(R^{-1})]. \quad (11.12a)$$

On the boundary $\theta = \frac{1}{2}\pi$ between regions II and III:

$$G_A(1,\epsilon;R,\tfrac{1}{2}\pi) \sim \frac{1}{(4\pi)^2\epsilon R}\left[\frac{\pi e^{iqR}}{R} + O(R^{-2})\right]. \quad (11.12b)$$

Form near the Origin:

$$G_0(\Delta,\epsilon;R,\theta) = (4\pi)^{-2}\Big\{-2\ln R + 2(1+\ln 2-\gamma) - \epsilon^{-1}(\epsilon+\Delta/\epsilon)\ln(1+\Delta) - \epsilon^{-1}(\epsilon-\Delta/\epsilon) \times \ln(1-\Delta) - \epsilon^{-2}[(\epsilon^2-\Delta^2)(\epsilon^2-1)]^{\frac{1}{2}} \times \ln\left[\frac{(\epsilon^2-\Delta^2)^{\frac{1}{2}}+(\epsilon^2-1)^{\frac{1}{2}}}{(\epsilon^2-\Delta^2)^{\frac{1}{2}}-(\epsilon^2-1)^{\frac{1}{2}}}\right]\Big\} + O(R\ln R), \quad (11.13)$$

which reduces for $\Delta = 1$ to

$$G_0(1,\epsilon;R,\theta) = (4\pi)^{-2}[-2\ln R + 2(1-\gamma) - (1-\epsilon^{-2})\ln(\epsilon^2-1)] + O(R\ln R). \quad (11.14)$$

12. CASE $m_a = m_b = 0$

From Eq. (2.4) we have

$$g(0,0,P;x) = \lim_{\substack{\xi\to0\\ \eta\to0}} \frac{1}{(2\pi)^4}\int \frac{e^{ip\cdot x}[dp]}{(p_a^2 - i\xi)(p_b^2 - i\eta)}. \quad (12.1)$$

Effectively $\mu_a = \mu_b = \frac{1}{2}$ so that (2.3) becomes

$$p = \tfrac{1}{2}(p_a - p_b), \quad (12.2)$$

and in the center-of-mass system this has no relative-energy component. (2.5) becomes

$$p_a = (\tfrac{1}{2}E, \mathbf{p}), \qquad p_b = (\tfrac{1}{2}E, -\mathbf{p}), \quad (12.3)$$

whence, defining $\epsilon = \frac{1}{2}E$, we obtain

$$g(0,0,2\epsilon;x) = \lim_{\substack{\xi\to0\\ \eta\to0}} \frac{1}{(2\pi)^4} \times \int \frac{e^{ip\cdot x}[dp]}{(\mathbf{p}^2 - \epsilon^2 - i\xi)(\mathbf{p}^2 - \epsilon^2 - i\eta)}. \quad (12.4)$$

We perform the p_0 integration, and put $\eta = \xi$, and $g_0(\epsilon;x)$ for the Green's function to obtain

$$g_0(\epsilon;x) = \lim_{\xi\to0}\frac{\delta(x_0)}{(2\pi)^3}\int \frac{e^{i\mathbf{p}\cdot\mathbf{x}}\,d^3\mathbf{p}}{(\mathbf{p}^2-\epsilon^2-i\xi)^2}. \quad (12.5)$$

Next, the angular integrations produce a factor $(4\pi/pr)\sin(pr)$ (where p now stands for $|\mathbf{p}|$) so that

$$g_0(\epsilon,x) = \lim_{\xi\to0}\frac{\delta(x_0)}{2\pi^2 r}\int_0^\infty \frac{p\sin(pr)}{(p^2-\epsilon^2-i\xi)^2}\,dp. \quad (12.6)$$

The integrand is an even function of p, so we extend the range of integration to $(-\infty, \infty)$, write the sine function as $(2i)^{-1}(e^{ipr}-e^{-ipr})$, and complete a contour C_1 for the first term in the upper half p-plane and a contour C_2 for the second term in the lower half p-plane. See Fig. 3.

$$g_0(\epsilon;x) = \lim_{\xi\to0} -\frac{i}{8\pi^2 r}\,\delta(x_0) \times \left[\int_{c_1}\frac{pe^{ipr}\,dp}{(p^2-\epsilon^2-i\xi)^2} - \int_{c_2}\frac{pe^{-ipr}\,dp}{(p^2-\epsilon^2-i\xi)^2}\right].$$

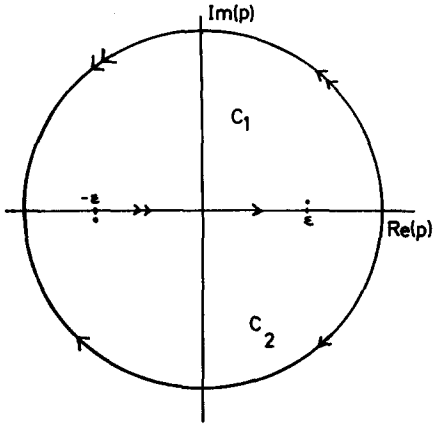

FIG. 3. Integration contours in the complex p-plane.

There are double poles just above and below the real axis at ϵ, $-\epsilon$ enclosed by C_1, C_2, respectively. Now, if $f(z)$ is analytic inside and on the simple contour C enclosing point a,

$$\int_c \frac{f(z)}{(z-a)^2}\,dz = 2\pi i f'(a),$$

whence we obtain

$$g_0(\epsilon; x) = (i/8\pi\epsilon)\ \delta(x_0)e^{i\epsilon r}. \tag{12.7}$$

13. CONCLUSION

In ranges of ϵ and θ, where the complementary integral term is dominant, the asymptotic form is given very accurately by this term, and this should be particularly important for weakly bound systems where the greater part of the solid angle is in region II.

The Green's function for the cases $\Delta = 1$ and $\Delta = 0$ exhibits nontypical behavior in several respects. Extension of previous studies for the equal-mass case to the more general unequal-mass case therefore have to be performed with care.

The form of the Green's function in the vicinity of the origin is a smooth function both of ϵ and Δ.

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APPENDIX

A Laplace Transform

The fundamental result that is proved here is[9]

$$I(\alpha,\beta) \equiv \int_0^\infty e^{-\beta x}K_0[x^{\frac{1}{2}}(x+2\alpha)^{\frac{1}{2}}]\,dx$$

$$= -\frac{\alpha}{z_1 - z_2}\,[e^{z_1}E_1(z_1) - e^{z_2}E_1(z_2)] \tag{A1}$$

for $\mathrm{Re}\,(\beta) > -1$ and arbitrary complex α, where $z_{1\atop 2} = \alpha e^{\pm\gamma}$, and $\gamma = \cosh^{-1}\beta$

$$\{\text{or } z_{1\atop 2} = \alpha[\beta \pm (\beta^2-1)^{\frac{1}{2}}]\}.$$

To be precise, we choose for γ the unique solution of $\cosh\gamma = \beta$ that satisfies

$$0 \le \mathrm{Im}\,(\gamma) < \pi \quad \text{for} \quad \mathrm{Re}\,(\gamma) > 0,$$
$$0 \le \mathrm{Im}\,(\gamma) \le \pi \quad \text{for} \quad \mathrm{Re}\,(\gamma) = 0,$$
$$0 < \mathrm{Im}\,(\gamma) \le \pi \quad \text{for} \quad \mathrm{Re}\,(\gamma) < 0.$$

We take $-\frac{1}{2}\pi \le \arg[(x+2\alpha)^{\frac{1}{2}}] < \frac{1}{2}\pi$, so that $I(\alpha,\beta)$ is an analytic function of α with a cut along the negative real axis.

It is also an analytic function of β as is clear from the integrand. The apparent cut, in the reduced form, along the positive real β axis from 1 to ∞ due to the boundary $\mathrm{Im}\,(\gamma) = 0$, has no discontinuity—crossing the boundary merely interchanges z_1, z_2 and the reduced form is clearly unchanged by this.

Notice that when $\mathrm{Im}\,(\gamma) \neq 0$, $|\arg z_1|$ and $|\arg z_2|$ are separately greater than π for a range of values of $\arg\alpha$, and in such a case the argument of the corresponding exponential integral function is not on its principal sheet.

Magnus and Oberhettinger[19] quote a version of the above for α, β real and nonnegative.

The method of proof is an extension of that used by Swift and Lee[20] in their attempt to determine the asymptotic form of the Green's function for $\Delta = 0$, $\epsilon > 1$.

Proof:

(a) $|\arg\alpha| < \pi$.

We start with the equation[21]

$$I_{\kappa,\mu}(\alpha,\beta) \equiv \int_0^\infty x^{-\kappa-\frac{1}{2}}(x+2\alpha)^{\kappa-\frac{1}{2}}e^{-\beta x} \times K_{2\mu}[x^{\frac{1}{2}}(x+2\alpha)^{\frac{1}{2}}]\,dx$$
$$= (2\alpha)^{-1}e^{\alpha\beta}\Gamma(\tfrac{1}{2}-\kappa+\mu)\Gamma(\tfrac{1}{2}-\kappa-\mu) \times W_{\kappa,\mu}(z_1)W_{\kappa,\mu}(z_2) \tag{A2}$$

with

$$|\arg\alpha| < \pi, \qquad \mathrm{Re}\,(\beta) > -1,$$
$$\mathrm{Re}\,(\kappa) + |\mathrm{Re}\,(\mu)| < \tfrac{1}{2}. \tag{A3}$$

[19] W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1949), p. 135.
[20] See Ref. 3, Appendix B.
[21] See Ref. 16, Vol. II, p. 377, Eq. (37).

With $\mu = 0$, if $\rho = \frac{1}{2} - \kappa$, the derivative of the integrand with respect to β is

$$x^{\rho}(x + 2\alpha)^{-\rho}e^{-\beta x}K_0[x^{\frac{1}{2}}(x + 2\alpha)^{\frac{1}{2}}].$$

Near the origin this is $\sim x^{\rho} \ln x$, and at infinity it is $\sim \exp[-\beta x - (x^2 + 2\alpha x)^{\frac{1}{2}}]$. It is therefore not difficult to prove rigorously that the integral from 0 to ∞ exists and converges uniformly with respect to β for Re $(\rho) > -1$, Re $(\beta) > -1$ and $|\arg \alpha| < \pi$.

Thus, for $|\arg \alpha| < \pi$, Re $(\beta) > -1$, Re $(\kappa) < \frac{3}{2}$,

$$-\frac{\partial}{\partial\beta} I_{\kappa,0}(\alpha, \beta) = \int_0^{\infty} x^{-\kappa+\frac{1}{2}}(x + 2\alpha)^{\kappa-\frac{1}{2}}e^{-\beta x} \times K_0[x^{\frac{1}{2}}(x + 2\alpha)^{\frac{1}{2}}]\, dx. \quad \text{(A4)}$$

From (A2), for Re $(\kappa) < \frac{1}{2}$,

$$\frac{\partial}{\partial\beta} I_{\kappa,0}(\alpha, \beta) = \frac{1}{2\alpha} e^{\alpha\beta}[\Gamma(\tfrac{1}{2} - \kappa)]^2\Big[\alpha W_{\kappa,0}(z_1)W_{\kappa,0}(z_2) + \frac{\partial W_{\kappa,0}(z_1)}{\partial z_1} W_{\kappa,0}(z_2) \frac{\partial z_1}{\partial\beta} + W_{\kappa,0}(z_1) \frac{\partial W_{\kappa,0}(z_2)}{\partial z_2} \frac{\partial z_2}{\partial\beta}\Big].$$

Now using

$$\frac{\partial z_1}{\partial\beta} = \frac{2\alpha z_1}{z_1 - z_2}, \qquad \frac{\partial z_2}{\partial\beta} = -\frac{2\alpha z_2}{z_1 - z_2}, \quad \text{(A5)}$$

and[22]

$$zW'_{\kappa,\mu}(z) = (\tfrac{1}{2}z - \kappa)W_{\kappa,\mu}(z) - W_{\kappa+1,\mu}(z), \quad \text{(A6)}$$

$$(2\kappa - z)W_{\kappa,\mu}(z) + W_{\kappa+1,\mu}(z) = (\mu - \kappa + \tfrac{1}{2})(\mu + \kappa - \tfrac{1}{2})W_{\kappa-1,\mu}(z), \quad \text{(A7)}$$

this becomes

$$\frac{\partial}{\partial\beta} I_{\kappa,0}(\alpha, \beta) = [e^{\alpha\beta}/(z_1 - z_2)][\Gamma(\tfrac{1}{2} - \kappa)]^2(\tfrac{1}{2} - \kappa)^2 \times [W_{\kappa-1,0}(z_1)W_{\kappa,0}(z_2) - W_{\kappa,0}(z_1)W_{\kappa-1,0}(z_2)].$$

Again, using $z\Gamma(z) = \Gamma(z + 1)$

and[23]

$$W_{\kappa,\mu}(z) = e^{-\frac{1}{2}z}z^{\frac{1}{2}+\mu}U(\tfrac{1}{2} + \mu - \kappa, 1 + 2\mu, z)$$

it becomes

$$\frac{\partial}{\partial\beta} I_{\kappa,0}(\alpha, \beta) = [\alpha/(z_1 - z_2)][\Gamma(\tfrac{3}{2} - \kappa)]^2 \times [U(\tfrac{3}{2} - \kappa, 1, z_1)U(\tfrac{1}{2} - \kappa, 1, z_2) - U(\tfrac{1}{2} - \kappa, 1, z_1)U(\tfrac{3}{2} - \kappa, 1, z_2)]. \quad \text{(A8)}$$

Now the integral in (A4) converges and is analytic in α, β, κ for Re $(\kappa) < \frac{3}{2}$, i.e., for a larger range of κ than that to which (A2) applies. The right-hand side of (A8) is also analytic for the extended range. Therefore, by analytic continuation, (A8) is true for the extended range Re $(\kappa) < \frac{3}{2}$. Putting $\kappa = \frac{1}{2}$ in (A4) and (A8) we obtain

$$-\lim_{\kappa\to\frac{1}{2}} \frac{\partial}{\partial\beta} I_{\kappa,0}(\alpha, \beta) = \int_0^{\infty} e^{-\beta x}K_0[x^{\frac{1}{2}}(x + 2\alpha)^{\frac{1}{2}}]\, dx = -\frac{\alpha}{z_1 - z_2}[U(1, 1, z_1)U(0, 1, z_2) - U(0, 1, z_1)U(1, 1, z_2)].$$

$U(0, 1, z) = 1$, and $U(1, 1, z) = e^z E_1(z)$, so that for $|\arg \alpha| < \pi$ we have indeed Eq. (A1).

(b) $\arg \alpha = -\pi$.

The reduced form clearly exists for $\arg \alpha = -\pi$, so that if we can prove that the limit as $\arg \alpha \to -\pi$ of the integral exists, then Eq. (A1) holds in this limit.

First define

$$J_s(\zeta, \beta) \equiv \int_0^{\pi} \sin\phi e^{-\beta\zeta\cos\phi}H_0^{(s)}(\zeta \sin\phi)\, d\phi, \quad \text{(A9)}$$

where $s = 1, 2$ and $H_0^{(s)}$ is the corresponding Hankel function. $J_s(\zeta, \beta)$ clearly exists for all β, and all $\gamma \neq 0$. If we put $y = \zeta \cos\phi$ we obtain

$$\zeta J_s(\zeta, \beta) = \int_{-\zeta}^{\zeta} e^{-\beta y}H_0^{(s)}[(\zeta^2 - y^2)^{\frac{1}{2}}]\, dy. \quad \text{(A10)}$$

Next suppose that $\alpha = re^{-i(\pi-\delta)}$, where r is real and δ is real, small, and positive.

Put $\zeta = \alpha e^{i\pi} = re^{i\delta}$. Notice that as $x \to 0$, $\arg[(x + 2\alpha)^{\frac{1}{2}}] \to -\frac{1}{2}\pi + \frac{1}{2}\delta$. We may write the integral in (A1) as

$$I(\alpha, \beta) = \Big(\int_0^{2r} + \int_{2r}^{\infty}\Big)e^{-\beta x}K_0[x^{\frac{1}{2}}(x - 2\zeta)^{\frac{1}{2}}]\, dx.$$

Now let us regard x as a complex variable, and change the path of integration. First, we insert two canceling straight integration contours between the points $2r$ and 2ζ, and split the total integration into

$$\int_0^{\infty} = \Big(\int_0^{2r} + \int_{2r}^{2\zeta}\Big) + \Big(\int_{2\zeta}^{2r} + \int_{2r}^{\infty}\Big).$$

This is allowed since the integrand is effectively logarithmic at the singularity at 2ζ so that the spur integrals exist (see Fig. 4). Also a logarithmic singularity has the property that the integral along a simple contour terminating at it is independent of the direction by which the contour approaches it. 0 and 2ζ are both effectively logarithmic singularities of the integrand so that we may replace the first bracketed pair of contours above by the straight segment between them. Instead of the second

[22] See Ref. 9, p. 507, Eqs. (13.4.31), (13.4.33).
[23] See Ref. 9, p. 505, Eq. (13.1.33).

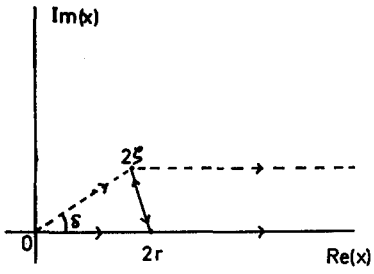

FIG. 4. Integration contours in the complex x-plane.

bracketed pair we may take a contour from 2ζ parallel to the real axis. It should return to the real axis at $+\infty$ by a short segment, but it is easily seen that the contribution is zero and we omit it. No singularities of the integrand are crossed by these deformations.

Therefore

$$I(\alpha,\beta) = \left(\int_0^{2\zeta} + \int_{2\zeta}^{\infty+2\zeta}\right) e^{-\beta x} K_0[x^{\frac{1}{2}}(x-2\zeta)^{\frac{1}{2}}]\,dx$$
$$= e^{-\beta\zeta}\int_{-\zeta}^{\zeta} e^{-\beta y} K_0[(y^2-\zeta^2)^{\frac{1}{2}}] + e^{-2\beta\zeta}\int_0^{\infty} e^{-\beta y} K_0[y^{\frac{1}{2}}(y+2\zeta)^{\frac{1}{2}}]\,dy,$$

where in the first integral $y = x - \zeta$, and in the second $y = x - 2\zeta$. For y on the open segment $(-\zeta, \zeta)$, $\arg[(y^2-\zeta^2)^{\frac{1}{2}}] = -\frac{1}{2}\pi + \delta$, so we put

$$(y^2-\zeta^2)^{\frac{1}{2}} = -i(\zeta^2-y^2)^{\frac{1}{2}}$$

with $\arg[(\zeta^2-y^2)^{\frac{1}{2}}] = \delta$. From the relations between the modified Bessel functions and the Hankel functions[24] we then have

$$I(\alpha,\beta) = \tfrac{1}{2}\pi i e^{-\beta\zeta}\int_{-\zeta}^{\zeta} e^{-\beta y} H_0^{(1)}[(\zeta^2-y^2)^{\frac{1}{2}}]\,dy + e^{-2\beta\zeta}\int_0^{\infty} e^{-\beta y} K_0[y^{\frac{1}{2}}(y+2\zeta)^{\frac{1}{2}}]\,dy. \quad \text{(A11)}$$

The limit of each integral as $\delta \to 0$ exists from (A10) and (A1), so that

$$\int_0^{\infty} e^{-\beta x} K_0[x^{\frac{1}{2}}(x-2r)^{\frac{1}{2}}]\,dx$$

exists. Thus (A1) is true for $\arg\alpha = -\pi$. We have proved incidentally with (A1) and (A11)

$$\int_{-\zeta}^{\zeta} e^{-\beta y} H_0^{(1)}[(\zeta^2-y^2)^{\frac{1}{2}}]\,dy = \left[-\frac{i}{(\pi\sinh\gamma)}\right]\{e^{\zeta\sinh\gamma}[E_1(\zeta e^{\gamma}) + E_1(\zeta e^{-\gamma-i\pi})] - e^{-\zeta\sinh\gamma}[E_1(\zeta e^{-\gamma}) + E_1(\zeta e^{\gamma-i\pi})]\} \quad \text{(A12)}$$

for $0 \le \arg\zeta < \pi$.

[24] See, e.g., Ref. 9, p. 375, Eq. (9.6.4).

Notice that if we had allowed $\arg\alpha$ to approach π rather than $-\pi$ we should have obtained

$$I(\alpha,\beta) = -\tfrac{1}{2}\pi i e^{-\beta\zeta}\int_{-\zeta}^{\zeta} e^{-\beta y} H_0^{(2)}[(\zeta^2-y^2)^{\frac{1}{2}}]\,dy + e^{-2\beta\zeta}\int_0^{\infty} e^{-\beta y} K_0[y^{\frac{1}{2}}(y+2\zeta)^{\frac{1}{2}}]\,dy \quad \text{(A13)}$$

with $\zeta = \alpha e^{-i\pi} = re^{-i\delta}$, $-\pi \le \arg\zeta < 0$. This would, at first sight, appear to give a different result for

$$\int_0^{\infty} e^{-\beta x} K_0[x^{\frac{1}{2}}(x-2r)^{\frac{1}{2}}]\,dx,$$

but the difference is due to taking $\arg[(x-2r)^{\frac{1}{2}}] = \frac{1}{2}\pi$ when $x < 2r$ rather than $-\frac{1}{2}\pi$, as is the case in (A11).

The analog of (A12) is[25]

$$\int_{-\zeta}^{\zeta} e^{-\beta y} H_0^{(2)}[(\zeta^2-y^2)^{\frac{1}{2}}]\,dy = \left[\frac{i}{(\pi\sinh y)}\right] \times \{e^{\zeta\sinh\gamma}[E_1(\zeta e^{\gamma}) + E_1(\zeta e^{-\gamma+i\pi})] - e^{-\zeta\sinh\gamma}[E_1(\zeta e^{-\gamma}) + E_1(\zeta e^{\gamma+i\pi})]\}. \quad \text{(A14)}$$

Now, if β is real and $|\beta| \le 1$, $\mathrm{Re}\,\gamma = 0$, i.e., $\gamma = i\theta$ with $0 \le \theta \le \pi$. Equation (A1) becomes

$$\int_0^{\infty} e^{-x\cos\theta} K_0[x^{\frac{1}{2}}(x+2\alpha)^{\frac{1}{2}}]\,dx = \frac{i}{2\sin\theta}[e^{z_1}E_1(z_1) - e^{z_2}E_1(z_2)]. \quad \text{(A15)}$$

with $z_1 = \alpha e^{\pm i\theta}$; $0 \le \theta < \pi$. For the special cases $\theta = \frac{1}{2}\pi$, 0, we have, respectively,

$$\int_0^{\infty} K_0[x^{\frac{1}{2}}(x+2\alpha)^{\frac{1}{2}}]\,dx = \{\tfrac{1}{2}\pi - \mathrm{Si}\,(\alpha)\}\cos\alpha + \mathrm{Ci}\,(\alpha)\sin\alpha \quad \text{(A16)}$$

for $|\arg\alpha| < \frac{1}{2}\pi$,

$$\int_0^{\infty} e^{-x} K_0[x^{\frac{1}{2}}(x+2\alpha)^{\frac{1}{2}}]\,dx = 1 - \alpha e^{\alpha} E_1(\alpha). \quad \text{(A17)}$$

Complementary Integral

We now evaluate

$$\int_{-\infty}^{\infty} e^{-y\cos\theta} K_0[(y^2-\alpha^2)^{\frac{1}{2}}]\,dy$$

[25] An alternative proof of Eqs. (A12), (A14) may be obtained by applying the operator sequence

$$\lim_{\nu\to 0}\left(1 \pm \frac{i}{\pi}\frac{\partial}{\partial\nu}\right)\lim_{\kappa\to\frac{1}{2}}\left(1 - \frac{\partial}{\partial\beta}\right)$$

to Eq. (17) of Ref. 16, Vol. II, p. 360.

for α an arbitrary complex number. From (A1)

$$I(\alpha, \cos\theta) = \int_0^\infty e^{-x\cos\theta} K_0\{[(x+\alpha)^2 - \alpha^2]^{\frac{1}{2}}\}\, dx$$

for $\theta \neq \pi$. Define $y = x + \alpha$ and modify the corresponding contour in the complex y plane, with the same justification as was used earlier so that

$$I(\alpha, \cos\theta) = e^{\alpha\cos\theta}\left(\int_\alpha^0 + \int_0^\infty\right) e^{-y\cos\theta} K_0[(y^2-\alpha^2)^{\frac{1}{2}}]\, dy.$$

Again, putting $y = -(x + \alpha e^{\pm i\pi})$, and excluding $\theta = 0$,

$$I(\alpha e^{\pm i\pi}, -\cos\theta) = e^{\alpha\cos\theta}\left(\int_0^\alpha + \int_{-\infty}^0\right) e^{-y\cos\theta} K_0[(y^2-\alpha^2)^{\frac{1}{2}}]\, dy,$$

where we choose the upper or lower sign according as $\arg\alpha < 0$ or $\arg\alpha \geq 0$. Therefore

$$\int_{-\infty}^\infty e^{-y\cos\theta} K_0[(y^2-\alpha^2)^{\frac{1}{2}}]\, dy = e^{-\alpha\cos\theta}[I(\alpha, \cos\theta) + I(\alpha e^{\pm i\pi}, -\cos\theta)]. \quad \text{(A18)}$$

Using (A15) and the property $E_1(ze^{\pm 2\pi i}) = E_1(z) \mp 2\pi i$ this then reduces to

$$\int_{-\infty}^\infty e^{-y\cos\theta} K_0[(y^2-\alpha^2)^{\frac{1}{2}}]\, dy = \frac{\pi}{\sin\theta} e^{\mp i\alpha\sin\theta} \quad \text{(A19)}$$

for $\theta \neq 0, \pi$.

For instance if $\alpha = \pm ia$ with a real and positive (A19) becomes

$$\int_{-\infty}^\infty e^{-y\cos\theta} K_0[(y^2+a^2)^{\frac{1}{2}}]\, dy = \frac{\pi}{\sin\theta} e^{-a\sin\theta} \quad \text{(A20)}$$

or if $\alpha = a$

$$\int_{-\infty}^\infty e^{-y\cos\theta} K_0[(y^2-a^2)^{\frac{1}{2}}]\, dy = \frac{\pi}{\sin\theta} e^{ia\sin\theta}. \quad \text{(A21)}$$

In physical applications of the causal Green's function we remember that small negative imaginary parts are added to the masses, and at the end the limit is taken where they vanish. If the development of Wick's form for the Green's function (5.1) is carefully followed one finds that U has a small negative imaginary part. It is for this reason that the range of arg α has been taken to include $-\pi$ rather than π, and (A21) gives the correct form for the complementary integral function needed here.

Asymptotic Forms

If we use the asymptotic form[26] for the exponential integral function

$$E_1(z) \underset{|z|\to\infty}{\sim} \frac{e^{-z}}{z} \sum_{t=0}^N (-1)^t \frac{t!}{z^t} + O(z^{-(N+1)}), \quad |\arg z| < \tfrac{3}{2}\pi \quad \text{(A22)}$$

we have for $\theta \neq \pi$, $|\arg\alpha| \leq \frac{1}{2}\pi$

$$I(\alpha, \cos\theta) \underset{|\alpha|\to\infty}{\sim} \frac{i}{2\sin\theta}\left[\sum_{t=0}^N (-1)^t \frac{t!}{\alpha^{t+1}} e^{-i(t+1)\theta} - \sum_{t=0}^N (-1)^t \frac{t!}{\alpha^{t+1}} e^{i(t+1)\theta}\right] = \sum_{t=0}^N (-1)^t \frac{t!}{\alpha^{t+1}} U_t(\cos\theta), \quad \text{(A23)}$$

where $U_t(\cos\theta) = \sin(t+1)\theta/\sin\theta$. We note that $U_t[\cos(\pi-\theta)] = (-1)^t U_t(\cos\theta)$ and $U_t(1) = t+1$. Thus

$$I(\alpha, 1) \underset{|\alpha|\to\infty}{\sim} \sum_{t=0}^N (-1)^t (t+1)!/\alpha^{t+1}. \quad \text{(A24)}$$

For $|\arg z|$ outside the range of application of (A22) we use $E_1(ze^{\pm 2\pi i}) = E_1(z) \mp 2\pi i$; e.g., for $|\arg\beta| \leq \frac{1}{2}\pi$, $\theta \neq 0, \pi$ we have

$$I(\beta e^{-i\pi}, \cos\theta) = \frac{\pi}{\sin\theta} e^{-\beta e^{-i\theta}} - \frac{i}{2\sin\theta}[e^{w_1} E_1(w_1) - e^{w_2} E_1(w_2)] \underset{|\beta|\to\infty}{\sim} \frac{\pi}{\sin\theta} e^{-\beta e^{-i\theta}} - \sum_{t=0}^N \frac{t!}{\beta^{t+1}} U_t(\cos\theta), \quad \text{(A25)}$$

where $w_{\frac{1}{2}} = \beta e^{\pm i(\pi-\theta)}$. For $\theta = 0$

$$I(\beta e^{-i\pi}, 1) \sim -\sum_{t=1}^N \frac{t!}{\beta^t}. \quad \text{(A26)}$$

For[27] $\theta = \frac{1}{2}\pi$

$$I(\beta e^{-i\pi}, 0) = \pi e^{i\beta} - [\mathrm{Ci}(\beta)\sin\beta - \mathrm{si}(\beta)\cos\beta] \sim \pi e^{i\beta} - \beta^{-1} \sum_{t=0}^N \frac{(-1)^t (2t)!}{\beta^{2t}}. \quad \text{(A27)}$$

[26] See Ref. 9, p. 231, Eq. (5.1.51).
[27] See Ref. 9, pp. 232, 233, Eqs. (5.2.5), (5.2.6), (5.2.21), (5.2.23), (5.2.34).

A New Derivation of the Kinetic Equation for an Inhomogeneous Plasma

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The kinetic equation for non-uniform plasma is derived from the Liouville equation by the Prigogine–Balescu diagram technique. The obtained equation is equivalent to the equation derived earlier by Balescu and this author, but has a little simpler form. The equation has a non-Markoffian form and is valid in both stable and unstable cases and for long and short times. Its explicit form is obtained by using the Resibois' summation procedure. The limiting form of the equation for long times in the stable case is derived.

1. INTRODUCTION

IN this paper a new way of deriving the kinetic equation for the slightly inhomogeneous plasma is studied. The kinetic equation for inhomogeneous plasma was first studied by Guernsey.[1] He derived the equation describing the inhomogeneous plasma in a state close to equilibrium. That problem was generalized by Balescu and this author[2] for the case of plasma far from equilibrium. In this paper the equation, obtained by Balescu and this author, is rederived in a slightly different form. It is obtained by using the Prigogine–Balescu[3-5] diagram technique and Résibois'[6] summation procedure.

The physical problem studied here is identical to the problem of Ref. 2. We consider an electron plasma for which an absolute variation of one-particle distribution is small but an arbitrary spatial gradients are allowed. In other words, we assume that the absolute value of the inhomogeneity factor is small compared to the velocity distribution function, but we assume practically nothing about the support of the inhomogeneity factor in $\mathbf{k}$ space. The inhomogeneity factor may not vanish for large $\mathbf{k}$.

The general form of the non-Markoffian equation is valid in both stable and unstable cases. The simplified Markoffian form derived later describes only sufficiently stable states. The generalization of this equation to the case of unstable or slightly stable plasma is completely analogous to the procedure described by Balescu.[7]

2. DERIVATION OF KINETIC EQUATION

The system studied in the present paper is an idealized plasma consisting of a slightly spatially inhomogeneous electron gas of mean density $c = N/\Omega$, where N is the total number of electrons, Ω is the volume. The electron gas is imbedded into a continuous neutralizing positive background.

The system is described by the classical Liouville equation

$$\mathfrak{L} f_N = (\mathfrak{L}^0 + e^2 \mathfrak{L}') f_N = 0, \tag{2.1}$$

where

$$\mathfrak{L}^0 = \partial_t + \sum_j \mathbf{v}_j \nabla_j;$$
$$\mathfrak{L}' = -m^{-1} \sum_{j<n} (\nabla_j V_{jn})(\partial_j - \partial_n); \tag{2.2}$$
$$\partial_t = \frac{\partial}{\partial t}; \qquad \nabla_j = \frac{\partial}{\partial \mathbf{x}_j}; \qquad \partial_j = \frac{\partial}{\partial \mathbf{v}_j};$$

$\mathbf{v}j$, $\mathbf{x}j$, and m are the velocity, position, and mass of j particle, respectively, and Coulomb potential can be written in the form

$$V_{jn} = (|\mathbf{x}_j - \mathbf{x}_n|)^{-1} = \frac{1}{2\pi} \int k^{-2} \exp\,[i\mathbf{k}(\mathbf{x}_j - \mathbf{x}_n)]\, d\mathbf{k}. \tag{2.3}$$

The problem considered here is, from the physical point of view, identical to the problem of Ref. 2. We therefore do not repeat here the proper approximation. We use here the approximation introduced there and called the slightly inhomogeneous ring approximation. A Prigogine–Balescu[3-5] diagram which gives a typical contribution in this approximation is shown in Fig. 1. The expression for inhomogeneity

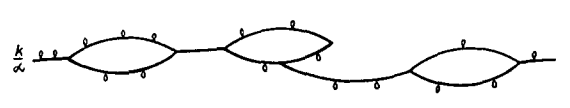

FIG. 1. A general contribution to $\rho_{\mathbf{k}}(\alpha, t)$ in slightly inhomogeneous ring approximation.

[1] R. Guernsey, Phys. Fluids 5, 322 (1962).
[2] R. Balescu and A. Kuszell, J. Math. Phys. 5, 1140 (1964).
[3] R. Balescu, *Statistical Mechanics of Charged Particles* (John Wiley & Sons, Inc., New York, 1963).
[4] I. Prigogine and R. Balescu, Physica 25, 281 (1959).
[5] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1962).
[6] P. Résibois, Phys. Fluids 6, 817 (1963).
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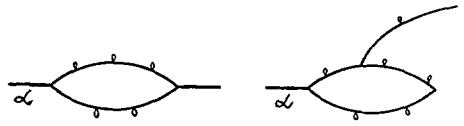

(a) (b)

FIG. 2. The typical slightly inhomogeneous rings.

factor was derived in Ref. 2 and can be written in the form

$$\tilde{\rho}_{\mathbf{k}}(\alpha; z) = \frac{1}{i[\mathbf{k}\mathbf{v}_\alpha - z]}\left\{\rho_{\mathbf{k}}(\alpha; 0) - \int_0^\infty d\tau \exp(iz\tau)\right.$$
$$\times\left[k^{-2}\omega_p^2 i\mathbf{k}\,\partial_\alpha\,\varphi(\alpha)\int d\mathbf{v}_1\,\rho_{\mathbf{k}}(1;\tau)\right.$$
$$\left.\left.+\sum_n\iint_{(n)}\sum_j R_{\mathbf{k}}^{(\alpha,j)}(z)\rho_{\mathbf{k}}(j\mid\alpha\cdots;\tau)\right]\right\}, \qquad (2.4)$$

where

$$\omega_p^2 = 4\pi e^2 c m^{-1} \qquad (2.5)$$

is the plasma frequency. The resolvent operator has the form

$$R_{\mathbf{k}}^{(\alpha,j)}(z) = \sum_{n=1}^{\infty}(-e^2)^{n+1}$$
$$\times\langle\mathbf{k}^{(\alpha)}|\,\mathfrak{L}'[R_0(z)\mathfrak{L}']^n\,|\mathbf{k}^{(j)}\rangle. \qquad (2.6)$$

The matrix elements of operator $R_0(2)$ on the set of wave vectors $\{k\}$ has the following form

$$\langle\{k\}|\,R_0(z)\,|\{k'\}\rangle$$
$$= \frac{1}{i[\sum_i \mathbf{k}_i\mathbf{v}_i - z]}\prod_i \delta(\mathbf{k}_i - \mathbf{k}_i'). \qquad (2.7)$$

The last term in (2.4) represents the effect of collision. In order to evaluate this term we can divide the slightly inhomogeneous rings into two separated classes. To the first group called A belong all rings whose right line is connected with the proper ring throught the inhomogeneous creation vertex  . To the second group B belong all diagrams whose connection vertex is of the type inhomogeneous destruction vertex  according to the terminology of Ref. 3. The general rings of Classes A and B are represented on Figs. 2(a) and 2(b), respectively.

For calculating the contribution of the general inhomogeneous rings we use the Résibois' theorem[6] on the factorization property, in the form exposed in Appendix 10 of Ref. 3.

Let us consider the diagram D which consists of two disconnected parts. We call the permutation class of diagrams generated by diagram D all diagrams obtained by the permutation of vertices of one subdiagram with respect to the vertices of the second subdiagram, but in such a way that the order of vertices of each subdiagram is unchanged. The diagram on which the all vertices of one subdiagram are on the left of all vertices of second subdiagram, is called the primitive diagram of the permutation class.

The Résibois theorem tells us that the contribution of the whole permutation class can be written in the form of the contribution of both subdiagrams of the primitive diagram.

$$R(z) = \frac{1}{2\pi}\int_{C'} P(z')Q(z - z')\,dz', \qquad (2.8)$$

where $R(z)$ is the contribution of the permutation class, $Q(z)$ and $P(z)$ are the contributions of the subdiagrams and the contour C' consists of a line parallel to the real axis lying above all singularities of $P(z')$ and below singularities of $Q(z - z')$.

The primitive rings of groups A and B are shown respectively by (a) and (b) in Fig. 3. The contribution of the permutation class of general way of type A can be evaluated as convolution of the contribution of two subdiagrams. This contribution can be directly evaluated and one can write it in the following form

$$Q_{n,n'}(\alpha, z) = \frac{\omega_p^2}{i(\mathbf{k}\mathbf{v}_\alpha - z)}\int l^{-2}\,d\mathbf{l}\;i\mathbf{l}\;\partial_\alpha\frac{1}{2\pi}\int_{C'}dz'\,\frac{d_{\mathbf{k}+\mathbf{l}}(\alpha,\tau)}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - z'}\prod_{q=1}^{n-1}\int d\mathbf{v}_q\,\frac{d_{\mathbf{k}+\mathbf{l}}(q,\tau)}{(\mathbf{k}+\mathbf{l})\mathbf{v}_q - z'}$$
$$\times\int\frac{d\mathbf{v}_n}{i[(\mathbf{k}+\mathbf{l})\mathbf{v}_n - z']}\prod_{s=1}^{n'-1}\int\frac{d_{-\mathbf{l}}(s,\tau)\,d\mathbf{v}_s}{z' - \mathbf{l}\mathbf{v}_s - z}\int\frac{d\mathbf{v}_{n'}}{i[-\mathbf{l}\mathbf{v}_{n'} - z + z']} \qquad (2.9)$$
$$\left\{\begin{array}{l} -\dfrac{\omega_p^2}{cl^2}\,i\mathbf{l}[(1-\delta_{n,0})\,\partial_{n,n'}\rho_{\mathbf{k}}(n;\tau) + \delta_{n,0}\,\partial_{\alpha,n'}\rho_{\mathbf{k}}(\alpha,\tau)]\varphi(n',\tau) \\ \text{or} \\ \dfrac{\omega_p^2}{|\mathbf{k}+\mathbf{l}|^2 c}\,i(\mathbf{k}+\mathbf{l})[(1-\delta_{n,0})\,\partial_{n',n}\varphi(n;\tau) + \delta_{n,0}\,\partial_{n',\alpha}\varphi(\alpha,\tau)]\rho_{\mathbf{k}}(n,\tau) \end{array}\right\},$$

where we use the notation

$$d_{\mathbf{k}}(\alpha, \tau) = \omega_p^2 k^{-2} \mathbf{k}\, \partial_\alpha \varphi(\alpha; \tau). \quad (2.10)$$

The upper value corresponds to the diagram whose right inhomogeneous line is labeled by index n (or α) and lower value when this line is labeled by index n'.

Performing summation over $n = 0, 1 \cdots \infty$ and $n' = 1, 2 \cdots \infty$ we get the contribution of all diagrams of type A in the following form:

$$\sum_{n=0}^{\infty} Q_{n,n'}(\alpha, z) = \frac{1}{i[\mathbf{k}\mathbf{v}_\alpha - z]} \int \frac{\omega_p^2}{l^2}\, d\mathbf{l}\, i\mathbf{l}\, \partial_\alpha \frac{1}{2\pi} \int_{C'} dz' \frac{1}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - z'} \int d\mathbf{v}_\beta \quad (2.11)$$

$$\left[\delta(\alpha - \beta) + \frac{d_{\mathbf{k}+\mathbf{l}}(\alpha, \tau)}{\varepsilon^+_{\mathbf{k}+\mathbf{l}}(z')} \frac{1}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - z'}\right] \int \frac{d\mathbf{v}_\gamma}{z' - \mathbf{l}\mathbf{v}_\gamma - z}$$

$$\times \left[\frac{\omega_p^2}{c\,|\mathbf{k}+\mathbf{l}|^2} (\mathbf{k}+\mathbf{l})\, \partial_{\gamma\beta} \rho_{\mathbf{k}}(\gamma)\varphi(\beta) - \frac{\omega_p^2}{cl^2}\, \mathbf{l}\, \partial_{\beta\gamma} \rho_{\mathbf{k}}(\beta)\varphi(\gamma)\right] = \frac{\omega_p^2}{i[\mathbf{k}\mathbf{v}_\alpha - z]} \int \frac{d\mathbf{l}}{l^2}\, i\mathbf{l}\, \partial_\alpha G^A_{\mathbf{k},\mathbf{l}}(\alpha, z; \tau),$$

where we have introduced Vlasov dielectric constant

$$\varepsilon^+_{\mathbf{k}}(z) = 1 - k^{-2}\omega_p^2 \int \frac{\mathbf{k}\, \partial_\alpha \varphi(\alpha; \tau)}{\mathbf{k}\mathbf{v}_\alpha - z}\, d\mathbf{v}_\alpha. \quad (2.12)$$

If we put $\mathbf{k} = 0$ and $\varphi(\alpha)$ instead of $\rho_{\mathbf{k}}(\alpha)$ in the expression (2.11), we obtain the expression identical to the respective collision operator for the homogeneous plasma (Refs. 3, 6–8) but multiplied by factor 2.

This factor 2 is explained by the fact that we have distinguished the diagrams whose right inhomogeneous lines were labeled by indices n or n'.

The summation of diagrams of type B is a little bit more complicated. For this purpose we introduce a new diagram line ——|$\psi(\alpha)$, which describes the operator acting on some function $\psi(\alpha)$ but in which the propagator is unchanged. The usual diagram line $\mathbf{k}/\alpha$ one can represent using new notation as $(\mathbf{k}/\alpha)|\rho_{\mathbf{k}}(\alpha, \tau)$. In our considerations we put instead of $\psi(\alpha)$ the function arising from the homogeneous creation vertex ⟩. We can represent the contribution of these diagrams as a convolution of contributions of subdiagrams. Denoting the contribution of subdiagrams with branch line by $P_{1,\mathbf{k}}(\alpha, z)$ we can write it as the sum of the series of diagrams shown in Fig. 4.

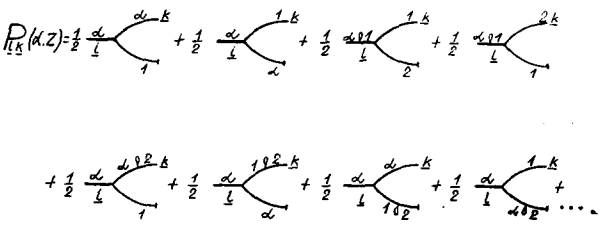

FIG. 4. The series for $P_{1,\mathbf{k}}(\alpha, 2)$.

Summing partially this series we obtain

$$P_{1,\mathbf{k}}(\alpha, z)\psi(\alpha) = T_{1,\mathbf{k}}(\alpha, z)\psi(\alpha)$$

$$+ \frac{d_1(\alpha, \tau)}{\mathbf{l}\mathbf{v}_\alpha - z} \int T_{1,\mathbf{k}}(1, z)\psi(1)\, d\mathbf{v}_1 + \frac{d_1(\alpha, \tau)}{\mathbf{l}\mathbf{v}_\alpha - z}$$

$$\times \int \frac{d_1(1, \tau)}{\mathbf{l}\mathbf{v}_1 - z}\, d\mathbf{v}_1 \int T_{1,\mathbf{k}}(2, z)\psi(2)\, d\mathbf{v}_2 + \cdots$$

$$= T_{1,\mathbf{k}}(\alpha, z)\psi(\alpha) + \frac{d_1(\alpha, \tau)}{\mathbf{l}\mathbf{v}_\alpha - z} \frac{1}{\varepsilon^+_1(z)} \int T_{1,\mathbf{k}}(1, z)\psi(1)\, d\mathbf{v}_1, \quad (2.13)$$

where

$$T_{1,\mathbf{k}}(\alpha, z) = T^{(1)}_{1,\mathbf{k}}(\alpha, z) + T^{(2)}_{1,\mathbf{k}}(\alpha, z) \quad (2.14)$$

and $T^{(1)}_{1,\mathbf{k}}(\alpha, z)$, $T^{(2)}_{1,\mathbf{k}}(\alpha, z)$ are defined by the series of diagrams shown in Fig. 5.

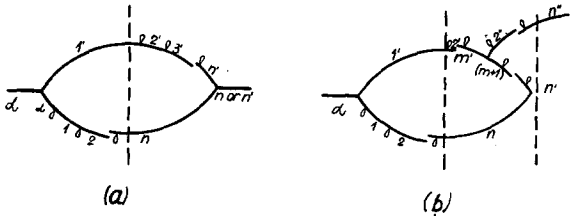

FIG. 3. The general primitive rings.

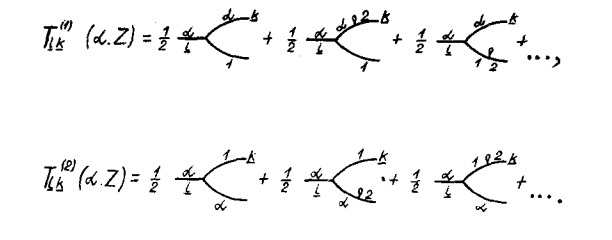

FIG. 5. The series for $T^{(1)}_{1,\mathbf{k}}$ and $T^{(2)}_{1,\mathbf{k}}$.

[8] R. Balescu, Phys. Fluids 3, 52 (1960).

The contribution $T^{(1)}_{1,\mathbf{k}}(\alpha, 2)$ can be written in the following form

$$T^{(1)}_{\mathbf{k},1}(\alpha, z)\psi(\alpha) = \frac{1}{2}\frac{\omega_p^2 |\mathbf{k}-1|^{-2}}{\mathbf{l}\mathbf{v}_\alpha - 2}(\mathbf{k}-\mathbf{l})\,\partial_\alpha \int d\mathbf{v}_1 \frac{1}{2\pi} \times \int_{C'} dz' R_{\mathbf{k}}(\alpha, z') S_{1-\mathbf{k}}(1, z-z')\psi(1), \quad (2.15)$$

where the function $R_{\mathbf{k}}(\alpha, z)$ is the Laplace transform of the solution of the linearized Vlasov equation $\tilde{R}_{\mathbf{k}}(\alpha, t)$ with the initial condition

$$\tilde{R}_{\mathbf{k}}(\alpha, 0) = \rho_{\mathbf{k}}(\alpha; \tau). \quad (2.16)$$

The function $R_{\mathbf{k}}(\alpha, z)$ has the well-known form

$$R_{\mathbf{k}}(\alpha, z) = \frac{\rho_{\mathbf{k}}(\alpha; z)}{\mathbf{k}\mathbf{v}_\alpha - z} + \frac{1}{\varepsilon^+_{\mathbf{k}}(z)}\frac{d_{\mathbf{k}}(\alpha, \tau)}{\mathbf{k}\mathbf{v}_\alpha - z}\int \frac{\rho_{\mathbf{k}}(1; \tau)\, d\mathbf{v}_n}{\mathbf{k}\mathbf{v}_1 - z}. \quad (2.17)$$

Similarly the operator $S_{\mathbf{k}}(\alpha, z)$ defined by the series of diagrams shown on Fig. 6, acting on the function $\psi(\alpha)$ can be written in the analytical form

$$S_{\mathbf{k}}(\alpha, z)\psi(\alpha) = \frac{\psi(\alpha)}{\mathbf{k}\mathbf{v}_\alpha - z} + \frac{1}{\varepsilon^+_{\mathbf{k}}(z)}\frac{d_{\mathbf{k}}(\alpha, \tau)}{\mathbf{k}\mathbf{v}_\alpha - z}\int \frac{\psi(1)\, d\mathbf{v}_1}{\mathbf{k}\mathbf{v}_1 - z}. \quad (2.18)$$

It is easy to see that if we put in the expresion (2.18) $\rho_{\mathbf{k}}(\alpha; \tau)$ instead of $\psi(\alpha)$ we obtain the function $R_{\mathbf{k}}(\alpha, z)$. Similarly we can express the operator $T^{(2)}_{1,\mathbf{k}}(\alpha, z)$ as follows:

$$T^{(2)}_{1,\mathbf{k}}(\alpha, z) = -\frac{1}{2}\frac{\omega_p^2 k^{-2}}{\mathbf{l}\mathbf{v}_\alpha - z}\mathbf{k}\,\partial_\alpha \int d\mathbf{v}_1 \frac{1}{2\pi} \times \int_{C'} dz' R_{\mathbf{k}}(1, z') S_{1-\mathbf{k}}(\alpha, z-z'). \quad (2.19)$$

Now we can complete the summation procedure by calculating the contribution of the whole class of diagrams of type B. It can be written in the form

$$Q^B_{\mathbf{k}}(\alpha, z) = \frac{\omega_p^2}{i[\mathbf{k}\mathbf{v}_\alpha - z]}\int d\mathbf{v}_1 \int d\mathbf{l}\, l^{-2} i\mathbf{l}\,\partial_\alpha \frac{1}{2\pi}\int_{C'} dz' \times [P_{-1,\mathbf{k}}(1, z')S_{\mathbf{k}+1}(\alpha, z-z') - P_{\mathbf{k}+1,\mathbf{k}}(\alpha, z')S_{-1}(1, z-z')]\frac{\omega_p^2}{|\mathbf{k}+1|^2}(\mathbf{k}+\mathbf{l})\,\partial_{\alpha 1}\varphi(\alpha; \tau)\varphi(1; \tau)$$

$$= \frac{\omega_p^2}{i[\mathbf{k}\mathbf{v}_\alpha - z]}\int l^{-2}\, d\mathbf{l}\, i\mathbf{l}\,\partial_\alpha G^B_{\mathbf{k},1}(\alpha, z; \tau). \quad (2.20)$$

3. KINETIC EQUATION IN THE STABLE CASE.

The expression for the Laplace transform of the inhomogeneity factor can be written in the form

$$\tilde{\rho}_{\mathbf{k}}(\alpha; z) = \frac{1}{i[\mathbf{k}\mathbf{v}_\alpha - z]}\left\{\rho_{\mathbf{k}}(\alpha; 0) - \int_0^\infty d\tau \exp(iz\tau) \times \left[id_{\mathbf{k}}(\alpha, \tau)\int d\mathbf{v}\, \rho_{\mathbf{k}}(\mathbf{v}; \tau) + \omega_p^2 \times \int 1^{-2}\, d\mathbf{l}\, i\mathbf{l}\,\partial_\alpha(G^A_{\mathbf{k},1}(\alpha, z, \tau) + G^B_{\mathbf{k},1}(\alpha, z, \tau))\right]\right\}. \quad (3.1)$$

Taking the inverse Laplace transformation of expression (3.1) and differentiating it with respect to time we can write the equation for $\rho_{\mathbf{k}}(\alpha; t)$ in the following form:

$$D_t\rho_{\mathbf{k}}(\alpha; t) = \int_0^t d\tau \frac{1}{2\pi}\int \exp(-iz\tau)\, dz \int \frac{\omega_p^2}{l^2}\, d\mathbf{l} \times \{i\mathbf{l}\,\partial_\alpha[G^A_{\mathbf{k},1}(\alpha, z, t-\tau) + G^B_{\mathbf{k},1}(\alpha, z, t-\tau)]\}, \quad (3.2)$$

where we have introduced the well-known linearized Vlasov operator,

$$D_t\rho_{\mathbf{k}}(\alpha; t) = \partial_t\rho_{\mathbf{k}}(\alpha; t) + i\mathbf{k}\mathbf{v}_\alpha\rho_{\mathbf{k}}(\alpha; t) - i\, d_{\mathbf{k}}(\alpha, t)\int d\mathbf{v}\, \rho_{\mathbf{k}}(\mathbf{v}; t). \quad (3.3)$$

Equation (3.2) has the most general form of the kinetic equation in a slightly inhomogeneous ring approximation. It is valid in the stable, as well as in unstable case, for long and short times. On the other hand it has a very complicated non-Markoffian form. The ring approximation according to the discussion given in Refs. 3, 7, and 8 is more correct for long times.

We get a Markoffian limit using the procedure exposed in detail in Refs. 3, 8. In the stable case

$$R_k(\alpha, z) = \frac{\alpha}{k} + \frac{\alpha\rho 1}{k} + \frac{\alpha\rho 1\rho 2}{k} + \dots,$$

$$S_k(\alpha, z) = \frac{\alpha}{k} + \frac{\alpha\rho 1}{k} + \frac{\alpha\rho 1\rho 2}{k} + \dots.$$

FIG. 6. The series for $R(\alpha, z)$ and $S(\alpha, z)$.

the limiting form of the equation can be written in the form

$$D_t\rho_{\mathbf{k}}(\alpha;t) = \frac{1}{2\pi}\int_C \frac{\exp(izt)}{-iz}\,dz \int d\mathbf{l}\,\frac{\omega_p^2}{l^2}\,i\mathbf{l}\,\partial_\alpha \times [G^A_{\mathbf{k},\mathbf{l}}(\alpha,z,t) + G^B_{\mathbf{k},\mathbf{l}}(\alpha,z,t)]. \quad (3.4)$$

Equation (3.4) is of a Markoffian type but still it contains the so-called transient terms which are very rapidly oscillating and damped. We assume now that the system is stable or, more precisely, strongly stable. This means that all singularities of functions are placed in the lower half-plane and separated from the real axis at least by the distance ω_p^{-1}. The contribution of this singularities is for the times longer than ω_p^{-1} negligible and we can take into account only the pole at $z = 0$. So we can write Eq. (3.4) in the following form:

$$D_t\rho_{\mathbf{k}}(\alpha,t) = \frac{1}{2\pi}\int_C d\mathbf{l}\,\frac{\omega_p^2}{l^2}\,i\mathbf{l}\,\partial_\alpha \times [G^A_{\mathbf{k},\mathbf{l}}(\alpha,0;t) + G^B_{\mathbf{k},\mathbf{l}}(\alpha,0;t)]. \quad (3.5)$$

Now we are going to evaluate functions $G^{A,B}_{\mathbf{k},\mathbf{l}}(\alpha,0;t)$. Because the functions $G^{A,B}_{\mathbf{k},\mathbf{l}}(\alpha,z;\alpha)$ are well defined only for z belong to the upper half-space, we take a limit when z is going to be real. We can rewrite expression for $G^A_{\mathbf{k},\mathbf{l}}(\alpha,z;t)$ in the more convenient form

$$G^A_{\mathbf{k},\mathbf{l}}(\alpha,z;t) = \frac{1}{\varepsilon^+_{-\mathbf{l}}[z-(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha]} \times \int \frac{d\mathbf{v}\,\psi(\mathbf{v}_\alpha,\mathbf{v})}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - \mathbf{l}\mathbf{v} - z} + \frac{1}{2\pi}\int_{C'} dz' \times \frac{d_{\mathbf{k}+\mathbf{l}}(\alpha,t)}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - z'}\,\frac{1}{\varepsilon^+_{-\mathbf{l}}(z-z')\varepsilon^+_{\mathbf{k}+\mathbf{l}}(z')} \times \int_{-\infty}^{\infty}\frac{ds}{|\mathbf{k}+\mathbf{l}|\,s-z'}\int\frac{du}{lu-z+z'} \times \int d\mathbf{v}_1\,\delta[(\mathbf{k}+\mathbf{l})\mathbf{v}_1 - |\mathbf{k}+\mathbf{l}|\,s] \times \int d\mathbf{v}_2\,\delta(l\mathbf{v}_2+lu)\psi(\mathbf{v}_1,\mathbf{v}_2), \quad (3.6)$$

where the notation is

$$\psi(\mathbf{v}_2,\mathbf{v}_\beta) = \frac{e^2}{2\pi^2 m} \times [|\mathbf{k}+\mathbf{l}|^{-2}(\mathbf{k}+\mathbf{l})\,\partial_{\alpha\beta}\rho_{\mathbf{k}}(\alpha)\varphi(\beta) - l^{-2}\mathbf{l}\,\partial_{\beta\alpha}\rho_{\mathbf{k}}(\beta)\varphi(\alpha)]. \quad (3.7)$$

Now let us take the contours C and C' in such a way that for $z \in C$ and $z' \in C'$ (and $\varepsilon > 0$)

$$z = x + 2i\varepsilon, \qquad z' = y + i\varepsilon, \quad (3.8)$$

where x and y are real.

Taking the limit $\varepsilon \to 0$ we find the expression for $G^A_{\mathbf{k},\mathbf{l}}(\alpha,0;t)$ in the following form:

$$G^A_{\mathbf{k},\mathbf{l}}(\alpha,0;t) = \frac{\pi}{\varepsilon^-_{\mathbf{l}}[(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - y]} \times \int d\mathbf{v}\,\delta_-[(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - \mathbf{l}\mathbf{v}]\psi(\mathbf{v}_\alpha,\mathbf{v}) + \frac{\pi^2}{2}\,d_{\mathbf{k}+\mathbf{l}}(\alpha,t)\int_{-\infty}^{\infty} dy\,\delta_-[(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - y] \times \frac{1}{\varepsilon^-_{\mathbf{l}}(y)\varepsilon^+_{\mathbf{k}+\mathbf{l}}(y)}\iint ds\,du\,\delta_-[|\mathbf{k}+\mathbf{l}|\,s-y]\,\delta_-[lu-y] \times \int d\mathbf{v}_1\,\delta[(\mathbf{k}+\mathbf{l})\mathbf{v}_1 - |\mathbf{k}+\mathbf{l}|\,s] \times \int d\mathbf{v}_2\,\delta(l\mathbf{v}_2+lu)\psi(\mathbf{v}_1,\mathbf{v}_2), \quad (3.9)$$

where we use the symmetry properties of the dielectric constant

$$\varepsilon^+_{\mathbf{k}}(z) = \varepsilon^-_{-\mathbf{k}}(-z). \quad (3.10)$$

One can easily see that the integral of the function $R_{\mathbf{k}}(\alpha,z)$ has the simple form

$$\int R_{\mathbf{k}}(\alpha,z)\,d\mathbf{v}_\alpha = \frac{1}{\varepsilon^+_{\mathbf{k}}(z)}\int\frac{\rho_{\mathbf{k}}(\mathbf{v})\,d\mathbf{v}}{\mathbf{k}\mathbf{v}-z}. \quad (3.11)$$

The similar expression can be found for integrals of operators

$$S_{\mathbf{k}}(\alpha,z) \quad \text{and} \quad P_{\mathbf{k},\mathbf{l}}(\alpha,z).$$

Using these formulas we can write

$$G^B_{\mathbf{k},\mathbf{l}}(\alpha,z;t) = \frac{1}{\varepsilon^+_{-\mathbf{l}}[z-(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha]}\int d\mathbf{v}_\beta T_{-\mathbf{l},\mathbf{k}}(\mathbf{v}_\beta, z-(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha)\varphi(\alpha,\beta) + \frac{1}{2\pi}\int_{C'} dz' \times \left\{\frac{d_{\mathbf{k}+\mathbf{l}}(\alpha,t)}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - z'}\,\frac{1}{\varepsilon^+_{\mathbf{k}+\mathbf{l}}(z')\varepsilon^-_{\mathbf{l}}(z-z')}\iint d\mathbf{v}_\beta\,d\mathbf{v}_\gamma\,\frac{T_{-\mathbf{l},\mathbf{k}}(\beta,z-z')}{(\mathbf{l}+\mathbf{k})\mathbf{v}_\gamma - z'} - T_{\mathbf{k}+\mathbf{l},\mathbf{k}}(\alpha,z')\,\frac{1}{\varepsilon^+_{-\mathbf{l}}(z-z')}\right. \times \left.\iint\frac{\delta(\alpha-\gamma)}{-\mathbf{l}\mathbf{v}_\beta - z + z'}\,d\mathbf{v}_\beta\,d\mathbf{v}_\gamma + \frac{d_{\mathbf{k}+\mathbf{l}}(\alpha,t)}{(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - z'}\,\frac{1}{\varepsilon^+_{-\mathbf{l}}(z-z')\varepsilon^+_{\mathbf{k}+\mathbf{l}}(z')}\iint\frac{T_{\mathbf{k}+\mathbf{l},\mathbf{k}}(\gamma,z')}{-\mathbf{l}\mathbf{v}_\beta - z + z'}\,d\mathbf{v}_\beta\,d\mathbf{v}_\gamma\right\}\varphi(\gamma,\beta), \quad (3.12)$$

where we denote

$$\varphi(\gamma, \beta) = \frac{\omega_p^2}{8\pi^2 c\,|\mathbf{k}+\mathbf{l}|^2}(\mathbf{k}+\mathbf{l})\,\partial_{\alpha\beta}\varphi(\alpha)\varphi(\beta). \tag{3.13}$$

The limit operators $T^{(i)}_{\mathbf{k},\mathbf{l}}(\alpha, x; t)$ where x is real have the forms

$$T^{(1)}_{\mathbf{l},\mathbf{k}}(\alpha, x)\psi(\alpha) = \frac{\pi}{2}\frac{\omega_p^2}{|\mathbf{k}-\mathbf{l}|^2}\,\delta_-(\mathbf{l}\mathbf{v}_\alpha - x)(\mathbf{k}-\mathbf{l})\,\partial_\alpha\Big\{\frac{\rho_{\mathbf{k}}(\alpha)}{\varepsilon^-_{\mathbf{k}-\mathbf{l}}(\mathbf{k}\mathbf{v}_\alpha - x)}\,\pi\int \delta_-[\mathbf{k}\mathbf{v}_\alpha + (\mathbf{l}-\mathbf{k})\mathbf{v}_1 - x]\psi(\mathbf{v}_1)\,d\mathbf{v}_1$$
$$+\frac{\pi^2}{2}\,d_{\mathbf{k}}(\alpha, t)\int_{-\infty}^{\infty} dy\;\delta_-[\mathbf{k}\mathbf{v}_\alpha - y]\,\frac{1}{\varepsilon^+_{\mathbf{k}}(y)\varepsilon^-_{\mathbf{k}-\mathbf{l}}(y-x)}$$
$$\times\iint \rho_{\mathbf{k}}(\mathbf{v})\psi(\mathbf{v}_1)\;\delta_-(\mathbf{k}\mathbf{v} - y)\;\delta[(\mathbf{l}-\mathbf{k})\mathbf{v}_1 - x + y]\,d\mathbf{v}_1\,d\mathbf{v}\Big\}, \tag{3.14}$$

and a similar expression for $T^{(2)}_{\mathbf{l},\mathbf{k}}(\alpha, x; t)$.

We can calculate now the final form of the second part of the collision operator:

$$G^B_{\mathbf{k},\mathbf{l}}(\alpha, 0; t) = \frac{1}{\varepsilon^-_{\mathbf{l}}[(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha]}$$
$$\times\int d\mathbf{v}\,T_{-\mathbf{l},\mathbf{k}}(\mathbf{v}, -(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha; t)$$
$$+\frac{\pi}{2}\int_{-\infty}^{\infty} dy\,\Big\{-T_{\mathbf{k}+\mathbf{l},\mathbf{k}}(\mathbf{v}_\alpha, y)\,\frac{1}{\varepsilon^-_{\mathbf{l}}(y)}$$
$$\times\iint d\mathbf{v}_1\,d\mathbf{v}\;\;\delta(\mathbf{v}_\alpha - \mathbf{v})\;\delta_-(y - \mathbf{l}\mathbf{v}_1)$$
$$+\frac{1}{\varepsilon^+_{\mathbf{k}+\mathbf{l}}(y)\varepsilon^-_{\mathbf{l}}(y)}\Big[d_{\mathbf{k}+\mathbf{l}}(\alpha, t)\;\delta_-[(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - y]$$
$$\times\iint d\mathbf{v}\,d\mathbf{v}_1 T_{-\mathbf{l},\mathbf{k}}(\mathbf{v}_1, y)\;\delta_-(\mathbf{k}\mathbf{v} - y)$$
$$+\,d_{\mathbf{k}+\mathbf{l}}(\alpha, t)\;\delta_-[(\mathbf{k}+\mathbf{l})\mathbf{v}_\alpha - y]$$
$$\times\iint d\mathbf{v}\,d\mathbf{v}_1 T_{\mathbf{l}+\mathbf{k},\mathbf{l}}(\mathbf{v}, y)\;\delta_-(y - \mathbf{k}\mathbf{v}_1)\Big]\Big\}\varphi(\mathbf{v}, \mathbf{v}_1). \tag{3.15}$$

The collision operator $G^B_{\mathbf{k},\mathbf{l}}(\alpha, 0; t)$ contains the double convolution terms. These terms correspond to the terms containing the convolution of the homogeneous correlation function with the solution of linearized Vlasov equation in Ref. 2. They contain the trace of non-Markoffian character of the process, the change of the correlations during collisions.

The obtained collision operator has a slightly simpler form than in Ref. 2 and can be more easily discussed.

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Global and Democratic Methods for Classifying N-Particle States

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The "global method" for describing N-particle systems (which relies on the existence of a large invariance group of the total Hamiltonian for N noninteracting particles, the "great group", whose Lie algebra is generated by the "grand angular momentum tensor"), is adapted to describe systems of identical particles by means of basis states with simple symmetry properties (with respect to permutations of the particles). We are led to define and study the concept of "democracy" among the particles, from which we obtain the "democratic" subgroups of the great group. The eigenvectors of a complete set of commuting observables, consisting essentially of Casimir operators of democratic subgroups, may furnish the desired basis. Unfortunately the scheme is seen to be sufficient only in the 3- and 4-particle cases, which, however, are most important. The Appendix contains a discussion of the possible relativistic generalizations of the global method.

INTRODUCTION

THE study of convenient basis systems for N-particle states is of considerable interest in that a correct choice of such a basis may greatly simplify the theoretical description of a given N-particle reaction. This is already true in the case $N = 2$; one needs only to think (for instance) of the general advantages offered by the helicity states[1] over other basis states. For $N > 2$, of course, there exists a very simple method for constructing basis states starting from the case $N = 2$ and using a step-by-step coupling, adding each particle in turn to the system consisting of the preceding ones. In recent years, great progress has been made towards a clear and practical classification of such basis systems, even in the relativistic case,[2] so that one may now immediately use such schemes to analyze concrete reactions, especially in the thoroughly studied case of $N = 3$.[3] This step-by-step scheme, however, suffers a major shortcoming in the fact that the N particles are, by construction, treated on a different footing. That is not very annoying if the particles play different roles in the process to be studied (there even exist important cases where this step-by-step coupling is most natural, for instance, cascade reactions such as: $A + B \to a + b, b \to c + d$). But when one has to treat reactions where identical particles are produced on the same footing (for example, multi-pion-production reactions), it is a very awkward scheme, completely destroying the physical symmetry between these particles. In these cases, one needs a "global" method to supersede the step-by-step coupling scheme. Such a global scheme may be devised[4,5,6] by introducing collective observables of the N-particle system, related to the "grand angular-momentum tensor".[7] Group-theoretical methods render very natural the introduction of this global scheme, at least in the nonrelativistic case, which may serve as a useful model for the more complicated situation encountered in the relativistic case. There also exist multiparticle reactions where the nonrelativistic approximation is valid: $^{12}C^* \to 3\alpha$, $^{16}O^* \to 4\alpha$, etc., and even $K \to 3\pi$.

The global method may be formally extended at once to the relativistic case and such generalizations have been proposed.[6,8] However, these generalizations are far from unique and, in our opinion, lack the physical content of the nonrelativistic theory. This important point is more thoroughly discussed in an Appendix to the present paper. In the absence of a convincing relativistic generalization, we adhere in the following to the nonrelativistic point of view.

If one adopts the global method for classifying the states of a system consisting of N identical particles, there still remains the problem of imposing the suitable symmetry conditions on these states, since we deal with particles obeying either Bose or Fermi statistics (in practice, multiple-particle states con-

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sist essentially of bosons). This is the main problem which we consider in this paper.

We first set the stage for our investigation with a brief review of the group-theoretical point of view on the classification of N-particle states, treatment of phase-space and the global method.[5] We then precisely state the problem to be solved concerning the symmetry properties of N-particle states and sketch a tentative simple method of solution based on the global coupling scheme. We are led to define and study a notion of "democracy" among the N particles, thereby giving a precise meaning to the idea introduced by Dragt under this same name in the case $N = 3$,[4] and at the same time generalizing this idea to higher N values. We conclude by examining the practical applications and the shortcomings of the democracy concept. Finally, the Appendix is devoted to the problem of devising a relativistic global method.

I. GENERALITIES ABOUT N-PARTICLE KINEMATICS

A. Kinematics and Phase-Space

Consider a system of N spinless particles with common mass m. The kinematical properties of the system are completely described by the associated representation of the Galilei group, that is the tensor product of the N equivalent irreducible representations corresponding to the individual particles. The state space of the system is the representation space, which we choose here as the space of square-integrable functions over the momentum-space, i.e., functions $\psi(\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_N)$ satisfying

$$\int |\psi(\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_N)|^2 \, d^3p_1 \cdots d^3p_N < +\infty.$$

To obtain a convenient basis in this state space, we have to choose a complete system of commuting observables whose common eigenvectors form such a basis. These observables naturally fall into two classes, describing on the one hand the kinematical properties of the N-particle system as a whole, and on the other hand its internal structure. In more technical terms, we look for a decomposition of the Galilei group representation into irreducible subspaces. We thus choose basis vectors belonging to these irreducible subspaces, so that they are labeled by two kinds of quantum numbers, ones giving the position of the basis states within the considered irreducible subspace (and corresponding to the observables of the first kind, such as the total energy, momentum, and intrinsic angular momentum of the system) and the others giving the position of this particular irreducible subspace within the global state space (and corresponding to the observables of the second kind, since the very irreducibility of the subspace, meaning that it is not affected by a kinematical transformation, shows that this subspace characterizes some internal property of the system).

There is not much freedom in choosing the observables in the first class, since experimental considerations lead us to diagonalize the energy, momentum, and total angular momentum of the composite system (here, as throughout this paper, "total angular momentum" of the system means "total *intrinsic* angular momentum," i.e., the total angular momentum in the center-of-mass frame). Fixing the energy–momentum 4-vector is a straightforward matter which leaves us with functions defined over the phase-space of the system, i.e., the manifold defined in momentum-space by the constraints

$$\sum_{i=1}^{N} \mathbf{p}_i = \mathbf{P}, \quad \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} = E, \qquad (1a, b)$$

where $(E, \mathbf{P})$ is obviously the energy–momentum of the system. What remains to be done is to diagonalize the angular momentum, that is, more precisely, to decompose into irreducible components the representation of the rotation group O_3 in the space of square-integrable functions over phase-space. This can be done by expanding these functions in spherical harmonics with respect to a suitable sequence of relative momenta: this corresponds to the usual step-by-step coupling scheme, where the internal observables are taken to be relative angular momenta and partial internal energies. A more global way to treat the problem, as shown in Ref. 5 (where the preceding analysis is given in detail) consists in choosing a complete set of commuting observables out of the algebra generated by the components of the "relative grand angular momentum tensor,"[7] which are operators commuting with the total energy (the Hamiltonian of N noninteracting particles) and the total momentum of the system. One gets collective observables, such as the "togetherness operator," which describe in an interesting way the global structure of the N-particle system.

Since the components of the relative grand angular momentum tensor form a Lie algebra, standard group-theoretical methods are at hand for finding a complete set of commuting observables, i.e., a maximal Abelian subalgebra in the enveloping algebra. The Lie algebra thus generated is the one of the orthogonal group O_{3N-3} leaving invariant the phase-space Π_N, which, according to (1), is obviously a sphere S_{3N-4}. We call O_{3N-3} the "great

group" of phase-space. The most natural way of obtaining a complete set of commuting observables is to choose the Casimir operators of the "great group" and a chain of its subgroups: $O_{3N-3} \supset \cdots \supset O_3 \supset O_2$, terminated by the ordinary three- and two-dimensional rotation groups (whose Casimir operators give the angular momentum of the system and its "third" component). Let us recall that the togetherness operator, for instance, is the first Casimir operator of the great group. Note that it may prove necessary to introduce additional "degeneracy parameters" if the irreducible representations of a given subgroup in the chain, when restricted to the following one, are not multiplicity-free, i.e., contain several equivalent irreducible representations of this smaller subgroup.

B. A General Parametrization of Phase-Space

Let us now introduce a useful general parametrization of the nonrelativistic phase-space Π_N defined in (1). In loose terms, we perform an orthogonal transformation on the N momenta in such a way as to "decouple" the total momentum $\mathbf{P}$, thus getting rid of (1a) and obtaining $(N-1)$ "relative momenta" which parametrize Π_N. Let $\{A_{ij}\}$ be an $N \times N$ orthogonal matrix with the property

$$A_{Ni} = N^{-\frac{1}{2}}, \qquad i = 1, \cdots, N. \tag{2}$$

Let us define new momenta:

$$\mathbf{q}_i = \sum_{j=1}^{N} A_{ij}\mathbf{p}_j, \qquad i = 1, \cdots, N, \tag{3}$$

so that, in particular, due to (2),

$$\mathbf{q}_N = N^{-\frac{1}{2}} \sum_{i=1}^{N} \mathbf{p}_i. \tag{4}$$

The constraints (1) may now be rewritten with the $\{\mathbf{q}\}$ variables in the form

$$\mathbf{q}_N = N^{-\frac{1}{2}}\mathbf{P}, \tag{5a}$$

$$\sum_{i=1}^{N-1} \frac{\mathbf{q}_i^2}{2m} = E - \frac{\mathbf{P}^2}{2Nm} = Q^2. \tag{5b}$$

We may thus forget about the (fixed) momentum $\mathbf{q}_N$ and consider a point on the phase-space Π_N to be defined by the $(N-1)$ momenta $(\mathbf{q}_1, \cdots, \mathbf{q}_{N-1})$ subjected to the constraint (5b). Note that $Q^2 = E - (\mathbf{P}^2/2Nm)$ is the internal (total minus kinetic) energy of the system, or equivalently its energy in the center-of-mass frame, which is a Galilean invariant quantity. More generally, the momenta $\mathbf{q}_i (i = 1, \cdots, N-1)$ are Galilean-invariant. Indeed, consider a pure Galilei transformation $\mathbf{v}$. The individual momenta $\mathbf{p}_i (i = 1, \cdots, N)$ transform according to

$$\mathbf{p}_i' = \mathbf{p}_i + m\mathbf{v}; \tag{6}$$

the new quantities $\mathbf{q}_i$ transform as follows:

$$\begin{aligned}\mathbf{q}_i' &= \sum_{j=1}^{N} A_{ij}\mathbf{p}_j' \\ &= \sum_{j=1}^{N} A_{ij}(\mathbf{p}_j + m\mathbf{v}) \\ &= \mathbf{q}_i + m\mathbf{v} \sum_{j=1}^{N} A_{ij}.\end{aligned}$$

But, the orthogonality of $\{A_{ij}\}$ reads

$$\delta_{ij} = \sum_{k=1}^{N} A_{ik}A_{jk}. \tag{7}$$

Putting $i \neq N$, $j = N$ in (7) and using (2), we get

$$0 = N^{-\frac{1}{2}} \sum_{i=1}^{N} A_{ij}, \qquad i \neq N, \tag{8}$$

so that

$$\mathbf{q}_i' = \mathbf{q}_i, \qquad i = 1, 2, \cdots, N-1 \tag{9}$$

as we have asserted.

We have thus obtained a quite general definition of relative momenta for our N particles, of which the definition used in Ref. 5, for instance, is a particular case;

$$\mathbf{q}_k = [k(k+1)]^{-\frac{1}{2}}\left(k\mathbf{p}_{k+1} - \sum_{i=1}^{k} \mathbf{p}_i\right), \qquad k = 1, \cdots, N-1. \tag{10}$$

This is, up to a factor $[k/(k+1)]^{\frac{1}{2}}$, the momentum of the $(k+1)$th particle relative to the system of the first k ones. Definition (10) is most suitable for the step-by-step coupling scheme, but there are other possibilities, some of which are more convenient for the global scheme (this we see later). The "relative grand angular momentum tensor" has a natural expression in terms of the relative momenta $\{\mathbf{q}_i\}$, independently of the precise form of the matrix $\{A_{ij}\}$;

$$L_{i\alpha;j\beta} = i\left(q_{i\alpha}\frac{\partial}{\partial q_{j\beta}} - q_{j\beta}\frac{\partial}{\partial q_{i\alpha}}\right), \qquad \begin{cases} i, j = 1, \cdots, N-1, \\ \alpha, \beta = 1, 2, 3. \end{cases}$$

These operators clearly define a basis for the Lie algebra of the orthogonal group O_{3N-3}, the great group.

C. Symmetry Considerations

A new problem now arises due to the symmetry or antisymmetry to be obeyed by the states of N identical particles.[9] In order to construct such states with simple symmetry properties, we need to consider the symmetric group S_N of permutations among the N particles, and its representation. Indeed, the state space of the N-particle system, being an N-fold tensor product of identical one-particle state spaces, is a representation space for S_N, a given permutation

$$P_{i_1 \cdots i_N} = \begin{pmatrix} 1 & 2 & \cdots & N \\ i_1 & i_2 & \cdots & i_N \end{pmatrix}$$

acting in the obvious way:

$$(P_{i_1 \cdots i_N} \psi)(\mathbf{p}_1, \cdots, \mathbf{p}_N) = \psi(\mathbf{p}_{i_1}, \cdots, \mathbf{p}_{i_N}). \qquad (11)$$

What we need is to reduce this representation of S_N, along with that of the Galilei group $\mathcal{G}$—that is to say, we consider the representation of the direct product $\mathcal{G} \otimes S_N$. Looking back at our decomposition scheme, one sees that its first stages (fixing the total energy–momentum of the system) do not break the invariance under S_N, since the constraints (1) are obviously symmetric in the N-particle momenta. In other words, the phase-space Π_N is invariant under S_N, and one is led to consider the representation of the direct product $O_3 \otimes S_N$ in the square-integrable functions over Π_N in order to reduce it. The intervening of the discrete group S_N gives rise to new technical problems in that there does not exist a Lie algebra with its Casimir operators to furnish adequate commuting observables. Doubtless, however, there are appropriate methods to solve the problem, since the symmetric group and its representations are well-known objects. But we do not wish to consider this approach here and tries instead a simpler technique, namely, an attempt to adapt our preceding considerations to the present situation.

It is clear that the step-by-step method is of no use, since, as we already noticed, it breaks the permutation invariance under S_N from the start. The global method, on the other hand, is more promising. As a matter of fact, $O_3 \otimes S_N$ is a subgroup of the great group O_{3N-3}, and the togetherness operator, for instance, is invariant under S_N. More generally, if the operators of our complete set of commuting observables had simple properties under the permutation group S_N, this would also be the case for their common eigenstates. The state space of the system would then be broken into small subspaces invariant under S_N (if not already irreducible), so that it would be easy to construct states with given symmetry properties.[9]

The simplest way to achieve this aim is to look for a chain of subgroups descending from O_{3N-3} to O_3 such that each one is invariant with respect to (the automorphisms generated by) the permutation group S_N. The set of invariants of the Lie algebra of such a group is then also stable under the action of S_N, that is to say, these Casimir operators possess simple symmetry properties as required. Such groups are called "democratic subgroups" of the great group. We investigate their existence and properties in the following paragraph.

Let us conclude these general considerations by studying the permutation properties of the relative momenta $\{\mathbf{q}\}$ introduced above. The momenta $\{\mathbf{p}\}$ whose N indices are permuted under the action of the symmetric group S_N are thus associated with an N-dimensional representation of the group S_N. It is easily proved that this is a reducible representation, since the total momentum $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$ obviously is invariant and thus corresponds to the identity one-dimensional representation. But it may be proved, for instance, by explicitly computing its character that the remaining $(N-1)$-dimensional representation is indeed irreducible and is associated with the partition

$$\{N-1, 1\} = \begin{array}{|c|c|c|c|c|c|}\hline \quad & \quad & \quad & \cdots & \quad & \quad \\ \hline \quad \\ \cline{1-1} \end{array}.$$

In other words, the relative momenta $\{\mathbf{q}\}$ (precisely obtained from the $\{\mathbf{p}\}$ by discarding the totally symmetric component $\mathbf{P}$) is transformed by permutation of the N particles under the irreducible representation $\{N-1, 1\}$ of the symmetric group S_N. Furthermore, the definition (10) of the $\{\mathbf{q}\}$ amounts to choosing a basis for this representation, where the representations of the subgroups S_k of permutations on the first k particles ($k = 1, \cdots, N-1$) are already in reduced form.

II. DEMOCRACY

Definition: a subgroup Γ of the great group O_{3N-3} is called *democratic* if it is (globally) invariant under

[9] Let us point out that we are not interested only in the totally symmetric or antisymmetric N-particle states. Indeed, if we consider internal symmetry properties of the particles involved in the process under study (isospin of pions, for instance), it is the total wavefunction of the system which must be made completely symmetric or antisymmetric. This is most easily done by coupling internal and spatial wavefunctions if they have simple symmetry properties. See, for instance, Dragt's treatment of the three-pion system in Ref. 4.

the internal automorphism group S_N:

$$PRP^{-1} \in \Gamma \quad \forall R \in \Gamma, \quad P \in S_N. \tag{12}$$

Lemma: To each democratic subgroup of the great group, there corresponds an invariant subgroup of the permutation group. Conversely, to each invariant subgroup of S_N, there corresponds at least one democratic subgroup.

Proof:

(i) Let Γ be a democratic subgroup of O_{3N-3}. Define Σ_Γ, the set of permutations in S_N which commute with each element of Γ, as

$$\Sigma_\Gamma = \{Q \in S_N; QRQ^{-1} = R, \forall R \in \Gamma\}. \tag{13}$$

It is obvious that Σ_Γ is a subgroup of S_N. It is, moreover, an invariant subgroup, since, for any $Q \in \Sigma_\Gamma$, $P \in S_N$, and $R \in \Gamma$, one has

$$\begin{aligned}(P^{-1}QP)R(P^{-1}QP)^{-1} &= P^{-1}Q(PRP^{-1})Q^{-1}P \\ &= P^{-1}(PRP^{-1})P \\ &= R,\end{aligned} \tag{14}$$

since $PRP^{-1} \in \Gamma$ [see (12)] and Q commutes with each element of Γ. Thus $P^{-1}QP$ also commutes with each element of Γ and belongs to Σ_Γ which is an invariant subgroup of S_N.

(ii) Let Σ be an invariant subgroup of S_N. Define Γ_Σ, the set of elements in the great group O_{3N-3} which commute with each permutation in Σ, as

$$\Gamma_\Sigma = \{R \in O_{3N-3}; RQR^{-1} = Q, \forall Q \in \Sigma\}. \tag{15}$$

Γ_Σ obviously is a subgroup of the great group. Moreover, it is a democratic subgroup, since, for any $Q \in \Sigma$, $P \in S_N$, $R \in \Gamma_\Sigma$, one has

$$\begin{aligned}Q(PRP^{-1})Q^{-1} &= P(P^{-1}QP)R(P^{-1}QP)^{-1}P^{-1} \\ &= PRP^{-1},\end{aligned} \tag{16}$$

since Σ is an invariant subgroup of S_N, for any $P \in S_N$, $P^{-1}QP \in \Sigma$ and commutes with $R \in \Gamma$. Thus $PRP^{-1} \in \Gamma_\Sigma$, which shows that Γ_Σ is a democratic subgroup.

Definition: Γ being a democratic subgroup of the great group and Σ the associated invariant subgroup of the permutation group, we call Γ a "*Σ-democratic*" subgroup and Σ the "*democracy group of* Γ".

Comments:

(i) We have *not* proved the existence of a one-to-one correspondence between the democratic subgroups of O_{3N-3} and the invariant subgroups of S_N. For, on the one hand, distinct democratic subgroups can have the same democracy group in S_N, and, on the other hand, distinct invariant subgroups of S_N can give rise, by the construction (ii) in the above proof, to identical democratic subgroups of the great group.

(ii) The interest of the notion of "democracy groups" stems from the fact that the Casimir operators of a given democratic subgroup Γ are obviously invariant under the action of the corresponding democracy group Σ. They transform among themselves in a simple way under the permutations of S_N not belonging to Σ (in many cases at most undergoing a change of sign), so that their common eigenvectors enjoy very simple symmetry properties, which is of course the motivation for our definition of democracy.

(iii) To use the appropriate technical vocabulary,[10] we may say that a democratic subgroup Γ is defined by the condition that the permutation group S_N be a subgroup of its *normalizer* in the great group O_{3N-3}. Its democracy group Σ_Γ then is the intersection of S_N and the *centralizer* of Γ; that Σ_Γ is an invariant subgroup of S_N derives from the fact that for any subgroup, its centralizer is an invariant subgroup of its normalizer. Conversely, given an invariant subgroup Σ of S_N, the democratic subgroup Γ_Σ, as constructed above, is its centralizer in the great group O_{3N-3}.

III. THE DEMOCRATIC GROUPS

Let us first quote the following well-known result:

Theorem: Except for the case $N = 4$, the only proper invariant subgroup of S_N is the alternating group A_N.[11]

In the case $N = 4$, besides the alternating group A_4, S_4 possesses another proper invariant subgroup $\mathfrak{V}_4$, isomorphic to Klein's "Vierergruppe".

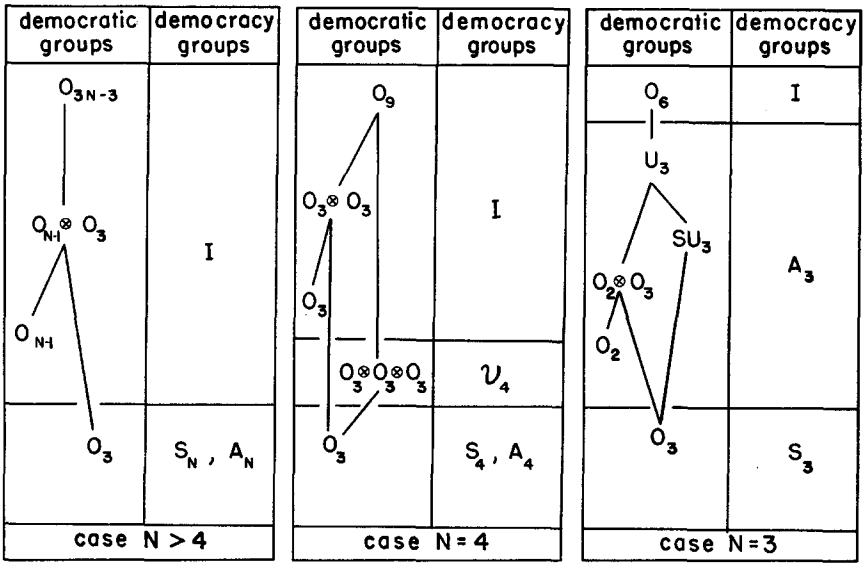
In fact, we are concerned with the notion of invariant subgroups of S_N in its largest sense, so that we add to the above list, the group S_N itself and the identity I.

The scarcity of these invariant subgroups leads us to foresee a corresponding scarcity of the democratic subgroups. Before stating and proving our main result, we wish to restrict slightly our notion of democracy: since we are ultimately interested in subgroups of the great group containing the usual

[10] N. Bourbaki, *Structures algébriques*, (Hermann & Cie., Paris, 1958), 3rd ed., Chap. 6, Exercice 13.

[11] See, for instance, J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959), Chap. VIII.

TABLE I. Democratic subgroups inclusion relations.



rotation group, we only consider such rotation-invariant democratic subgroups. With this proviso, we have:

Theorem D: For each value of N, the democratic subgroups of the great group and the corresponding democracy subgroups of the symmetric group are given by Table I, where the inclusion relations between the democratic subgroups are displayed.

Proof: The concrete definition of the democratic subgroups and the way in which they act on the phase-space Π_N is now exhibited. Let us consider the Lie algebra A of the great group O_{3N-3}, consisting of the antisymmetric operators $L_{i\alpha,j\beta}(i = 1, \cdots, N-1; \alpha = 1, 2, 3)$ obeying the commutation rules:

$$[L_{i\alpha,j\beta}, L_{m\rho,n\sigma}] = i(\delta_{jm}\,\delta_{\beta\rho}L_{i\alpha,n\sigma} - \delta_{jn}\,\delta_{\beta\sigma}L_{i\alpha,m\rho} + \delta_{in}\,\delta_{\alpha\sigma}L_{j\beta,m\rho} - \delta_{im}\,\delta_{\alpha\rho}L_{j\beta,n\sigma}). \quad (17)$$

The automorphism group S_N of the great group naturally induces automorphism of its Lie algebra A by acting on the indices (i, j). The Lie algebra of a democratic subgroup, i.e., a democratic Lie algebra, has to be invariant under such automorphisms. But we observe that the Lie algebra A, possessing a vector-space structure, is a representation space for S_N. As a consequence, it may be decomposed into a sum of irreducible subspaces. A democratic Lie algebra, being an invariant subspace, is a sum of such irreducible subspaces which has the property of being closed under the Lie bracket law. Our quest for democratic subalgebras thus will be accomplished in two steps—first, decomposing A into irreducible subspaces, and second, investigating the Lie bracket properties of these irreducible subspaces.

(a) As already noticed [Sec Ic], the $(N-1)$-component vector $q_{i\alpha}$ for each fixed value of $\alpha(= 1, 2, 3)$ transforms under the $\{N-1, 1\}$ representation of the symmetric group S_N. Accordingly, for each value (α, β), the operators $L_{i\alpha,j\beta}$ transform under the tensor product representation $\{N-1, 1\} \times \{N-1, 1\}$ of S_N, and we obtain irreducible subspaces simply by decomposing this representation into irreducible components. The result of such a decomposition is given by[11]

$$\{N-1, 1\} \times \{N-1, 1\} = \{N-2, 1^2\} + [\{N\} + \{N-1, 1\} + \{N-2, 2\}], \quad (18)$$

where, as usual, an irreducible representation of S_N is labeled by a partition of $N(\{N\}$ is the identity representation); the second line corresponds to the symmetrized tensor product of $\{N-1, 1\}$ by itself and the first line to the antisymmetrized product. Now, as already stated, we are only interested in rotation-invariant subalgebras. The rotation group O_3 acts on the indices (α, β) of $L_{i\alpha,j\beta}$, which, for given (i, j), transform under the tensor product $D^1 \times D^1$ of the rotation group representations [D^l denotes the irreducible $(2j+1)$-dimensional representation of the rotation group] which decomposes in the well-known way:

$$D^1 \times D^1 = [D^0 + D^2] + D^1, \quad (19)$$

where we have separated the symmetrized and antisymmetrized products. We are thus led to consider

the Lie algebra A as a representation space for the group $S_N \otimes O_3$, and to decompose it into irreducible subspaces. Due to the antisymmetry of the $L_{i\alpha,j\beta}$ tensor, the representation of $S_N \otimes O_3$ acting in A is the antisymmetrized tensor product of $\{N-1,1\} \otimes D^1$ by itself, whose decomposition into irreducible components, easily computed from (18) and (19) by combining the respective symmetrized and antisymmetrized parts, is given by

$$\begin{aligned}[\{N-1,1\} \otimes D^1] \times^a [\{N-1,1\} \otimes D^1] \\ = \{N\} \otimes D^1 + \{N-1,1\} \otimes D^1 \\ + \{N-2,2\} \otimes D^1 + \{N-2,1^2\} \otimes D^0 \\ + \{N-2,1^2\} \otimes D^2. \end{aligned} \tag{20}$$

We denote the corresponding decomposition of A into irreducible subspaces by:

$$A = V_0 + V_1 + V_2 + S + T. \tag{21}$$

V_0, transforming under $\{N\} \otimes D^1$ (that is, being a completely symmetric vector operator), is a three-dimensional subspace of A, a basis of which is given by

$$\epsilon_{\alpha\beta\gamma} \sum_{i=1}^{N-1} L_{i\beta,i\gamma} = l_\alpha, \quad \alpha = 1, 2, 3. \tag{22}$$

The operator 1 is obviously the total (intrinsic) angular momentum which generates the ordinary rotation group O_3.

V_1 and V_2, transforming under $\{N-1,1\} \otimes D^1$ and $\{N-2,2\} \otimes D^1$, are respectively, $3(N-1)$- and $\frac{3}{2}N(N-3)$-dimensional subspaces, which together with V_0, span the subspace of A antisymmetrized with respect to the space indices.

S and T, transforming under $\{N-2,1^2\} \otimes D^0$ and $\{N-2,1^2\} \otimes D^2$ are, respectively, $\frac{1}{2}(N-1)(N-2)$- and $\frac{5}{2}(N-1)(N-2)$-dimensional subspaces, whose sum gives the subspace of A symmetrized with respect to the space indices.

By construction, the operators in each of these subspaces transform under rotations as irreducible tensor operators of scalar, vector, tensor character, respectively, for S, $V_i (i = 0, 1, 2)$, T.

(b) We now undertake to examine the Lie-bracket properties of these various subspaces whose number fortunately is rather small. A_1 and A_2 being two such irreducible subspaces, we denote as usual by $[A_1, A_2]$ the set of all Lie-algebra elements of the form $[M_1, M_2]$, where $M_i \in A_i$ $(i = 1, 2)$. Let Δ_1 and Δ_2 be the two irreducible representations of $S_N \otimes O_3$ under which A_1 and A_2 transform. Then it is clear that $[A_1, A_2]$ is itself an invariant subspace of A which defines a representation space for $S_N \otimes O_3$. The associated representation is a subrepresentation of $\Delta_1 \times \Delta_2$. In other words, $[A_1, A_2]$ is a sum of irreducible subspaces, such that the corresponding irreducible representations appear in the decomposition of the tensor product $\Delta_1 \times \Delta_2$. Furthermore, in the case where $A_1 = A_2$, the subspace is a representation space for a subrepresentation of the antisymmetrized product $\Delta_1 \times^a \Delta_1$. Thus, by simply using the Clebsch–Gordan series for the product of irreducible representations of $S_N \otimes O_3$, we obtain strong limitations on the Lie-bracket properties of the irreducible subspaces. Of course, explicit computations, using the above described characterization of these subspaces, are necessary in order to check if a given irreducible subspace corresponding to a component of $\Delta_1 \times \Delta_2$ really belongs to $[A_1, A_2]$; indeed, this is generally true. We do not reproduce here these rather trivial calculations, but simply state the results in the form of a table (Table II) whose entry corresponding to the line A_1 and column A_2 gives the decomposition of $[A_1, A_2]$ into a sum of irreducible subspaces. Due to the low dimensionalities of the representations for $N = 3$ and $N = 4$, these are exceptional cases which are treated separately (Tables III and IV)

(c) $N > 4$. It suffices now to use Table II in order to find the democratic subalgebras, that is,

TABLE II. Decomposition of $[A_1, A_2]$, $N > 4$.

	T	S	V_2	V_1	V_0
V_0	T	0	V_2	V_1	V_0
V_1	$V_1 + V_2 + T$	$V_1 + V_2$	$V_1 + V_2 + S + T$	$V_0 + V_1 + V_2 + S + T$	
V_2	$V_1 + V_2 + T$	$V_1 + V_2$	$V_0 + V_1 + V_2 + S + T$		
S	T	S			
T	$V_0 + V_1 + V_2 + S + T$				

invariant subspaces closed under the Lie-bracket composition law. The only possibilities are:

V_0, which, as already mentioned, generates the ordinary three-dimensional rotation group O_3.

S, a convenient basis in the subspace S consists of the $\frac{1}{2}(N-1)(N-2)$ operators

$$S_{ij} = \sum_{\alpha=1}^{3} L_{i\alpha,j\alpha}, \qquad 1 \leq i < j \leq N-1. \tag{23}$$

Their commutation relations are easily derived from (17):

$$[S_{ij}, S_{kl}] = i(\delta_{ik}S_{jl} - \delta_{jl}S_{ik} + \delta_{il}S_{jk} - \delta_{ik}S_{jl}),$$

which characterize S as the Lie algebra of a rotation group in an $(N-1)$-dimensional space, O_{N-1}. It is an easy matter to understand the nature of this group and its action on the phase-space Π_N. Write the constraint (5b) in the form

$$Q^2 = \sum_{\alpha=1}^{3}\left[\sum_{i=1}^{N-1}(q_{i\alpha})^2\right] = \sum_{\alpha=1}^{3} Q_\alpha^2,$$

where we define three $(N-1)$-dimensional vectors $Q_\alpha = (q_{1\alpha}, \cdots, q_{(N-1)\alpha})$. Then our O_{N-1} group acts on Π_N by rotating each vector Q_α by the same $(N-1)$-dimensional rotation. It is clear that this group O_{N-1} commutes with the rotation group O_3 (their operators act on different indices), as is also verified from the fact that $[V_0, S] = 0$ (see Table II).

$V_0 + S$, which is, in fact, a direct sum $V_0 \oplus S$ and the resulting Lie algebra generates the direct product $O_3 \otimes O_{N-1}$ of the previously characterized democratic groups.

$A = V_0 + V_1 + V_2 + S + T$, which is the whole Lie algebra of the great group, is the only possibility left.

The groups O_{3N-3}, $O_{N-1} \otimes O_3$, O_{N-1}, O_3 thus found are easily verified to be democratic groups. As to their democracy groups, one sees that no permutation is in the center of O_{N-1} (nor *a fortiori* in the center of O_{3N-3}) so that the democracy groups for O_{N-1}, $O_3 \otimes O_{N-1}$, and O_{3N-3} reduce to the identity. The rotation group O_3 instead is left pointwise-invariant by any permutation so that the whole symmetric group S_N (and its alternating subgroup A_N as well) is the corresponding democracy group. We have now justified the part $N > 4$ of Table I.

(d) $N = 4$. Table III presents the Lie-bracket properties of the irreducible subspaces in this case.

As in the general case, we find here as democratic subalgebras: V_0 which generates the ordinary rotation group O_3; S which here generates also an O_3 group but with an entirely different interpretation (mixing the three relative momenta); $V_0 \oplus S$ generating an $O_3 \otimes O_3$ group; and A generating the whole O_9 great group. But in addition to these, there is another democratic subalgebra generated by $V_0 + V_2$, which is nine-dimensional. The nature of this algebra is most clearly exhibited if one notices that V_2 corresponds to the $\{2^2\}$ partition of S_4. This gives us a clue as to the parametrization of Π_4 most adapted to the present situation. Indeed, let us define:

$$\begin{aligned} \mathbf{q}_1 &= \tfrac{1}{2}(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4), \\ \mathbf{q}_2 &= \tfrac{1}{2}(\mathbf{p}_2 + \mathbf{p}_3 - \mathbf{p}_1 - \mathbf{p}_4), \\ \mathbf{q}_3 &= \tfrac{1}{2}(\mathbf{p}_1 + \mathbf{p}_3 - \mathbf{p}_2 - \mathbf{p}_4), \end{aligned} \tag{24}$$

which is of the general form (2), (3).

A convenient basis in $V_0 + V_2$ is then given by

$$K_{i\alpha} = \epsilon_{\alpha\beta\gamma}L_{i\beta,i\gamma}\begin{cases}\text{no summation on } i = 1, 2, 3, \\ \alpha = 1, 2, 3; \end{cases} \tag{25}$$

that is,

$$K_{i\alpha} = i\epsilon_{\alpha\beta\gamma}\left(q_{i\beta}\frac{\partial}{\partial q_{i\gamma}} - q_{i\gamma}\frac{\partial}{\partial q_{i\beta}}\right),$$

where the $\{\mathbf{q}\}$ are given by (24). The commutation relations now read

$$[K_{i\alpha}, K_{j\beta}] = i\,\delta_{ij}\epsilon_{\alpha\beta\gamma}K_{i\gamma}, \tag{26}$$

clearly showing that $V_0 + V_2$ generates a group

TABLE III. Decomposition of $[A_1, A_2]$, $N = 4$.

	T	S	V_2	V_1	V_0
V_0	T	O	V_2	V_1	V_0
V_1	$V_1 + V_2 + T$	$V_1 + V_2$	$V_1 + S + T$	$V_0 + V_1 + V_2 + S + T$	
V_2	$V_1 + T$	V_2	$V_0 + V_2$		
S	T	S			
T	$V_0 + V_1 + V_2 + S + T$				

isomorphic to $O_3 \otimes O_3 \otimes O_3$. The action of the group at large on Π_4 is given by

$$\mathbf{q}_i' = R_i \mathbf{q}_i, \qquad i = 1, 2, 3, \tag{27}$$

where (R_1, R_2, R_3) are three 3×3 orthogonal matrices defining an element of the group. The usual rotation group O_3 is the "diagonal" subgroup of the triple product $O_3 \otimes O_3 \otimes O_3$, that is to say, is defined by $R_1 = R_2 = R_3$. Its Lie algebra V_0 has the standard basis [see (22)]

$$l_\alpha = \sum_{i=1}^{3} K_{i\alpha}, \qquad \alpha = 1, 2, 3. \tag{28}$$

It is not surprising, when computing the democracy group of $O_3 \otimes O_3 \otimes O_3$, to find precisely the invariant subgroup $\mathcal{U}_4$ [characteristic of the case $N = 4$ and consisting of (besides the identity) the permutations belonging to the class $\{2^2\}$].

(e) $N = 3$. The situation is simplified by the fact that the subspace V_2 [with dimension $\frac{1}{2}N(N-3) = 0$] vanishes. We are left with Table IV.

As in the general case, we find the democratic subalgebras consisting, respectively, of V_0, S, $V_0 \oplus S$, and A. Observe that here S is one-dimensional, thus generating an Abelian O_2 group. But we also find a new democratic subalgebra, $V_0 + T$, which is eight-dimensional. It is easily shown[4] that it generates an SU_3 subgroup of the great group O_6 (itself isomorphic to SU_4). Observe also that the 9-dimensional democratic subalgebra $(V_0 + T) \oplus S$ generates a complete U_3 group. In order to exhibit the way it acts on Π_3, define [see (10)]

$$\begin{aligned} \mathbf{q}_1 &= (1/\sqrt{2})(\mathbf{p}_2 - \mathbf{p}_1), \\ \mathbf{q}_2 &= 6^{-\frac{1}{2}}(2\mathbf{p}_3 - \mathbf{p}_2 - \mathbf{p}_1), \end{aligned} \tag{29}$$

consider now the 3-dimensional *complex* vector:

$$\begin{aligned} \mathbf{q} &= \mathbf{q}_2 + i\mathbf{q}_1 \\ &= 2(6)^{-\frac{1}{2}}(\mathbf{p}_3 + \omega \mathbf{p}_2 + \omega^2 \mathbf{p}_1) \quad \omega = e^{\frac{2}{3}i\pi} \end{aligned} \tag{30}$$

with fixed length:

$$|\mathbf{q}|^2 = Q^2, \tag{31}$$

TABLE IV. Decomposition of $[A_1, A_2]$, $N = 3$.

	T	S	V_1	V_0
V_0	T	O	V_1	V_0
V_1	V_1	V_1	V_0+V_1+S+T	
S	O	O		
T	V_0			

which parametrizes Π_3. The transformations

$$\mathbf{q}' = u\mathbf{q}, \qquad u \in U_3, \tag{32}$$

where u is an unitary 3×3 matrix leaving the constraint (31) invariant, defines the action of U_3 on Π_3.

It is not difficult to show that this whole U_3 group is left point-wise invariant by the alternating group A_3 which constitutes its democracy group. We have now completed the proof of our Theorem D and proceeds to comment on its physical applications.

IV. PHYSICAL DISCUSSION AND CONCLUSIONS

Case $N = 3$

Besides the great group O_6 (I-democratic), and the rotation group O_3(S_3-democratic), there exists an A_3-democratic subgroup, U_3. It turns out that this group, and even its unimodular subgroup SU_3, equally A_3-democratic, is big enough to play the role of the great group, since it is transitive on the sphere $S_5 (= \Pi_3)$ and its representation in the square-summable functions on S_5 is multiplicity-free. Furthermore, its quadratic Casimir operator coincides with the one of O_6, that is the togetherness operator. This is the SU_3 group first introduced by Dragt,[4] who invented the democracy concept to which we have given here a precise and more general meaning. Let us recall that the 3-particle states corresponding to this democratic method have been thoroughly studied[4,12-16] and prove to be very interesting: when analyzing, for instance, the final state of the $K \to 3\pi$ decay, it practically suffices to consider the lowest possible state of Dragt's basis,[4] instead of a complicated superposition of basis states in the step-by-step coupling schemes.[17] Moreover, these Dragt states present, as expected, very simple symmetry properties, and should be very appealing to the experimentalists since they permit an immediate computation of the associated Dalitz diagram densities. We think that they may find other applications, for instance in the nuclear reactions[18]

$$^{11}\mathrm{B} + p \to 3\alpha, \qquad ^{9}\mathrm{Be} + {}^{3}\mathrm{He} \to 3\alpha, \qquad 2(^{6}\mathrm{Li}) \to 3\alpha.$$

[12] Z. Koba, Phys. Letters **1**, 34 (1962); Acta Phys. Polon. **22**, 103 (1962).
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[18] See the entire issue of Rev. Mod. Phys. **37**, No. 3 (1965); P. Kramer, *ibid.* **37**, 346 (1965). N. McDonald, Phys. Letters **19**, 293 (1965).

Of course, a convincing relativistic generalization (see the Appendix) would be most interesting for the analysis of reactions such as: η or $\omega \to 3\pi$, $p + \bar{p} \to 3\pi$, etc.

Case $N = 4$

Between the great group O_9 (I-democratic) and the rotation group O_3(S_4- and A_4-democratic), we find here a group $O_3 \otimes O_3 \otimes O_3$ ($\mathcal{U}_4$-democratic), which has an interesting physical interpretation. The relevant $\{q\}$ momenta [see (24)] are in fact the relative momenta of two pairs of particles, i.e., for each couple of such pairs which can be formed out of the four particles. As a consequence, the Casimir operators of the group $O_3 \otimes O_3 \otimes O_3$, (that is, the three angular momenta corresponding to these three rotation groups), are the relative angular momenta of two pairs of particles for each one of the three couples of pairs. The usual rotation group (S_4-democratic) is the diagonal O_3 subgroup of the direct product $O_3 \otimes O_3 \otimes O_3$ [i.e., $R_1 = R_2 = R_3$ in (27)]. This means that the total angular momenta of the four-particle system is finally obtained by recoupling the three partial angular momenta just discussed. It is most desirable to do this recoupling in such a way as to preserve the attractive symmetry properties of the scheme. Fortunately, there exists a symmetrical coupling method for three angular momenta[19] which finds here a natural application. There still remains an open question: do the quantum numbers just introduced in connection with the $O_3 \otimes O_3 \otimes O_3$ and O_3 groups, along with the Casimir operators of O_9, suffice to constitute a complete set of commuting observables? In other words: are the irreducible representations of the great group O_9, when restricted to the $O_3 \otimes O_3 \otimes O_3$ subgroup, multiplicity-free, or are some new degeneracy parameters necessary? This question must be answered before the method may be fully used, and, in the (most probable) case of a positive answer to this last question, democratic degeneracy parameters must be found.

On the other hand, it might be possible still to obtain interesting results by just using the $O_3 \otimes O_3 \otimes O_3$ group, without applying the complete apparatus of the global method: take, for instance, commuting observables consisting of the internal energies and internal angular momenta of the three couples of pairs of particles (and couple these angular momenta as above). This simply replaces the discrete and collective quantum numbers associated with the great group by the three partial internal energies and represents a sort of compromise between the global and step-by-step methods. In this connection, let us note that, in the relativistic case, these internal energies, simply related to the relative momenta (24), have been used in order to analyze four-particle states by a kind of Dalitz diagram[20] which has proven useful to discuss the B resonance.[21]

Besides the analysis of four-pion processes—which must await the desired relativistic generalization of the scheme—the present method could be applied to nuclear reactions such as $^{16}O^* \to 4\alpha$.[18]

Observe that we have not proposed the use of the I-democratic $O_3 \otimes O_3$ subgroup—being smaller than the $\mathcal{U}_4$-democratic $O_3 \otimes O_3 \otimes O_3$ subgroup and having a smaller democracy group, it is probably not worth considering.

Case $N > 4$

Here, between the I-democratic great group O_{3N-3} and the S_N-democratic rotation group O_3, we find only the $O_3 \otimes O_{N-1}$ I-democratic subgroup. Though interesting, it is certainly not sufficient to constitute, with O_{3N-3} and O_3, a chain of groups furnishing enough Casimir operators to serve as a complete set of commuting observables. One can no longer escape the problem of dealing with the symmetric group S_N itself. More precisely, what has to be done is to reduce the irreducible representations of the great group O_{3N-3} when restricted to its "semi-discrete" subgroup $O_3 \otimes S_N$. This requires completely different, noninfinitesimal, methods.[22]

We undertook this work with the hope that the democracy concept, so useful in the case $N = 3$, could be generalized and used for any number of particles. Unfortunately, this proves not to be completely feasible. However, although being of a limited scope, this notion enables one to obtain interesting classifications at least of three- and four- particle states, enjoying simple symmetry properties. The practical importance of three- and four-particle processes (with identical particles), in our opinion, sufficiently justifies further investigations along these lines; in particular, the four-particle case now requires explicit calculations. Of course, the problem of devising a physically meaningful relativistic generalization remains to be solved. It is our hope that the tools thus devised may prove helpful in the

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analysis of experimental results as well as in theoretical studies on three- and four-particle processes.

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APPENDIX. ON THE RELATIVISTIC GENERALIZATION OF THE GLOBAL COUPLING SCHEME

The kinematical description of a relativistic N-particle system proceeds along exactly the same lines as in the nonrelativistic case (Sec. IA). One is led to consider the representation of the Poincaré group consisting of the tensor product of the N irreducible representations corresponding to the individual particles. The problem now is to reduce this representation into irreducible components. Working in the Hilbert space of functions defined over the momentum-space with the invariant norm

$$||\psi||^2 = \int |\psi(\mathbf{p}_1, \cdots, \mathbf{p}_N)|^2 \frac{d^3p_1}{2\omega_1} \cdots \frac{d^3p_N}{2\omega_N}, \qquad \omega_i^2 = m_i^2 + \mathbf{p}_i^2, \tag{A1}$$

we first fix the total energy-momentum of the system, so that we are left with functions over the phase-space Π_N^r, now defined by the constraints:

$$\sum_{i=1}^{N} \mathbf{p}_i = \mathbf{P}, \quad \sum_{i=1}^{N} (m_i^2 + \mathbf{p}_i^2)^{\frac{1}{2}} = E, \tag{A2}$$

and we have to decompose (into irreducible components) the representation of the rotation group O_3 in the space of square-integrable functions over phase-space.

The step-by-step coupling method works without great modifications, by expanding any function on Π_N^r in spherical harmonics with respect to a sequence of relative momenta (whose definition, however, is the delicate point), and by successively recoupling the orbital angular momenta thus obtained.[2]

The global method, on the other hand, may be formally adapted quite simply as follows. Let us first define some notations: Π_N^n and Π_N^r, with elements π^n and π^r, are, respectively, the nonrelativistic and relativistic phase-spaces. $L^2(\Pi_N^n)$ and $L^2(\Pi_N^r)$ are, respectively, the Hilbert spaces of functions on Π_N^n and Π_N^r square-integrable with respect to the measures $d\mu^n$ and $d\mu^r$ induced in Π_N^n and Π_N^r by the measures $d^3p_1 \cdots d^3p_n$ and $d^3p_1/2\omega_1 \cdots d^3p_N/2\omega_N$, respectively, in the surrounding momentum-space. That is to say, $L^2(\Pi_N^n)$ and $L^2(\Pi_N^r)$ are defined by the norms:

$$\phi \in L^2(\Pi_N^n): \quad ||\phi||_n^2 = \int_{\Pi_N^n} |\phi(\pi^n)|^2 \, d\mu^n(\pi^n) < +\infty, \tag{A3}$$

$$\psi \in L^2(\Pi_N^r): \quad ||\psi||_r^2 = \int_{\Pi N^n} |\psi(\pi^r)|^2 \, d\mu^r(\pi^r) < +\infty.$$

Now, let T be a one-to-one mapping from Π_N^r onto Π_N^n:

$$T: \pi^r \in \Pi_N^r \to \pi^n = T(\pi^r) \in \Pi_N^n. \tag{A4}$$

Call $J_T(\pi^r)$ the associated Jacobian:

$$J_T(\pi^r) = d\mu^n[T(\pi^r)]/d\mu^r(\pi^r), \tag{A5}$$

where T induces a canonical mapping U_T from $L^2(\Pi_N^n)$ onto $L^2(\Pi_N^r)$ defined by:

$$(U_T\phi)(\pi^r) = [J_T(\pi^r)]^{\frac{1}{2}}\phi[T(\pi^r)]. \tag{A6}$$

It is easily seen that this is an isometry of these Hilbert spaces, since if $\phi \in L^2(\Pi_N^n)$ then

$$||U_T\phi||_r^2 = \int_{\Pi_N^r} |(U_T\phi)(\pi^r)|^2 \, d\mu^r(\pi^r) = \int_{\Pi_N^r} |\phi[T(\pi^r)]|^2 \frac{d\mu^n[T(\pi^r)]}{d\mu^R(\pi^r)} \, d\mu^r(\pi^r) = \int_{\Pi_N^n} |\phi(\pi^r)|^2 \, d\mu^n(\pi^n) = ||\phi||_n^2.$$

In other terms, to each one-to-one mapping of the relativistic phase-space onto the nonrelativistic one, corresponds a mapping of the physical state spaces onto each other. The transformation (A6) thus acts as a dictionary which enables us to translate at once a list of nonrelativistic N-particle basis states into a corresponding relativistic list. The transformation T also takes any group acting on Π_N^n into an isomorphic group acting on Π_N^r, so that by this device, complete sets of relativistic basis states labeled according to the representations of a great group, etc., are obtained.

Indeed, this is the device used by Halpern[6] and

Dragt.[8] They both choose a "radial" mapping of Π_N^r onto Π_N^n; since both are convex compact manifolds embedded in a $3N$-dimensional Euclidean (momentum) space and containing the origin O ($\mathbf{p}_1 = \cdots \mathbf{p}_N = 0$), any radius vector extending from O will intersect each of these at one and only one point, thus establishing a one-to-one correspondence. More precisely, let $\pi^r = (\mathbf{p}_1, \cdots, \mathbf{p}_N) \in \Pi_N^r$. Define a function $\lambda(\mathbf{p}_1, \cdots, \mathbf{p}_N)$ by

$$\lambda(\mathbf{p}_1, \cdots, \mathbf{p}_N) = \left[\frac{\sum_i (\mathbf{p}_i^2 + m_i^2)^{\frac{1}{2}}}{\sum_i \mathbf{p}_i^2/2m_i}\right]^{\frac{1}{2}}, \qquad \text{(A7)}$$

then $\pi^n = (\lambda\mathbf{p}_1, \cdots, \lambda\mathbf{p}_N)$ obviously defines a point of the nonrelativistic phase-space Π_N^n.

We wish to emphasize strongly in this Appendix that this is a perfectly arbitrary procedure. There is a nondenumerably infinite number of admissible correspondences between Π_N^n and Π_N^r, even if one requires this mapping to reduce to the identity at the nonrelativistic limit (that is when the total kinetic energy of the N-particle system is small compared to its total mass). Even on the purely formal ground of mere simplicity, the "radial" mapping is not privileged. For instance, in the three-particle case, it can be seen that it induces a complicated correspondence between the relativistic and nonrelativistic Dalitz diagrams (which are two-dimensional projections of the corresponding phase-spaces). It would seem much simpler and more convenient for practical purposes to take a "radial" correspondence directly between the Dalitz diagrams. More precisely, (ρ, φ) being the polar coordinates of a point on the relativistic Dalitz diagram Δ^r, i.e., a point on the two-dimensional plane lying inside the boundary curve $\rho = f^r(\varphi)$ (the well-known cubic), define a point (ρ', φ') of the nonrelativistic Dalitz diagram Δ^n (the unit circle in the plane) through the mapping:

$$\begin{cases} \varphi' = \varphi, \\ \rho' = \rho/f^r(\varphi). \end{cases} \qquad \text{(A8)}$$

The remaining parameters of the three-dimensional phase-spaces may be easily identified, since they are, in both the relativistic and the nonrelativistic cases, three Euler angles specifying the spatial orientation of the momenta $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$ (whose lengths are fixed by the Dalitz diagram point).

In the present state of affairs, we would recommend this very simple mapping (A8) to be used instead of the radial case (A7) (if one wants to apply the global scheme to three-particle relativistic states).

However, we feel that the classification schemes thus obtained in the relativistic case are rather formal and lack most of the physical content which, to our opinion, gives its interest to the global method in the nonrelativistic case.[5] Indeed, the components of the nonrelativistic grand angular momentum tensor are the quantum transcriptions of the classical dynamical variables:

$$\mathcal{L}^n_{i\alpha,j\beta} = p_{i\alpha}x_{j\beta} - p_{j\beta}x_{i\alpha}, \quad \begin{cases} i = 1, \cdots, N, \\ \alpha = 1, 2, 3, \end{cases} \qquad \text{(A9)}$$

which possess a real physical meaning,[7] describing the relations between the world lines of pairs of particles ($x_{i\alpha}$ is the αth configuration-space coordinate of the ith particle). In the same way, the togetherness operator

$$\Lambda = \sum_{i,j;\alpha,\beta} (L_{i\alpha,j\beta})^2$$

(L being the *relative* grand angular momentum tensor) describes the minimal spatial extension of the N-particle system. This enables us to generalize the well-known centrifugal barrier argument in the sense that, for closely packed systems such as those with which one ordinarily deals, we know in advance that only the eigenstates with low eigenvalues of Λ are important.

Now, the mappings U_T (A6) in general [and in particular for the radial mapping (A7)] map the nonrelativistic angular momentum tensor onto some Lie algebra of operators with the same formal properties but unrelated to what one would like to call a relativistic grand angular momentum tensor.

Indeed, if one tries to generalize the expressions (A9) to obtain relativistic operators $\mathcal{L}^r_{i\alpha,j\beta}$ with the following properties:

(1) they only depend on the i and j particles;

(2) the $i = j$ components are proportional to the angular momentum of the ith particle;

(3) they are constants of the motion for free particles, one obtains the following dynamical variables:

$$\mathcal{L}^r_{i\alpha,j\beta} = f(\omega_i, \omega_j)\left(\frac{p_{i\alpha}}{\omega_i}x_{j\beta} - \frac{p_{j\beta}}{\omega_j}x_{i\alpha}\right), \qquad \text{(A10)}$$

where the ω's are the energies and f an arbitrary function. Obviously, in the relativistic case as well as in the nonrelativistic case, any quantity of the form $f(\omega_i, \omega_j)[v_{i\alpha}x_{j\beta} - v_{j\beta}x_{i\alpha}]$, where the v's are the velocities of the particles, are constants of the motion for free particles.

The great advantage of the nonrelativistic expression (A9), which enables us to use them for

setting up the global coupling scheme, is that they close under commutation on a Lie-algebra structure. One would like this also to be true in the relativistic case. Unfortunately, it can be shown that for no choice of the function f do the operators $\mathfrak{L}^r$ (A10) close under commutation. That is to say, it is impossible to define a relativistic grand angular momentum tensor in such a way as to form a Lie algebra out of its components.

One could still want to use this $\mathfrak{L}^r$ to form a complete set of commuting observables. But, without relying on Lie-algebraic methods, this seems a rather difficult task and, in any event, a new problem in quantum mechanics (where, up to now, the set of all interesting observables was kind enough to close under commutation).

As far as we can see, two possibilities are thus open for obtaining a relativistic generalization of the global coupling scheme:

(1) One may insist on the formal method, relying upon a given one-to-one correspondence between the relativistic and nonrelativistic phase-spaces, but tries to find a privileged correspondence by means of a physical motivation, yet to be imagined.

(2) One may try to obtain a maximal Abelian subalgebra (a complete set of commuting observables) out of the components of the relativistic grand angular momentum tensor. This cannot be done by group-theoretical (or Lie-algebraic) methods, and one has to devise completely new approaches. Let us also notice that one has to define a *relative* grand angular momentum tensor, i.e., the subalgebra of the grand angular momentum tensor which commutes with the total 3-momentum. It would be very helpful for that purpose to have a convenient general parametrization of the relativistic phase-space by means of "relativistic relative momenta", as the one presented for nonrelativistic case in Sec. IB.

We felt that it might be useful to ask these questions, even if we have not been able, up to now, to answer them.

Hermitian Analyticity and S-Matrix Singularity Structure*

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It is shown that the requirement of Hermitian analyticity can be used to determine the Riemann sheet structure of S-matrix singularities. The examples of the square-diagram Landau curve and of a single anomalous threshold are discussed for the $(2 \rightarrow 2)$-particle amplitude.

I. INTRODUCTION

IT has long been known[1] that the singularities of unitary integrals lie on Landau curves. Since unitary integrals represent the difference of S-matrix elements evaluated in different limits, it remains a problem how to determine the way in which these singularities are distributed among the different Riemann sheets of the actual S-matrix amplitudes. The original attempt[1] was based on the assumption of cut-plane analyticity in a limited region, but this is clearly a more drastic assumption than one would ideally wish to make. Recently, Landshoff and Olive[2] have shown that unitarity determines the Riemann sheet structure of the triangle singularity in the physical region, and the method has been extended to other singularities occurring in the the physical region.[3-5] In each case, it is found that the singularity is only present on those arcs of Landau curves which correspond to positive α's, and the corresponding discontinuity is given by the Cutkosky formula.[6] The method is based on the fact that the physical unitarity equations satisfied on either side of the Landau curve are not analytic continuations of each other, so that the requirement that both are true imposes additional restrictions on the S-matrix amplitudes that suffice to determine the Riemann sheet structure. While this argument can only be applied to physical region singularities, the information there obtained can be analytically continued to other regions. In particular, by the evaluation of residues at poles in higher amplitudes, it is possible, in principle, to obtain information about the sheet structure of singularities which, like the anomalous thresholds in $(2 \rightarrow 2)$-particle amplitudes, cannot have any part lying in a physical region.

Our assumptions in this paper are the customary S-matrix assumptions of unitarity, analyticity, connectedness-structure, and crossing in the form in which they are fully described in Ref. 6. We make only minimal use of connectedness-structure, since we deal only with $2 \rightarrow 2$ amplitudes. In addition, we make the explicit assumption of Hermitian analyticity.[6,7] This enables us to regard the $+$ and $-$ amplitudes of S-matrix theory as analytic continuations of a single function along complex conjugate paths. This assumption was not used in the approach of Refs. 2–5. From these assumptions, we obtain the singularity structure associated with the square and the triangle Landau diagrams for values of the external masses such that, in perturbation theory, there is not more than one singular anomalous threshold. We also find the corresponding discontinuity for the square diagram. The results deduced in this S-matrix approach are the same as those deduced in finite-order perturbation theory. We obtain our conditions on the Riemann sheet structure by continuing the unitarity relations from two different channels into a crossed-cut region and interlock them by using Hermitian analyticity. Compared with the physical region method, this approach suffers from the need to make a larger initial assumption. Nevertheless, we feel that it has some interest, since we do not at present have sufficient general knowledge of S-matrix singularity structure to know what ingredients are necessary for an eventual complete specification. Thus, any inter-relation between Riemann sheet structure and other properties seems worth elucidating, and this discussion can be thought of as a complement to the discussions of how to derive Hermitian analyticity from singularity assumptions.[7,8] Finally, it is an

* This research was supported in part by the Air Force Office of Scientific Research, OAR, under Grant AF-EOAR 65-36 with the European Office of Aerospace Research, United States Air Force.

[1] J. C. Polkinghorne, Nuovo Cimento **23**, 360 (1962); *ibid.* **25**, 901 (1962).

[2] P. V. Landshoff and D. I. Olive, J. Math. Phys. **7**, 1464 (1966).

[3] P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, J. Math. Phys. **7**, 1600 (1966).

[4] P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, J. Math. Phys. **7**, 1593 (1966).

[5] M. J. W. Bloxham, Nuovo Cimento **44**, A796 (1966).

[6] R. J. Eden, P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, *The Analytic S-Matrix* (Cambridge University Press, Cambridge, England, 1966).

[7] D. I. Olive, Phys. Rev. **135**, B745 (1964).

[8] J. B. Boyling, Nuovo Cimento **33**, 1356 (1964).

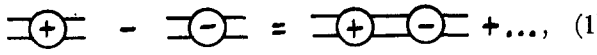
approach which deals with the amplitude of interest directly, rather than by embedding it in higher amplitudes.

For simplicity, we consider the case of a real analytic function, and the real coupling constants, defined by residues of S-matrix elements at single-particle poles. (It would be possible to relax this at the expense of introducing many phase factors into the subsequent argument.) The relation of this reality assumption to symmetry principles has been discussed by Olive.[9] He shows, in particular, that this relation follows from charge-conjugation invariance.

II. THE SQUARE DIAGRAM

We now consider the Landau curve associated with the square diagram of Fig. 1. We do not suppose that all the masses are equal, but we do require that the relationships among them are such that the part Γ of the Landau curve lying in the region of crossed normal-threshold cuts has the form of Fig. 2. Some other cases are discussed in the following section.

We consider the two-particle term in unitarity relation in the s channel. If s lies below the three-particle threshold, this is the only term in the relation. If s lies above that threshold, multi-particle terms appear, but, since they play no part in generating Γ, we need not explicitly take them into account. We write, therefore



(1)

where the Hermitian analyticity implies that the

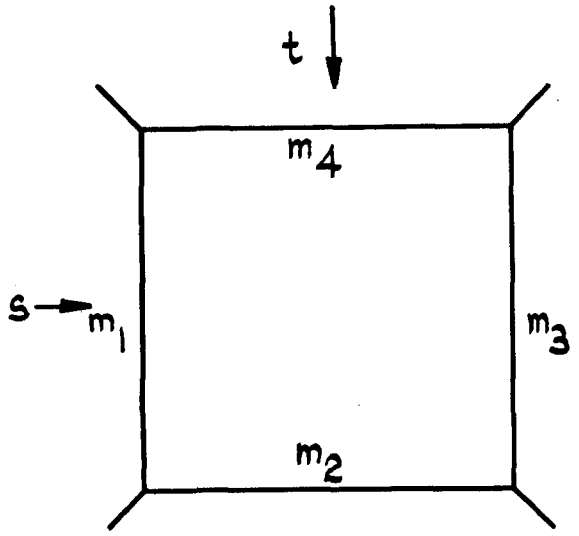


FIG. 1. The square diagram.

[9] D. I. Olive, Nuovo Cimento **26** 73, (1962).

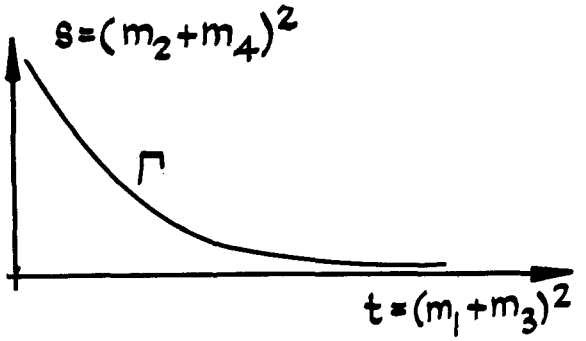


FIG. 2. The Landau curve of Fig. 1 in the crossed-cut region.

$+$ and $-$ signs indicate the continuation of a common function along paths in s given by $\pm i\epsilon$ prescriptions respectively.[10]

The integral appearing on the right-hand side of (1) may be expressed in terms of invariants[11] in the form

$$i\int_{\Delta\geq 0}\frac{dt_1\,dt_2}{\Delta^{\frac{1}{2}}(s,\,t,\,t_1,\,t_2,\,m_2^2,\,m_4^2)}f^+(s,\,t_1)f^-(s,\,t_2), \tag{2}$$

where

$$\Delta \equiv \det(q_i\cdot q_j) \tag{3}$$

with q_i being the momentum associated with the internal line of mass m_i in Fig. 1. The region of integration in t_1 and t_2 for (2) in the physical region is a closed curve and corresponds to real negative values of these two invariants.

As relation (1) is continued outside the physical region, the form of the integration region in t_1 and t_2 is distorted. At the edge of the physical region, the closed curve degenerates, and thereafter the region of integration is bounded by complex parts of the curve $\Delta = 0$. Eventually, further distortions are required by the presence of the poles of $f^{\pm}$ at $t_1 = m_1^2$ and $t_2 = m_3^2$; finally, the singularity associated with the Landau curve of Fig. 1 may be encountered when these two poles trap the edge of the t_1, t_2 region of integration.

These distortions are not easy to follow explicitly, but fortunately it is not necessary to do so. Instead, we revive the idea[1] of using the Feynman integral as a mathematical probe to follow the distortions of the contour. The Feynman integral associated with Fig. 1 satisfies, in the physical region, the equation

$$F(s+i\epsilon,\,t)-F(s-i\epsilon,\,t) = i\int_{\Delta\geq 0}\frac{dt_1\,dt_2}{\Delta^{\frac{1}{2}}(s,\,t;\,t_1,\,t_2,\,m_2^2,\,m_4^2)}\frac{1}{t_1-m_1^2}\frac{1}{t_2-m_3^2}. \tag{4}$$

[10] We use conventional S-matrix bubble notation[6] with certain modifications explained explicitly as required.

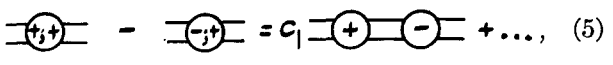
[11] I. T. Drummond, Nuovo Cimento **29**, 720 (1963).

If Eq. (4) is continued outside the physical region, the integration region suffers the same distortions as does (2) due to the single-particle poles in f^+ and f^-. Notice that we do not have to cross the normal threshold cuts in t_1 and t_2. These cuts are known to switch off the poles in f^+ and f^-, but they do not affect the poles in the Feynman integral.[6]

In both (2) and (4) any singularity of Γ is due to the poles being trapped at $t_1 = m_1^2$, $t_2 = m_3^2$ by the edge of the region of integration, $\Delta = 0$. The functions obtained by continuing above or below Γ differ in the relative configurations of the poles and the integration region. The discontinuity, which is the difference between these two continuations, must, therefore, involve taking the residues at the two poles, as has long been known.[1] It is therefore necessarily of the Cutkosky mass-shell integral form,

in the usual S-matrix notation for integrals.[6] For Eq. (2), the small circles represent the residues at single-particle poles and correspond to the S-matrix definition of coupling constants; for Eq. (4), these circles directly represent the coupling constants in the Feynman integral. The factor λ is a topologically determined number corresponding to the number of times, and the sense in which, the poles encircle the integration region when a path is followed in the external variables completely encircling Γ. A case of nonsingularity would correspond to $\lambda = 0$. Because of the similarity of the integration region and the location of the poles in Eqs. (2) and (4), λ must be the same for both. It is in this sense of determining λ that we use Feynman integrals as a mathematical probe.

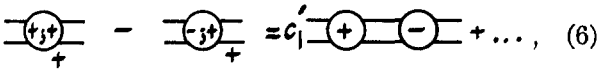
If now Eq. (4) is continued outside the physical region through real values of t, we eventually encounter the normal threshold $t = (m_1 + m_3)^2$. This is not present on the right-hand side of (4), but it is present in each of the terms on the left-hand side of (4), and, if the continuation is to be valid, we must take each of them round the threshold in the same sense. If we choose to do this with a $+i\epsilon$ prescription, then the left-hand side becomes $F(s + i\epsilon, t + i\epsilon) - F(s - i\epsilon, t + i\epsilon)$. We know that, for the Feynman integral, this is singular on the Landau curve Γ in the crossed cuts, since the first term is singular there.[6] Similarly, we continue (1) to give



(5)

where the second $+$ in the left-hand-side bubbles represents the fact that t has been continued over the normal threshold with a $+i\epsilon$ prescription, and the C_1 on the right-hand side is a symbol indicating that (2) is appropriately continued. It then follows from the equivalence of the relevant distortions of (2) and (4) that the right-hand side of (5) is also usinglar on Γ.

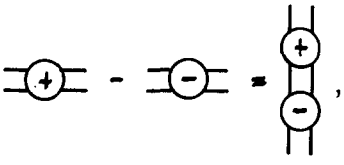
It is necessary, for further continuation, to specify how we continue past Γ. We use the type of prescription found appropriate elsewhere[2,3] and introduce a variable η in the plane normal to Γ so that $\eta < 0$ corresponds to real points below Γ and $\eta > 0$ corresponds to real points above Γ. There are two possible distinct continuations corresponding to a $\pm i\epsilon$ prescription in the η plane: we denote them by subscripts attached to the bubbles on the left-hand side of the unitarity relation. Choosing the $+i\epsilon$ prescription, we obtain



(6)

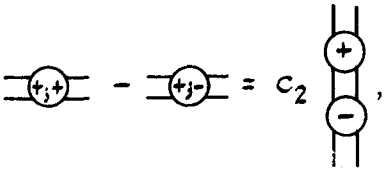
where the symbol C_1' denotes the appropriate continuation of the integral on the right.

Instead of starting with (1), the unitarity relation in the s channel, we might have started with

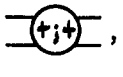


(7)

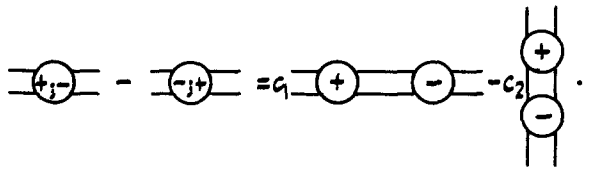
the unitarity relation in the t channel. In (7) the $+$ and $-$ signs refer to the variable t. When we continue (7) into the crossed cut region, it is necessary to choose a particular continuation across the $s = (m_2 + m_4)^2$ normal threshold. With a $+i\epsilon$ prescription, we obtain



(8)

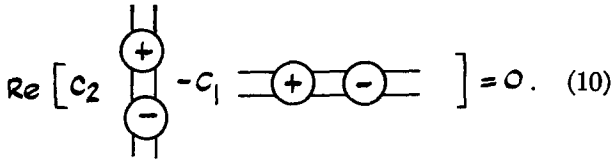
where the first $+$ in the bubbles on the left-hand side denotes the prescription for s, and the C_2 on the right-hand side denotes the appropriate continuation of the unitarity integral. Notice that the sign convention in the bubbles is used consistently in both (5) and (8) so that  , for example, in

both equations denotes an S-matrix amplitude with a $+i\epsilon$ prescription for both s and t. Subtracting (8) from (5) gives



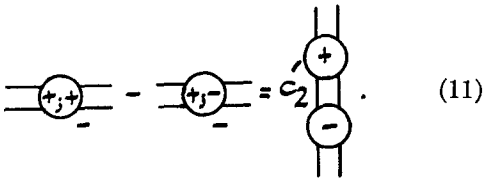
(9)

On the assumption of real Hermitian analyticity, the amplitudes on the left-hand side are complex conjugates of each other so that we can deduce



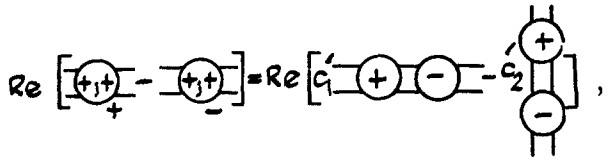
(10)

This will hold in the region below Γ, where (5) and (8) hold. It is now possible to continue (8) around Γ, and we do so by using a $-i\epsilon$ prescription, which



(11)

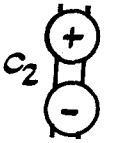
Subtracting (11) from (6), and taking the real part of the resulting equation yields



(12)

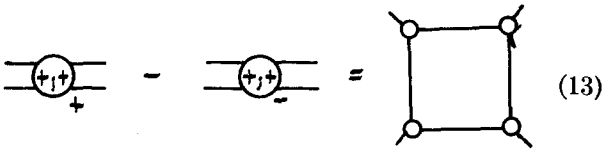
where Hermitian analyticity is used to show that the real parts of the second bubbles on the left-hand sides of (6) and (11) cancel, since the amplitudes correspond to complex conjugate paths of continuation and are complex conjugates of each other.

The function $\mathfrak{F}$ [in square brackets in (10)] is a pure imaginary analytic function below Γ. It ceases to be so above Γ because it is singular on Γ, and it acquires a real part directly related to its discontinuity across Γ. The function in square brackets on the right-hand side of (12) is not a continuation of $\mathfrak{F}$, because C_1' corresponds to a continuation across Γ with $+i\epsilon$ and C_2' corresponds to a continuation across Γ with $-i\epsilon$. However, it differs from a continuation of $\mathfrak{F}$ only by the discontinuity of



across Γ. This discontinuity is real since it is given by $(2\pi i)^2$ times the residue of two poles, replacing $f^{\pm}$ [in an expression similar to (2)] with the function Δ, which now has a value <0. From this, we conclude that the effect of the singularity Γ on the expression in square brackets on the left-hand side of (12) is wholly contained in the real part, and that the real part on the right-hand side of (12) is wholly due to the singularity-generating mechanism. Moreover, the effect of this mechanism is, according to our previous arguments, identical in the perturbation theory model of Eq. (4) and in a general S-matrix theory. The former theory is known to give the answer

, where all the internal lines are on the mass shell. Hence, we deduce that

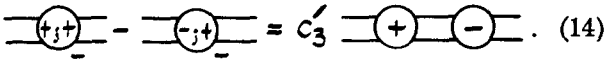


(13)

on the arc Γ. It is not necessary to put $\pm$ signs in the bubbles on the right-hand side of (13) since they are just coupling constants which, according to our assumptions, are real. Equation (13) shows that the

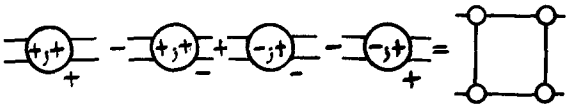
amplitude is singular on Γ and evaluates its discontinuity.

If (4) is continued across Γ with a $-i\epsilon$ prescription, we obtain



(14)

The difference between the C_1' continuation of (6) and the C_3' continuation of (14) is due to the Γ generating mechanism. Once again, this can be evaluated from the model (4) to get



(15)

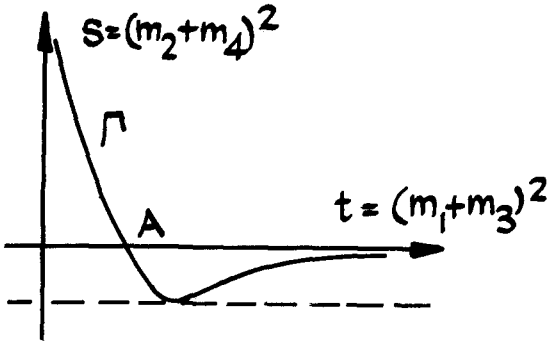
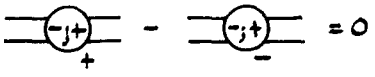


FIG. 3. The Landau curve in the presence of one t-channel anomalous threshold.

Together with (2) this gives



(16)

so that the  amplitude is not singular on Γ.

III. ANOMALOUS THRESHOLDS

We now consider cases in which anomalous thresholds exist in perturbation theory. The appearance of singular anomalous thresholds on the physical sheet is correlated with a change in the Landau curve.[6] Figure 3 shows the form of Γ when there is one anomalous threshold corresponding to the broken line of the figure.

The t-channel anomalous threshold is not present in the s-channel two-particle unitarity integral.[12] Thus, in this case, the continuation of (1) does not directly indicate the anomalous threshold in the S-matrix theory. Moreover, in the t channel, the physical unitarity relation only operates above the anomalous threshold, and so it is equally uninformative. There has been a long standing difficulty in S-matrix theory about the sheet structure of anomalous thresholds.[1] Landshoff and Olive[2] have determined the sheet structure of the triangle singularity in the physical region of the (3 → 3)-particle amplitude; this structure can then be used to determine, by analytic continuation to the appropriate single-particle poles, the condition for the triangle anomalous threshold to be present in the (2 → 2)-particle amplitude. Here we use what is essentially the argument of an earlier paper[13] improved by the use of the ideas of the preceding section.

The arguments of Sec. II can be applied in the arc of Γ lying above A in Fig. 3. The + and − signs associated with the continuations in t now refer to both the encirclement of the t-channel normal threshold and the anomalous threshold (if it is singular). Thus this arc of Γ is a singularity of the  amplitude, but not of the  amplitude. If the anomalous threshold were not singular below A, there would be no distinction between the different t limits in these two amplitudes, which then would need to have the same analytic behavior. However, the point A does not represent a critical intersection of Γ with the normal threshold, and so it is not a point at which the analytic behavior of the amplitudes can change. Hence, there is a contradiction, if the assumption that the anomalous threshold is not singular were correct[14]. Thus we conclude that the anomalous threshold must also be singular in the S-matrix theory.

If the external masses are sufficiently large, an anomalous threshold in the s-channel may also become singular in perturbation theory. The Landau curve is now shown in Fig. 4. The methods used previously now run into complications, since the continuations from the two physical regions are across different arcs of Γ, and it is nontrivial to correlate the different continuations. We do not pursue the matter further in this paper.

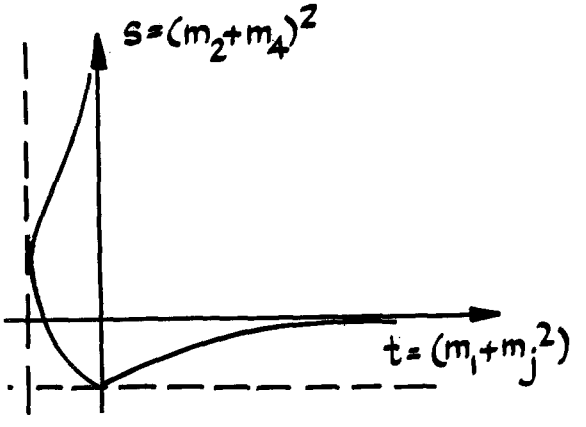


FIG. 4. The Landau curve in the presence of two anomalous thresholds.

[12] While this is true for the Landau singularity associated with Fig. 1, it is not necessarily true for singularities associated with n-particle unitary integrals. See P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, Nuovo Cimento **43**, 444 (1966). This causes no difficulty here since we can continue from regions of elastic unitarity.

[13] J. C. Polkinghorne, Phys. Rev. **128**, 2898 (1962).

[14] Further detailed contradictions can also be obtained by arguments relating to discontinuities.

Representations of the Homogeneous Galilei Group in a Spherical Basis and the Asymptotic Behavior of Relativistic Special Functions*

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The irreducible unitary representations of the Galilei group G_h are obtained in the base $|lm\rangle$ from their expression in the base $|q\rangle$ (Mackey's representation). The faithful representations are then considered as asymptotic expressions for the representation matrices of the principal series of the Lorentz group.

INTRODUCTION

IT is of physical interest to know the representations of a given group in different bases. In Mackey's formalism, which generalizes the Frobenius–Wigner results, the irreducible unitary representations (iur) of the homogeneous Galilei group G_h are based on the velocity transformations (Sec. I). We derive here the expression of these representations in the base $|lm\rangle$ corresponding to the (compact) subgroup of rotations. We thus extend to the group a previous result obtained for the Lie algebra[1] (Sec. 2).

On the other hand, the Galilei group can be obtained by contraction of the Lorentz group L with respect to the rotations[2] and we have shown that the faithful representations of G can be derived from sequences of (iur) of L belonging to the principal series,[1] in a way which generalizes the results of Inonu–Wigner for the rotation group.[3] It follows from this that the matrices corresponding to faithful representations of G_h give the asymptotic behavior of the matrices of the representations of L. We consider this aspect in Sec. 3, making use of Dolzinov–Toptyzin's representations of L.[4]

I. REPRESENTATIONS OF G_h IN THE BASE $|q\rangle$

The homogeneous Galilei group G_h contains the rotations R and the pure Galilei transformations $\mathbf{V}$ (the so-called velocity transformations). It is the set of all transformations, in the space (x_1, x_2, x_3, t), of the type

$$\begin{pmatrix}\mathbf{x}\\ t\end{pmatrix} \to \begin{pmatrix}\mathbf{x}'\\ t'\end{pmatrix} = \begin{pmatrix}R\mathbf{x} + \mathbf{v}t\\ t\end{pmatrix}, \tag{1}$$

where

$$R = (R_{ij}) \quad \begin{cases} R_{ik}R_{jl} = \delta_{kl}, \\ \det R = 1, \end{cases}$$

$\mathbf{v}$ = any vector in space $(\mathbf{x})$.

The transformation (1) is denoted by $(\mathbf{v}, R)$, the order of application being from the right to the left. The multiplication law is

$$(\mathbf{v}_2, R_2)(\mathbf{v}_1, R_1) = (\mathbf{v}_2 + R_2\mathbf{v}_1, R_2R_1). \tag{2}$$

G_h has two kinds of (iur),[1] namely, those in which the translations are trivially represented and other ones which are faithful.

In the present work, we are concerned only with the latter representations which, in fact, on the basis of the isomorphism between G_h and the Euclidean group in three dimensions E_3, can be derived from results obtained by Wightman for E_3.[5,6] Wightman worked out these representations in Mackey's formalism and obtained the following results which we state in a slightly different but equivalent manner.

Let T be the subgroup of accelerations. Let $\mathbf{q}_0 = |q|\mathbf{e}_3$ be the vector parametrizing a particular character of T. Let K be the semidirect product of T by the group corresponding to the rotations φ about the axis $0x_3(e_3)$. K is called "little group of second kind" corresponding to $\mathbf{q}_0$. Also let $\{\exp(i\mathbf{q}_0\cdot\mathbf{v})\exp(is\varphi)\}$ be a particular iur. $\{L(\mathbf{v}, \varphi)\}$ of $K = \{(\mathbf{v}, \varphi)\}$. $\mathfrak{K}(L, K)$ is the space of this representation. We now consider the (homogeneous) left quotient

* This work was supported in part by the U. S. Atomic Energy Commission.

[1] J. Voisin, J. Math. Phys. (to be published).

[2] E. Inönü and E. P. Wigner, Proc. Natl. Acad. Sci. (U. S.) **39**, 510 (1953); E. J. Saletan, J. Math. Phys. **2**, 1 (1961).

[3] E. Inönü and E. P. Wigner, Ref. 2.

[4] A. Z. Dolginov and I. N. Toptygin, Zh. Eksperim. i Teor. Fiz. **37**, 1441 (1959) [English transl.: Soviet Phys.—JETP **37**, 1022 (1960)].

[5] A. S. Wightman, Rev. Mod. Phys. **34**, 845 (1962).

[6] For the application of Mackey's theory to the inhomogeneous Galilei group, see A. S. Wightman, Ref. 5, and J. Voisin, J. Math. Phys. **6**, 1822 (1965); Proc. Indian Acad. Sci. **63**, 39 A (1966).

space G/K. Its points can be labeled by the characters of the type $\mathbf{q} = R\mathbf{q}_0$ (orbit of $\mathbf{q}_0$). We obtain a set of representatives for G/K by taking in each class $\mathbf{q}$ a particular rotation $R_\mathbf{q}$ leading from $\mathbf{q}_0$ to $\mathbf{q}$.

Now let $\{f\}$ be a family of functions from G_h into $\mathcal{H}(L, K)$. These functions satisfy certain conditions of measurability in order to make sure that the representation be continuous (these conditions are of no interest here) and further, they are such that

$$f(g\cdot k) = f(g)L^*(k) \tag{3}$$

[$L^*(k)$ is the complex conjugate of the representative $L(k)$] if k belongs to K. Finally, the functions f have a finite norm with respect to the left-invariant scalar product

$$f_2\cdot f_1 = \int_{\text{orbit}} d\mathbf{q}\,[f_2(R_\mathbf{q})f_1(R_\mathbf{q})]. \tag{4}$$

$[f_2(R_\mathbf{q})f_1(R_\mathbf{q})]$ is the scalar product in $\mathcal{H}(L, K)$.

With this notation, the representation ($\Xi = |\mathbf{q}|$, s) of G_h induced by the representation $L(K)$ of K can be written

$$[U(\mathbf{v}, R)f](R_\mathbf{q}) = \exp(is\varphi)\exp(i\mathbf{q}\cdot\mathbf{v})f(R_{R^{-1}\mathbf{q}}), \tag{5}$$

where $\varphi = R_\mathbf{q}^{-1}RR_{R\mathbf{q}}{}^{-1}$ describes rotation about $\mathbf{e}_3$. This representation (5) is unitary, continuous, and irreducible, and is based on the accelerations. We now obtain an equivalent representation based on the rotations.

II. REPRESENTATION (Ξ, s) IN THE BASE $|lm\rangle$

Let us expand $f(R_\mathbf{q})$ in terms of the irreducible representations of the rotation group. We first write formally

$$f(R_\mathbf{q}) = f^l_{mn}(1)\,D^{(l)}_{mn}{}^*(R_\mathbf{q}). \tag{6}$$

Now, because of the covariance law (3), we must take $n = s$. For, if φ is a rotation about $\mathbf{e}_3$, we have from (3) and (6)

$$\begin{aligned} f(R_\mathbf{q}\varphi) &= f(R_\mathbf{q})\exp(-is\varphi) \\ &= f^l_{mn}(1)\,D^l_{nm}(R_\mathbf{q}^{-1})\exp(-is\varphi) \end{aligned}$$

and, on the other hand, from (3)

$$\begin{aligned} f(R_\mathbf{q}\varphi) &= f^l_{mn}(1)\,D^l_{nm}(\varphi^{-1}R_\mathbf{q}) \\ &= f^l_{mn}(1)\,D^l_{n\mu}(\varphi^{-1})\,D^l_{\mu m}(R_\mathbf{q}^{-1}) \\ &= f^l_{mn}(1)\,D^l_{nm}(R_\mathbf{q}^{-1})\exp(-in\varphi). \end{aligned}$$

Hence $n = s$ and

$$f(R_\mathbf{q}) = f^l_{ms}(1)\,D^l_{sm}(R_\mathbf{q}^{-1}). \tag{7}$$

We also write

$$f(R_\mathbf{q}) = \tilde{f}^l_m(1)\,D^l_{sm}(R_\mathbf{q}^{-1}). \tag{7'}$$

From (7), it follows immediately that $l \geq s$, i.e., $l = |s| + k$ with k any positive integer, and we see that the irreducible representations $l = |s|, |s| + 1, \cdots$ of the rotation group—and only these—are contained in the irreducible representation (Ξ, s) of G_h. Further, as can be checked directly by using (5) and (7), the rotation R is obviously represented by the matrix

$$D(R) = \sum_{l=|s|,|s|+1,\cdots}{}^{\oplus} D^l(R). \tag{8}$$

What about the acceleration $(\mathbf{v}, 1)$? In the base $|\mathbf{q}\rangle$, we have

$$\langle\mathbf{q}'|\,U(\mathbf{v}, 1)\,|\mathbf{q}\rangle = \exp(i\mathbf{q}\cdot\mathbf{v})\,\delta(\mathbf{q} - \mathbf{q}'). \tag{9}$$

Now, the relation between the basis $|\mathbf{q}\rangle$ and $|lm\rangle$ is, from (7),

$$|lm\rangle = \int_{\text{sphere }\Xi} d\mathbf{q}\,D^l_{sm}(R_\mathbf{q}^{-1})\,|\mathbf{q}\rangle. \tag{10}$$

Let $R_\mathbf{q}$ be of the type $(\varphi, \theta, 0)$ with $\mathbf{q} = (\Xi, \theta, \varphi)$. We have[7]

$$\int d\mu\,(\theta, \varphi)\,D^{(j_1)}_{sm_1}{}^*(0, \theta, \varphi)\,D^{(j_2)}_{sm_2}(0, \theta, \varphi) = \delta_{m_1m_2}\,\delta_{j_1j_2}\frac{4\pi}{2j_1 + 1}. \tag{11}$$

Hence

$$\tilde{f}^l_m = \frac{2l + 1}{4\pi}\int d\mathbf{q}\,f(\mathbf{q})\,D^{(l)}_{sm}{}^*(R_\mathbf{q}^{-1}). \tag{12}$$

Thus

$$\begin{aligned} |\mathbf{q}\rangle &= \sum_{l'=|s|}^{\infty}\sum_{m'=-l'}^{l'}\frac{2l' + 1}{4\pi}D^{(l')}_{sm'}{}^*(R_\mathbf{q}^{-1})\,|l'm'\rangle \\ &= \sum_{l'=|s|}^{\infty}\sum_{m'=-l'}^{l'}\frac{2l' + 1}{4\pi}D^{l'}_{m's}(R_\mathbf{q})\,|l'm'\rangle. \end{aligned} \tag{13}$$

On the other hand, if $q = (\Xi, \theta, \varphi)$ and $\mathbf{v} = (r, \theta_v, \varphi_v)$, we have[8]

$$\exp(i\mathbf{q}\cdot\mathbf{v}) = 4\pi\sum_{l_3=0}^{\infty}\sum_{m_3=-l_3}^{l_3}(i)^{l_3}J_{l_3}(\Xi r) \times Y_{l_3m_3}(\theta_v, \varphi_v)Y^*_{l_3m_3}(\theta, \varphi) \tag{14}$$

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[7] See, e.g., A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

[8] Reference 7, p. 81.

with

$$D^{l}_{m0}(\varphi,\ \theta,\ 0) = (-1)^{m}\left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}} Y_{lm}(\theta,\ \varphi)$$
$$= D^{l}_{m0}(R_{\mathfrak{q}}),$$

$R_{\mathfrak{q}}$ being the rotation of Euler angles $(\varphi,\ \theta,\ 0)$. Now, from (10),

$$\langle l_2 m_2|\ U(\mathbf{v},\ 1)\ |l_1 m_1\rangle = \int d\mathfrak{q}_2\ d\mathfrak{q}_1\ D^{(l_2)}_{sm_2}{}^{*}(R^{-1}_{\mathfrak{q}_2})$$
$$\times\ D^{l_1}_{sm_1}(R^{-1}_{\mathfrak{q}_1})\langle \mathfrak{q}_2|\ U(\mathbf{v},\ 1)\ |\mathfrak{q}_1\rangle, \qquad (15)$$

and thus, from (9), (14), and (15),

$$\langle l_2 m_2|\ U(\mathbf{v},\ 1)\ |l_1 m_1\rangle$$
$$= \sum_{l_3=0}^{\infty}\sum_{m_3=-l_3}^{l_3} (-1)^{m_3}[4\pi(2l_3+1)]^{\frac{1}{2}} i^{l_3}\ D^{l_3}_{0m_3}(R^{-1}_{\mathfrak{q}})$$
$$\times\ J_{l_3}(\Xi r) Y_{l_3 m_3}(\theta_v \varphi_v) \int dq\ D^{(l_2)}_{sm_2}{}^{*}(R^{-1}_{\mathfrak{q}})\ D^{l_1}_{sm_1}(R^{-1}_{\mathfrak{q}}). \qquad (16)$$

On the other hand,[9]

$$D^{l_1}_{sm_1}(R^{-1}_{\mathfrak{q}})\ D^{l_3}_{0m_3}(R^{-1}_{\mathfrak{q}})$$
$$= \sum_{l=|l_1-l_3|}^{|l_1+l_3|} (l_1 s l_3 0\ |\ l_1 l_3 l_s)$$
$$\times\ D^{l}_{sm_1+m_3}(R^{-1}_{\mathfrak{q}})(l_1 l_3 l m_1 + m_3\ |\ l_1 m_1 l_3 m_3).$$

It follows from this that

$$\langle l_2 m_2|\ U(\mathbf{v},\ 1)\ |l_1 m_1\rangle$$
$$= \sum_{l_3=0}^{\infty}\sum_{m_3=-l_3}^{l_3} (-1)^{m_3} i^{l_3}[4\pi(2l_3+1)]^{\frac{1}{2}} J_{l_3}(\Xi r)$$
$$\times\ Y_{l_3 m_3}(\theta_v \varphi_v) \sum_{l=|l_1-l_3|}^{l_1+l_3} (l_1 s l_3 0\ |\ l_1 l_3 l s)$$
$$\times\ (l_1 l_3 l m_1 + m_3\ |\ l_1 m_1 l_3 m_3)$$
$$\times \int d\mathfrak{q}\ D^{(l_2)}_{sm_2}{}^{*}(R^{-1}_{\mathfrak{q}})\ D^{l}_{sm_1+m_3}(R^{-1}_{\mathfrak{q}}).$$

We have, finally,

$$\langle l_2 m_2|\ U(\mathbf{v},\ 1)\ |l_1 m_1\rangle = \sum_{l_3=0}^{\infty}\sum_{m_3=-l_3}^{l_3}\sum_{l=|l_1-l_3|}^{l_1+l_3} A(l_1 l l_3$$
$$\times\ m_1 s m_3)\ \delta_{l_2 l}\ \delta_{m_2 m_1+m_3}\ Y_{l_3 m_3}(\theta_v,\ \varphi_v) J_{l_3}(\Xi r), \qquad (17)$$

with

$$A(l_1 l l_3 m_1 s m_3)$$
$$= (-1)^{l_3}[4\pi(2l_3+1)]^{\frac{1}{2}}[4\pi/(2l_2+1)]$$
$$\times\ (l_1 s l_3 0\ |\ l_1 l_3 l s)(l_1 l_3 l m_1 + m_3\ |\ l_1 m_1 l_3 m_3). \qquad (18)$$

[9] Reference 7, p. 60.

III. ASYMPTOTIC BEHAVIOR OF SPECIAL FUNCTIONS RELATED TO L

Dolginov and Toptygin[4] have constructed the iur of the Lorentz group L in the base $|lm\rangle$. In the case of the principal series, if the lowest weight for the rotation subgroup is zero, the iur are characterized by a second invariant N, which is any pure imaginary number.

Let us consider the representation

$$\{T^{N}_{lml'm'}[0,\ \epsilon(r/\Xi),\ 0]\}$$

of the pure Lorentz transformation $v = \tanh(\epsilon r/\Xi)$ along 0_3. Let then ϵ go to zero and $|N|$ tend to infinity in such a way that

$$\lim_{\substack{|N|\to\infty \\ \epsilon\to 0}} \epsilon\ |N| = \Xi. \qquad (19)$$

By definition of the contraction procedure,[2,1] we have

$$\lim_{\substack{\epsilon\to 0 \\ |N|\to\infty}} T^{N}_{lml'm'}\left(0,\ \frac{\epsilon r}{\Xi},\ 0\right) = T^{\Xi}_{lml'm'}\left(\mathbf{v} = \frac{r\mathbf{e}_3}{\Xi},\ 1\right). \qquad (20)$$

The second member of (20) is the matrix element $\langle lm|\ \cdots\ |l'm'\rangle$ of the representative of the pure Galilean transformation $\mathbf{v} = r\mathbf{e}_3/\Xi$ in the representation $(\Xi,\ s = 0)$. The relation (20) gives the asymptotic behavior of the functions $T^{N}_{lml'm'}(0,\ \alpha,\ 0)$. In particular,[4]

$$T^{N}_{l000}(0,\ \alpha,\ 0) = \frac{(2l+1)^{\frac{1}{2}}}{N} \prod_{l}(N,\ \alpha), \qquad (21)$$

with

$$\prod(N,\ \alpha) = \frac{(-1)^{l+1} M_l}{\sinh^{l+1}\alpha}$$
$$\times \int_0^{\alpha} \cos N\beta\ \frac{(\cosh\alpha - \cosh\beta)^{l}}{l!}\ d\beta,$$
$$M_l = [N^2(N^2+1^2)\cdots N^2+l^2]^{\frac{1}{2}},$$

and hence from (17) and (18)

$$\lim_{\substack{N\to\infty \\ \epsilon\to 0}} T^{N}_{l000}\left(0,\ \frac{r}{|N|},\ 0\right) = i^{l} 4\pi J_l(r). \qquad (22)$$

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Drum Shapes and Isospectral Graphs*

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We analyze the discrete drum model of Fisher and show that the information on the shape of a smooth drum contained in its low-order spectral moments is, at best, the area, length of its boundary, and number and type of corners. We produce a counter example which proves that one cannot always hear the shape of a discrete drum.

I. INTRODUCTION

IN a recent lecture entitled "Can you Hear the Shape of a Drum?" Kac[1] propounded the following question, which he attributes to Bochner. Consider a membrane whose vertical displacement satisfies the wave equation

$$\nabla^2 F = \partial^2 F/\partial t^2 \tag{1.1}$$

in a region Ω, held fixed along its boundary Γ. We may reduce this equation by separation of variables through the substitution

$$F = u(\mathbf{r})e^{i\omega t} \tag{1.2}$$

so that (1.1) becomes

$$\nabla^2 u + \omega^2 u = 0 \tag{1.3}$$

subject to the boundary conditions

$$u(\mathbf{r}) = 0 \qquad \text{for } \mathbf{r} \text{ on } \Gamma. \tag{1.4}$$

Kac points out that it is well known that this problem defines uniquely an infinite sequence of discrete eigenvalues

$$\omega^2 = \lambda_1 \leq \lambda_2 \leq \lambda_3, \cdots, \tag{1.5}$$

or correspondingly a unique characteristic function

$$C(t) = \sum_{n=1}^{\infty} e^{-\lambda_n t}. \tag{1.6}$$

His question is, if two regions Ω_1 and Ω_2 have the same $C(t)$, are they congruent? As a partial answer he summarizes and extends previous work to show for a smooth drum that

$$C(t) \sim (|\Omega|/2\pi t) - \tfrac{1}{4}L(2\pi t)^{-\frac{1}{2}} + \tfrac{1}{6}(1 - r), \tag{1.7}$$

where $|\Omega|$ is the area, L the length of the boundary, and r the number of holes.

Fisher[2] introduces a discrete model drum. In his model the drum consists of a regular lattice array of atoms coupled by a Hooke's law force along the lattice bonds to their nearest neighbors. His discrete model has the virtue that one can analyze in complete detail the eigenspectrum of at least small drums. He proceeds to show that the same information as given in (1.7) about continuous drums can be readily extracted from the low-order moments of the eigenspectrum for discrete drums.

We investigate the moment problem for Fisher's discrete model and show that there is a certain large class of large, smooth, discrete drums for which the low-order spectral moments give, at best, very little additional information about the drum shape. We point out that the higher-order moments are related to the shape in such a way that they do not clearly correspond uniquely to the shape. We give a number of examples which illustrate how quirks can cause very differently shaped graphs (related by Fisher directly to the discrete drum problem) to be isospectral (have exactly the same eigenvalue spectrum). In particular, we exhibit an isospectral pair of graphs which satisfy the spirit of all of Fisher's criteria to be drum graphs. As Fisher[2] points out, this counter example provides strong presumptive evidence that one cannot always hear the shape of a drum.

II. CALCULATION OF THE SPECTRAL MOMENTS

We review the formulation of the discrete drum problem as given by Fisher[2] and recast the calculation of the spectral moments in a form more suitable to our purposes. The discrete model is a regular two-dimensional lattice (coordinate number q) of atoms cut in some arbitrary shape. These atoms are thought to interact along the nearest-neighbor bonds of the lattice by a Hooke's law force. The boundary atoms are considered to be clamped in place. Thus the equations of motion for the displacement of

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[1] M. Kac; this lecture was filmed under the auspices of the Committee on Educational Media of the Mathematical Association of America and an expanded version is to be published in the American Mathematical Monthly.

[2] M. E. Fisher, J. Combinatorial Theory, 1, 105 (1966).

the jth atom $\varphi_j(t)$ are

$$\varphi_j(t) = 0 \qquad (j \text{ a boundary site}), \tag{2.1a}$$

$$m\frac{d^2\varphi_j}{dt^2} = -K\sum_{k(j)}^{q}(\varphi_j - \varphi_{k(j)}) \qquad (j \text{ an interior site}), \tag{2.1b}$$

where K is the effective "spring constant" and $k(j)$ are the q nearest neighbors of j. If we make the standard substitution[3]

$$\varphi_j(t) = u_j \exp\,[i(K/m)^{\frac{1}{2}}\omega t], \tag{2.2}$$

then the eigenvalues are given by the solution of the set of homogeneous equations,

$$\omega^2 u_j = qu_j - \sum_{k(j)}^{q} u_{k(j)}, \tag{2.3}$$

where j runs over all the interior sites. The eigenvalues are given by

$$\omega^2 = q - g, \tag{2.4}$$

where g is any eigenvalue of the $N \times N$ graph matrix

$$\begin{aligned} \mathbf{G}_{ij} &= 1, \text{ if } i \text{ and } j \text{ are nearest neighbors,} \\ &= 0, \text{ otherwise.} \end{aligned} \tag{2.5}$$

Consequently, two discrete drums have the same set of eigenvalues if and only if their graph matrices do.

The knowledge of the N eigenvalues of an $N \times N$ matrix is equivalent, through the use of Newton's indentities and the solution for the roots of a polynomial, to the knowledge of the first N spectral moments

$$M_s = \sum_{n=1}^{N} g_n^s, \tag{2.6}$$

where the g_n are the eigenvalues of the matrix. However, as the trace is invariant, under a diagonalizing similarity transformation, we can readily see that

$$M_s = \mathrm{Tr}\,\{\mathbf{G}^s\} = \sum_{i=1}^{N}(\mathbf{G}^s)_{ii}. \tag{2.7}$$

Fisher[2] now shows that $(\mathbf{G}^s)_{ij}$ is exactly equal to the number of closed paths on the N-point graph $\mathcal{G}$ of interior points of exactly s steps which begin and end at site j. Consequently we may evaluate the spectral moments by counting closed paths. We now recast this result in a more convenient form.

First let us introduce the notion of the support of a path. A path is a sequence of steps between vertices which may double back on itself or intersect itself. The support of a path is defined as the undirected graph which results by placing a bond between every pair of vertices which are connected by some step of the path.

If we now consider all paths of s steps on $\mathcal{G}$, they may be classified according to their supports. If any support is embeddable on $\mathcal{G}$ then all paths of s steps with that support occur for each such embedding. Thus the number of paths of s steps are given by the sum over all supports of the number of embeddings times the number of s step paths with that support. The number of embeddings of a support on the graph $\mathcal{G}$ is just a row from the Rushbrooke $\mathbf{T}$ matrix[4] which is the number of topologically distinct ways one graph may be embedded in another. As this matrix can be put in triangular form with $\mathbf{T}_{ii} = 1$ it is not singular (det $\mathbf{T} = 1$).

Let us now introduce the moment generating function of a graph $\mathcal{G}_k$ with graph matrix $\mathbf{G}_k$ as

$$M_k(z) = \sum_{s=0}^{\infty}\frac{M_s z^s}{s!} = \mathrm{Tr}\,\{\exp\,[z\mathbf{G}_k]\}, \tag{2.8}$$

and the irreducible moment generating function

$$R_k(z) = \sum_{s=0}^{\infty}\frac{r_{k,s}z^s}{s!}, \tag{2.9}$$

where

$$r_{k,s} \text{ is the number of paths with exactly } s \text{ steps having } \mathcal{G}_k \text{ as their support.} \tag{2.10}$$

We discuss only connected graphs, since a disconnected graph is never the support of a path.

It follows from the above argument that

$$M_k(z) = \sum_i \mathbf{T}_{ki}R_i(z). \tag{2.11}$$

A knowledge of either the set $\{M_k(z)\}$ or $\{R_k(z)\}$ allows one to solve for the other as $\mathbf{T}$ is nonsingular. The point of relation (2.11) is that the low-order irreducible moments vanish, except for very small graphs and hence the low-order moments of any graph can be discussed in terms of the number of embeddings of small graphs alone.

In order to determine which graphs contribute to the sth moment, it is necessary to classify graphs according to their circumference. By the circumference of a graph, we mean the least number of steps of any path which has that graph as its support. For example, a simple closed loop has a cir-

[3] See, for example, W. V. Houston, *Principles of Mathematical Physics* (McGraw-Hill Book Company Inc., New York, 1948), Chap. 7.

[4] G. S. Rushbrooke, J. Math. Phys. 5, 1106 (1964).

cumference equal to the number of its bonds. A tree has a circumference equal to twice the number of its bonds. All other graphs lie in between. We illustrate in Figs. 1–5 all graphs of circumference 2 to 6. The point has circumference zero and there is no graph of circumference one. The number accompanying each graph is its serial number in an extensive compilation of graphs collected in connection with work on the Heisenberg model of ferromagnetism.[5] Graphs are referred to herein by these serial numbers insofar as possible. As an illustration, we give the first few terms of $R_k(z)$ for the first three graphs. They are

$$R_1(z) = 2z^2/(2!) + 2z^4/(4!) + 2z^6/(6!) + \cdots,$$
$$R_2(z) = 4z^4/(4!) + 12z^6/(6!) + \cdots, \qquad (2.12)$$
$$R_3(z) = 6z^3/(3!) + 30z^5/(5!) + 24z^6/(6!) + \cdots.$$

If we work out the rest of the $R_k(z)$ for the graphs in Figs. 1–5 we may write out (2.11) explicitly for the first six moments. Thus

$$\begin{aligned} M_k(z) = N &+ 2\mathbf{T}_{k1}\, z^2/(2!) + 6\mathbf{T}_{k3}\, z^3/(3!) \\ &+ [2\mathbf{T}_{k1} + 4\mathbf{T}_{k2} + 8\mathbf{T}_{k6}]z^4/(4!) \\ &+ [30\mathbf{T}_{k3} + 10\mathbf{T}_{k7} + 10\mathbf{T}_{k12}]z^5/(5!) \\ &+ [2\mathbf{T}_{k1} + 12\mathbf{T}_{k2} + 24\mathbf{T}_{k3} + 12\mathbf{T}_{k4} + 6\mathbf{T}_{k5} \\ &+ 48\mathbf{T}_{k6} + 36\mathbf{T}_{k11} + 12\mathbf{T}_{k13} + 24\mathbf{T}_{k26} \\ &+ 12\mathbf{T}_{k29}]z^6/(6!) + \cdots. \qquad (2.13) \end{aligned}$$

We now apply this formalism to the problem of determining what can be learned from the early moments about the shape of a macroscopic discrete drum. In order to simplify the discussion we restrict the allowed drum shapes to a large connected region (N points, possibly multiply-connected) of a plane lattice bounded by straight lines parallel to the nearest-neighbor bonds of the lattice of a length of the order of $N^{\frac{1}{2}}$. What can we tell about this kind of drum from a finite number of spectral moments? Fisher[2] has shown that the first three (or four depending on the lattice) spectral moments suffice to determine the area, the length of the boundary, and the connectivity of the drum. The contributions to any finite number, $s \ll N^{\frac{1}{2}}$, of moments can be seen to be composed of three parts. Firstly N times the moment per site on an infinite lattice. Secondly, $N^{\frac{1}{2}}$ order of magnitude corrections due to the length of the boundary as moments of order s can "see" only a distance $\frac{1}{2}s$ from the boundary, and lastly terms of order unity arising from the corners. Information about the length of various edges, for example, cannot come in, since it involves graphs of a length of the order of $N^{\frac{1}{2}}$ which do not contribute to the first s spectral moments. One can probably determine the number of each type of corner. (The connectivity is a certain simple function of these numbers.) Beyond that, there is no more information contained in the low-order moments of this simple type of graph. For moments of the order of the size of the graph $[O(N^{\frac{1}{2}})]$, quirks of one sort or another can arise to cause very different graphs to have the same spectrum for their graph matrices, as we see in the next section.

FIG. 1. The graph of circumference 2.

FIG. 2. The graph of circumference 3.

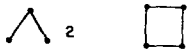

FIG. 3. The graphs of circumference 4.

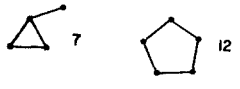

FIG. 4. The graphs of circumference 5.

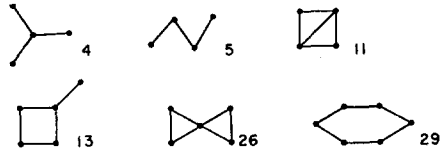

FIG. 5. The graphs of circumference 6.

III. ISOSPECTRAL GRAPHS

We have surveyed a collection of 1443 different graphs[5] containing at least all graphs (save one) of at most seven points and ten lines, all of less than eight lines, all with less than three loose ends of nine lines, odd graphs, less than four loose ends of nine lines, even graphs, and less than three loose ends ten lines, even graphs. We checked for isospectral graphs (two or more graphs with the same spectral moments). We programmed the IBM 7094 to compute the moments (as the trace of powers of the graph matrix) and compare them for identity. We found approximately 120 pairs, 5 triples, and 1 quadruple of isospectral graphs. We illustrate these results with several examples.

The smallest pair of isospectral graphs are shown in Fig. 6. They have six points and seven lines. They also appear to have been missed by Fisher in his search of all six point or smaller graphs. For the convenience of the reader the relevant, nonzero

[5] G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters **20**, 146 (1966) and fuller account in preparation.

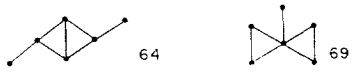

FIG. 6. The smallest pair of isospectral graphs.

T matrix elements required to evaluate the first six moments are listed in Table I. The reader may note that the differences in 2 and 6 compensate in fourth order and those in 2, 4, 5, 6, 11, 13, and 26 in sixth order. The moments are

$$6, 0, 14, 12, 70, 120, 446, \cdots . \quad (3.1)$$

TABLE I. T Matrix elements.

j	1	2	3	4	5	6	7	11	13	26
$T_{64,j}$	7	12	2	4	14	1	6	1	2	0
$T_{69,j}$	7	14	2	10	12	0	6	0	0	1

As we have examined all graphs of five or fewer points we may hereby provide the answer to Harary's question[6]: What is the smallest number of points for which there exists a pair of isospectral graphs?

This represents a reduction from the smallest known previous pair with 15 points[2] to six points (see note added in proof). The smallest pair of nonisomorphic, isospectral trees are illustrated in Fig. 7.

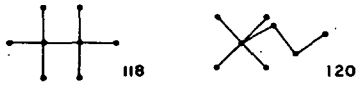

FIG. 7. The smallest pair of isospectral trees.

They have seven lines and eight points. Their moments are

$$8, 0, 14, 0, 62, 0, 308, 0, 1598, \cdots . \quad (3.2)$$

An example of a pair of isospectral graphs, one with a pendant bond and one without is afforded by the graphs illustrated in Fig. 8. Their moments are

$$7, 0, 16, 6, 64, 60, 310, 448, \cdots . \quad (3.3)$$

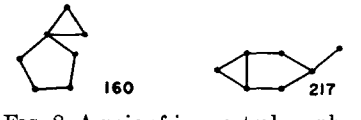

FIG. 8. A pair of isospectral graphs.

An example of a triple of isospectral graphs with nine lines and nine points is given by Fig. 9 with moments

$$9, 0, 18, 0, 78, 0, 402, 0, 2214, 0, \cdots . \quad (3.4)$$

[6] F. Harary, SIAM Rev. 4, 202 (1962).

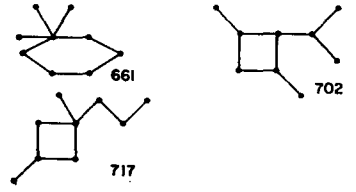

FIG. 9. A triple of isospectral graphs.

An example of a quadruple of isospectral graphs with ten lines and nine points is shown in Fig. 10. The moments for this case are

$$9, 0, 20, 0, 116, 0, 812, 0, 5924, 0, \cdots . \quad (3.5)$$

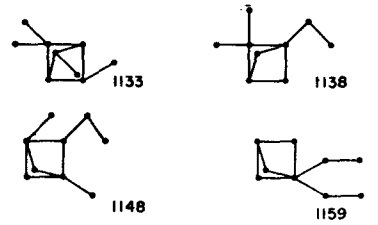

FIG. 10. A quadruple of isospectral graphs.

None of these examples are suitable for the drum problem. Fisher[2] has set up criterion for a pair of isospectral graphs, which, if met, "would be strong presumptive evidence that one cannot always hear the shape of drum!" His criteria are (a) that the graphs be planar, (b) that they can be strongly embedded in the triangular (or other) plane lattice, and (c) that the embedding is free of pendant bonds and (x) configurations.[7] There is precisely one isospectral pair in the compilation of graphs[5] which is free of pendant bonds. It has 10 lines and 7 points and is illustrated in Fig. 11. The spectral moments are

$$7, 0, 20, 12, 132, 180, 1076, 2044, \cdots . \quad (3.6)$$

However, this example does not satisfy (b), for example.

We have, however, succeeded, taking this pair as a

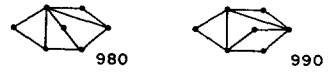

FIG. 11. A pair of isospectral graphs free of pendant bonds.

[7] He, in addition, requires that the graphs be built up of rigid subgraphs in order to obtain a class of graphs for which the graph matrix corresponds to a unique shape. We take the liberty of relaxing his conditions somewhat by including, in addition, graphs which, by virtue of (b), have a unique shape. The reason for this change is that, for example, the smallest "rigid" graph with one hole has 18 points and 36 lines while 6 points and 6 lines suffice for a "(b) rigid" graph.

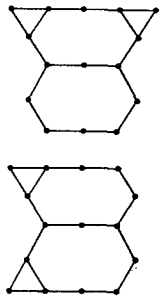

FIG. 12. A pair of isospectral drum graphs.

starting point, in constructing a pair of 18 lines, 15 interior sites isospectral graphs which do satisfy all the criterion of drum graphs. They are shown in Fig. 12. Their moments are

$$15, 0, 36, 12, 144, 100, 684, 700, 3584, 4692,$$
$$19996, 30976, 116412,$$
$$203424, 698356, 1334092, \cdots . \quad (3.7)$$

This pair of graphs, together with the evidence of the statistical frequency of isospectral graphs given earlier in this section plus the analysis of the previous section suggest strongly that one cannot always hear the shape of a drum.

Note added in proof: Recently we were apprised of the fact that the pair of eight-point, non-isomorphic, isospectral trees (Fig. 7) was previously given by L. Collatz and U. Sinogowitz, Abh. Math. Sem. Univ. Hamburg **21**, 63(1957).

Factorization Theorems

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(Received 3 January 1966)

A precise set of conditions is given for which the momentum correlation functions of quantum mechanical, weakly interacting, many-particle systems can be factorized.

1. INTRODUCTION

IN this paper we consider the time evolution of the momentum correlation functions for many-particle systems of fermions and bosons.

For a system in a pure state $|\phi_0\rangle$ at time $t = 0$, the momentum correlation functions at time t are defined by

$$f_1(\mathbf{k}_1; t) = \langle\phi_0| U_{-t} n_{\mathbf{k}_1} U_t |\phi_0\rangle,$$

$$f_2(\mathbf{k}_1, \mathbf{k}_2; t) = \langle\phi_0| U_{-t} n_{\mathbf{k}_1} n_{\mathbf{k}_2} U_t |\phi_0\rangle,$$

and in general

$$f_m(\mathbf{k}_1 \cdots \mathbf{k}_m; t) = \langle\phi_0| U_{-t} n_{\mathbf{k}_1} \cdots n_{\mathbf{k}_m} U_t |\phi_0\rangle. \quad (1)$$

$n_{\mathbf{k}}$ is the number operator for the particles with momentum $\mathbf{k}$ and

$$U_t = e^{-iHt}, \quad (2)$$

where H is the Hamiltonian of the system.

Van Hove[1] has shown how the time evolution of a large class of operators can be calculated using the Pauli master equation.[2] The use of this equation is limited to weakly coupled or low-density systems. We confine our attention to weakly coupled systems, although the same methods can be applied to low-density systems.

We prove the following theorem: given at $t = 0$ the state $|\phi_0\rangle$ is such that

$$f_2(\mathbf{k}_1, \mathbf{k}_2; 0) = f_1(\mathbf{k}_1; 0) f_1(\mathbf{k}_2; 0) \quad (3)$$

and that the time evolution of the functions f_1 and f_2 is governed by the Pauli master equation, then

$$f_2(\mathbf{k}_1, \mathbf{k}_2; t) = f_1(\mathbf{k}_1; t) f_1(\mathbf{k}_2; t) \quad (4)$$

at all later times. Such a theorem is called a factorization theorem. This terminology was first used by Kac,[3] who proved the theorem for a system described by a model master equation.

So far, the theorem has been proved explicitly only for classical, low-density systems (McLennan and Swenson[4]). We wish to generalize these proofs to quantum mechanical, weakly interacting systems.

The theorem has an underlying physical content apart from its use in "contracting" the master equation and deriving a Boltzmann equation for $f_1(\mathbf{k}_1; t)$ (Kac,[3] Brout,[5] Van Hove[6]). It tells us that if there are no momentum correlations present initially in a weakly coupled system, then they do not develop at any later time during the evolution of the system. We show during the course of the proof that the theorem is only true in the thermodynamic limit. There is no reason to believe the theorem to be true for a small system.

The plan of the paper is as follows. In Secs. 2 and 3, we describe the Pauli master equation in Van Hove's formalism and specialize this formalism to a weakly interacting system of fermions. Section 4 contains the proof of the factorization theorem. The conditions under which the theorem is valid are discussed in Sec. 5. In Sec. 6 we generalize the results to bosons and mixtures of bosons and fermions. In a later paper, we use the factorization theorem to discuss the derivation of the nonlinear Boltzmann equation for these systems.

2. VAN HOVE'S WEAK COUPLING MASTER EQUATION

Consider a quantum mechanical many-particle system with Hamiltonian

$$H = H_0 + \lambda H_1, \quad (5)$$

where, for a system of fermions, H_0 would be the free-particle kinetic energy and λH_1 the interaction

* Part of a thesis submitted by J. Sykes in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mathematical Physics at Birmingham University, England (1964).

[1] L. Van Hove, Physica 21, 517 (1955).

[2] W. Pauli, *Festschrift zum 60. Geburtstage A. Sommerfelds* (S. Hirzel Verlag, Leipzig, 1928).

[3] M. Kac, *Lectures on Probability Theory* (Interscience Publishers, Inc., New York, 1959).

[4] J. A. McLennan, and R. J. Swenson, J. Math. Phys. 4, 1527 (1963).

[5] R. Brout, Physica 22, 509 (1956).

[6] L. Van Hove, *The Theory of Neutral and Ionised Gases* (John Wiley & Sons, Inc., New York, 1960), p. 149.

potential in which λ is a dimensionless parameter. The unperturbed Hamiltonian H_0 is assumed to have a complete set of eigenstates $|\alpha\rangle$:

$$H_0 \, |\alpha\rangle = |\alpha\rangle \epsilon(\alpha). \tag{6}$$

In the limit of an infinite system, the energy $\epsilon(\alpha)$ and the quantum numbers α are assumed to be continuous so that spin must be excluded. The eigenstates are normalized such that

$$\langle \alpha \mid \alpha' \rangle = \delta^D(\alpha - \alpha'). \tag{7}$$

The state $|\phi_t\rangle$ at time t of an isolated system which at $t = 0$ has been prepared in the pure state $|\phi_0\rangle$ is given by

$$i \, |\dot{\phi}_t\rangle = H \, |\phi_t\rangle \tag{8}$$

in which we have put $\hbar = 1$. This equation has the formal solution

$$|\phi_t\rangle = U_t \, |\phi_0\rangle = e^{-iHt} \, |\phi_0\rangle. \tag{9}$$

The expectation value of any operator A, diagonal in the $|\alpha\rangle$ representation, is

$$\bar{A}(t) = \langle \phi_t | \, A \, |\phi_t\rangle = \langle \phi_0 | \, A(t) \, |\phi_0\rangle, \tag{10}$$

where $A(t)$ is the Heisenberg operator

$$A(t) = U_{-t} A U_t. \tag{11}$$

Since the eigenstates $|\alpha\rangle$ form a complete set, $|\phi_0\rangle$ can be expanded as

$$|\phi_0\rangle = \int d\alpha' \, c(\alpha') \, |\alpha'\rangle \tag{12}$$

and substituted into Eq. (10). The resulting expression is of the form

$$\bar{A}(t) = \int d\alpha \int d\alpha' \, |c(\alpha)|^2 \, P_{\alpha|\alpha'}(t) A(\alpha')$$

$$+ \int d\alpha \int d\alpha' \int d\alpha'' \, c^*(\alpha) c(\alpha') I_{\alpha\alpha'|\alpha''}(t) A(\alpha''), \tag{13}$$

which defines the master function $P(t)$ and the interference function $I(t)$.

Van Hove[1] has shown by imposing simple conditions on (a) the initial state of the system, (b) the diagonal operators A being considered, (c) the interaction and by taking two limiting processes: (i) the thermodynamic limit (N/V), $N \to \infty$, $V \to \infty$ with N/V constant; (ii) the $\lambda^2 t$ limit, $\lambda \to 0$, $t \to \infty$ with $\lambda^2 t$ constant, that the master function $P(t)$ can be "coarse-grained" and satisfies the Pauli master equation

$$\frac{d}{d\tau} P_{\alpha\alpha'}(t) = \int d\alpha'' \, \Omega_{\alpha\alpha''} P_{\alpha''\alpha'}(t), \tag{14}$$

where

$$\tau = 2\pi\lambda^2 t. \tag{15}$$

The operator Ω can be expressed in terms of the transition probabilities

$$W_{\alpha\alpha''} = |\langle \alpha | \, H_1 \, |\alpha''\rangle|^2 \, \delta[\epsilon(\alpha) - \epsilon(\alpha'')] \tag{16}$$

by the equation

$$\Omega_{\alpha\alpha''} = W_{\alpha\alpha''} - \int d\alpha_1 \, W_{\alpha\alpha_1} \, \delta^D(\alpha - \alpha''). \tag{17}$$

The initial condition is

$$P_{\alpha\alpha'}(0) = \delta^D(\alpha - \alpha'). \tag{18}$$

The formal solution of Eq. (14) is

$$P_{\alpha\alpha'}(t) = \sum_{m=0}^{\infty} \frac{\tau^m}{m!} \, \Omega^{(m)}_{\alpha\alpha'}, \tag{19}$$

where

$$\Omega^{(m)}_{\alpha\alpha'} = \int d\alpha_1 \cdots \int d\alpha_{m-1} \, \Omega_{\alpha,\alpha_1} \cdots \Omega_{\alpha_{m-1},\alpha'} \tag{20}$$

and

$$\Omega^{(0)}_{\alpha\alpha'} = \delta^D(\alpha - \alpha'). \tag{21}$$

Janner[7] has shown for weakly coupled systems that the interference function $I(t)$ behaves as $\lambda P(t)$, so for states independent of λ and in the $\lambda^2 t$ limit, the master function $P(t)$ dominates the time evolution of the system.

3. SYSTEM OF FERMIONS

The Hamiltonian is taken to be of the form (5) with

$$H_0 = -\frac{1}{2m} \sum_i \nabla_i^2, \tag{22}$$

$$H_1 = \tfrac{1}{2} \sum_{i,j}{}' \, v(\mathbf{r}_i - \mathbf{r}_j). \tag{23}$$

In second quantization, this becomes

$$H = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}} c_{\mathbf{p}} + \frac{\lambda}{V} \sum_{\mathbf{pqr}} v_{\mathbf{q}} c^\dagger_{\mathbf{p}+\mathbf{q}} c^\dagger_{\mathbf{r}-\mathbf{q}} c_{\mathbf{r}} c_{\mathbf{p}}, \tag{24}$$

where

$$v_{\mathbf{q}} = \frac{1}{2} \int d\mathbf{r} \, e^{-i\mathbf{q}\cdot\mathbf{r}} v(\mathbf{r}). \tag{25}$$

In the summation over $\mathbf{q}$, the terms with $\mathbf{q} = 0$ have been included in the unperturbed part of the Hamiltonian. $v_{\mathbf{q}=0}$ is required to converge.

The basic representation is the set of normalized

[7] A. Janner, Helv. Phys. Acta, **35**, 47 (1962).

eigenstates

$$|\alpha\rangle = |\{n_{\mathbf{k}}\}\rangle \tag{26}$$

of the free system, where $\{n_{\mathbf{k}}\}$ is the set of occupation numbers of the fermion plane-wave states.

We start with a discrete representation and later, when the (N/V) limit is taken, put

$$\sum_{\mathbf{k}} \to \frac{V}{(2\pi)^3}\int d\mathbf{k}$$

and

$$\frac{V}{(2\pi)^3}\,\delta^K_{\mathbf{p},0} \to \delta^D(\mathbf{p}), \tag{27}$$

where δ^K and δ^D are the Kronecker and Dirac delta-functions, respectively.

For the fermion interaction, the matrix element $\langle\{n_{\mathbf{k}}\}\ |H_1|\ \{n_{\mathbf{k}}\}\rangle$ is different from zero only if for some $\mathbf{p}, \mathbf{q}, \mathbf{r}$

$$n''_{\mathbf{k}} = n_{\mathbf{k}} - \delta_{\mathbf{k},\mathbf{p}} - \delta_{\mathbf{k},\mathbf{r}} + \delta_{\mathbf{k},\mathbf{p}+\mathbf{q}} + \delta_{\mathbf{k},\mathbf{r}-\mathbf{q}},$$

subject to the condition $n_{\mathbf{k}} = 0$ or 1. The transition probability W is then

$$W_{\{n\mathbf{k}\}\{n\mathbf{k}''\}} = \sum_{\mathbf{pqr}} \frac{|v_{\mathbf{q}}|^2}{V^2}\,\delta(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{r}};\,\epsilon_{\mathbf{p}+\mathbf{q}}+\epsilon_{\mathbf{r}-\mathbf{q}})n_{\mathbf{p}}(1-n_{\mathbf{p}+\mathbf{q}})n_{\mathbf{r}}(1-n_{\mathbf{r}-\mathbf{q}})$$
$$\times\,\delta\{n''_{\mathbf{k}};\,n_{\mathbf{k}}-\delta_{\mathbf{p},\mathbf{k}}-\delta_{\mathbf{r},\mathbf{k}}+\delta_{\mathbf{p}+\mathbf{q},\mathbf{k}}+\delta_{\mathbf{r}-\mathbf{q},\mathbf{k}}\} \tag{28}$$

in which all elements of the set $(\mathbf{p}, \mathbf{r}, \mathbf{p}+\mathbf{q}, \mathbf{r}-\mathbf{q})$ are distinct. The symmetry relation

$$W_{\{n\mathbf{k}\}\{n\mathbf{k}''\}} = W_{\{n\mathbf{k}''\}\{n\mathbf{k}\}} \tag{29}$$

follows by rearranging the summations and using the condition

$$v_{\mathbf{q}} = v_{-\mathbf{q}}.$$

From the relations (17) and (28), for example,

$$\sum_{\{n\mathbf{k}'\}} \Omega_{\{n\mathbf{k}\}\{n\mathbf{k}'\}} n'_{\mathbf{k}_1}$$
$$= \frac{2}{V^2}\sum_{\mathbf{p},\mathbf{q}} |v_{\mathbf{q}}|^2\,\delta(\epsilon_{\mathbf{k}_1}+\epsilon_{\mathbf{p}};\,\epsilon_{\mathbf{p}+\mathbf{q}}+\epsilon_{\mathbf{k}_1-\mathbf{q}})$$
$$\times\,[n_{\mathbf{k}_1-\mathbf{q}}(1-n_{\mathbf{k}_1})n_{\mathbf{p}+\mathbf{q}}(1-n_{\mathbf{p}})$$
$$-\,(1-n_{\mathbf{k}_1-\mathbf{q}})n_{\mathbf{k}_1}(1-n_{\mathbf{p}+\mathbf{q}})n_{\mathbf{p}}]. \tag{30}$$

4. FACTORIZATION THEOREMS

Define the expectation value of the fermion occupation number $n_{\mathbf{k}_1}$ at time t as

$$\langle n_{\mathbf{k}_1}\rangle_t = \sum_{\{n\mathbf{k}''\}} P_{\{n\mathbf{k}\}\{n\mathbf{k}''\}}(t)n''_{\mathbf{k}_1}, \tag{31}$$

where $P(t)$ is given by Eq. (19). Similarly,

$$\langle n_{\mathbf{k}_1}n_{\mathbf{k}_2}\rangle_t = \sum_{\{n\mathbf{k}''\}} P_{\{n\mathbf{k}\}\{n\mathbf{k}''\}}(t)n''_{\mathbf{k}_1}n''_{\mathbf{k}_2}. \tag{32}$$

From Eqs. (1), (13), and (31),

$$f_1(\mathbf{k}_1;\,t) = \sum_{\{n\mathbf{k}\}} |c(\{n_{\mathbf{k}}\})|^2\,\langle n_{\mathbf{k}_1}\rangle_t,$$
$$f_2(\mathbf{k}_1,\mathbf{k}_2;\,t) = \sum_{\{n\mathbf{k}\}} |c(\{n_{\mathbf{k}}\})|^2\,\langle n_{\mathbf{k}_1}n_{\mathbf{k}_2}\rangle_t. \tag{33}$$

We start by proving factorization theorems, such as

$$\langle n_{\mathbf{k}_1}n_{\mathbf{k}_2}\rangle_t = \langle n_{\mathbf{k}_1}\rangle_t\langle n_{\mathbf{k}_2}\rangle_t, \tag{34}$$

and then use these theorems to prove a factorization theorem for the momentum correlation functions.

The factorization theorem in the $|\alpha\rangle$ representation is stated in the most general way in the following theorem.

Theorem 1: Given any two functions $G(n : \{\kappa\})$, $H(n : \{\mathbf{K}\})$, where G is a product of fermion occupation numbers over the set of states $\{\kappa\}$ and H a product over the set $\{\mathbf{K}\}$ and all elements of the set $\{\kappa, \mathbf{K}\}$ are distinct, then in the N/V limit

$$\langle G(n : \{\kappa\})\cdot H(n : \{\mathbf{K}\})\rangle_t$$
$$= \langle G(n : \{\kappa\})\rangle_t\cdot\langle H(n : \{\mathbf{K}\})\rangle_t. \tag{35}$$

This theorem can be written in a different way.

Lemma 1: A necessary and sufficient condition for the validity of Theorem 1. For $m = 1, 2, 3 \cdots$,

$$\sum_{\{n\mathbf{k}'\}} \frac{1}{m!}\,\Omega^{(m)}_{\{n\mathbf{k}\}\{n\mathbf{k}'\}} G(n' : \{\kappa\})H(n' : \{\mathbf{K}\})$$
$$= \sum_{s=0}^{m}\sum_{\{n\mathbf{k}''\}} \frac{1}{s!}\,\Omega^{(s)}_{\{n\mathbf{k}\}\{n\mathbf{k}''\}} G(n'' : \{\kappa\})$$
$$\cdot \sum_{\{n\mathbf{k}'''\}} \frac{1}{(m-s)!}\,\Omega^{(m-s)}_{\{n\mathbf{k}''\}\{n\mathbf{k}'''\}} H(n''' : \{\mathbf{K}\}). \tag{36}$$

Proof:

(a) *Sufficiency.* Multiply Eq. (36) by τ^m and sum over all m from 0 to ∞. Then the summations on the right-hand side can be rearranged and Eqs. (19) and (32) used to give (35).

(b) *Necessity.* Substitute the expansion (19) into (35). Since (35) is assumed to be valid for all values of $\tau/2\pi\lambda^2 \gg \tau_c$ (which is explained in the next section), the power series on the left- and right-hand sides must be identical, term by term, in powers of τ. Equation (36) must then hold for each value of m.

We now discuss the ordering of the terms in the N/V limit.

Consider the second-order transition $\Omega^{(2)}$ operating on $n_{\mathbf{k}_1}$. A typical term of this is

$$\frac{1}{V^4}\sum_{\mathbf{wpqr}} |v_{\mathbf{w}}|^2\,|v_{\mathbf{q}}|^2$$
$$\times\,\delta(\epsilon_{\mathbf{k}_1};\,\epsilon_{\mathbf{k}_1+\mathbf{w}}+\epsilon_{\mathbf{r}-\mathbf{w}}-\epsilon_{\mathbf{r}};\,\epsilon_{\mathbf{k}_1+\mathbf{q}}+\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}+\mathbf{q}})$$
$$\times\,n_{\mathbf{k}_1+\mathbf{w}}n_{\mathbf{r}-\mathbf{w}}(1-n_{\mathbf{r}})n_{\mathbf{k}_1}(1-n_{\mathbf{k}_1+\mathbf{q}})(1-n_{\mathbf{p}})n_{\mathbf{p}+\mathbf{q}},$$

where

$$\delta(x;y;z)\equiv\delta_{x,y}\,\delta_{y,z},$$

and in which all the elements of the set $\{\mathbf{k}_1,\ \mathbf{k}_1+\mathbf{w},\ \mathbf{r}-\mathbf{w},\ \mathbf{r}\}$ and all the elements of $\{\mathbf{k}_1,\ \mathbf{k}_1+\mathbf{q},\ \mathbf{p},\ \mathbf{p}+\mathbf{q}\}$ must be distinct. However, an element of the first set (apart from $\mathbf{k}_1$) may be equal to an element of the second which would result in a contraction of the above expression. We thus adopt the following summation convention: whenever a summation over states of occupation numbers is written, it is done so on the understanding that all contractions between those states are excluded from the summation.

With this summation convention, the first two terms of $\langle n_{\mathbf{k}_1}n_{\mathbf{k}_2}\rangle_t$ and $\langle n_{\mathbf{k}_1}\rangle_t\langle n_{\mathbf{k}_2}\rangle_t$ become

$$\langle n_{\mathbf{k}_1}n_{\mathbf{k}_2}\rangle_t = n_{\mathbf{k}_1}n_{\mathbf{k}_2} + 2\tau\{A(\mathbf{k}_1,\mathbf{k}_2)+A(\mathbf{k}_2,\mathbf{k}_1)+B(\mathbf{k}_1,\mathbf{k}_2)\}+O(\tau^2) \tag{37}$$

and

$$\langle n_{\mathbf{k}_1}\rangle_t\langle n_{\mathbf{k}_2}\rangle_t = n_{\mathbf{k}_1}n_{\mathbf{k}_2} + 2\tau\{A(\mathbf{k}_1,\mathbf{k}_2)+A(\mathbf{k}_2,\mathbf{k}_1)+C(\mathbf{k}_1,\mathbf{k}_2)\}+O(\tau^2), \tag{38}$$

where

$$A(\mathbf{k}_1,\mathbf{k}_2)=\frac{1}{V^2}\sum_{\mathbf{p},\mathbf{q}}|v_{\mathbf{q}}|^2\,\delta(\epsilon_{\mathbf{k}_2}+\epsilon_{\mathbf{p}+\mathbf{q}};\,\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{k}_2+\mathbf{q}})$$
$$\times\,n_{\mathbf{k}_1}[n_{\mathbf{p}}(1-n_{\mathbf{p}+\mathbf{q}})n_{\mathbf{k}_2+\mathbf{q}}(1-n_{\mathbf{k}_2})$$
$$-(1-n_{\mathbf{p}})n_{\mathbf{p}+\mathbf{q}}(1-n_{\mathbf{k}_2+\mathbf{q}})n_{\mathbf{k}_2}], \tag{39}$$

and although B and C are not identical they contain terms with similar structures, a typical term being

$$\frac{1}{V^2}\sum_{\mathbf{q}}|v_{\mathbf{q}}|^2\,\delta(\epsilon_{\mathbf{k}_1}+\epsilon_{\mathbf{k}_2};\,\epsilon_{\mathbf{k}_1+\mathbf{q}}+\epsilon_{\mathbf{k}_2-\mathbf{q}})$$
$$\times\,[(1-n_{\mathbf{k}_1})n_{\mathbf{k}_1+\mathbf{q}}(1-n_{\mathbf{k}_2})n_{\mathbf{k}_2-\mathbf{q}}$$
$$-n_{\mathbf{k}_1}(1-n_{\mathbf{k}_1+\mathbf{q}})n_{\mathbf{k}_2}(1-n_{\mathbf{k}_2-\mathbf{q}})]. \tag{40}$$

Terms A are "more probable" than B or C. For, in $A(\mathbf{k}_1,\mathbf{k}_2)$, particle $\mathbf{k}_2$ undergoes a collision with any particle other than the particular particle $\mathbf{k}_1$. In the typical term of B and C, particles $\mathbf{k}_1$ and $\mathbf{k}_2$ collide with each other.

This "probable" description must now be formulated mathematically.

The order of magnitude of each term in the series of an expectation value resulting from the expansion of $P(t)$ [Eq. (19)] is estimated in powers of N and V and only those terms kept which remain nonvanishing in the N/V limit. In particular, a term Q_a which satisfies the condition

$$0\le Q_a\lesssim R_a(N/V)^r;\qquad r\ge 0,$$

where R_a is real, finite, and independent of N, and V is retained when the N/V limit is taken. However, a term Q_b which satisfies

$$0\le Q_b\lesssim R_b(N/V)^r(1/V)^s;\qquad r\ge 0,\qquad s\ge 1,$$

where R_b is real, finite, and independent of N and V, has an upper bound which approaches zero in the N/V limit. Such a term is discarded.

As an example, consider the first part of $A(\mathbf{k}_1,\mathbf{k}_2)$, where $\mathbf{k}_1$ and $\mathbf{k}_2$ are fixed momenta. The δ function in the energies only imposes a restriction on the angular coordinates of the momenta. The occupation numbers are bounded,

$$0\le n_{\mathbf{k}}\le 1;\qquad 0\le(1-n_{\mathbf{k}})\le 1.$$

Thus

$$0\le\frac{1}{V^2}\sum_{\mathbf{p},\mathbf{q}}|v_{\mathbf{q}}|^2\,\delta(\epsilon_{\mathbf{k}_2}+\epsilon_{\mathbf{p}+\mathbf{q}};\,\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{k}_2+\mathbf{q}})$$
$$\times\,n_{\mathbf{k}_1}n_{\mathbf{p}}(1-n_{\mathbf{p}+\mathbf{q}})n_{\mathbf{k}_2+\mathbf{q}}(1-n_{\mathbf{k}_2})$$
$$\le\frac{1}{V^2}\sum_{\mathbf{p},\mathbf{q}}|v_{\mathbf{q}}|^2\,n_{\mathbf{p}}\frac{1}{E},$$

where E is some typical energy of the system and must be introduced because the δ function has been removed. Now, $\sum_{\mathbf{p}}n_{\mathbf{p}}=N$ and with the limiting forms (27), the upper bound becomes of the order of

$$\frac{N}{V^2}\frac{V}{(2\pi)^3}\int d\mathbf{q}\,|v_{\mathbf{q}}|^2\frac{1}{E}.$$

But

$$\int d\mathbf{q}\,|v_{\mathbf{q}}|^2=(2\pi)^3V_2, \tag{41}$$

where

$$V_n=\int d\mathbf{r}\,[\tfrac{1}{2}v(r)]^n. \tag{42}$$

We have already assumed that V_1 converges. We must now assume V_2 does also. The upper bound then becomes $(V_2/E)(N/V)$. A similar argument holds for the second part of $A(\mathbf{k}_1, \mathbf{k}_2)$. The term $A(\mathbf{k}_1, \mathbf{k}_2)$ is retained.

Now consider the typical term (40) of B and C. By the same arguments, it has an upper bound of the form $(V_2/E)(1/V)$ and so is discarded in the N/V limit.

If all the terms of A, B, and C are considered in this way, Eqs. (37), (38) give

$$\langle n_{\mathbf{k}_1} n_{\mathbf{k}_2}\rangle_t - \langle n_{\mathbf{k}_1}\rangle_t \langle n_{\mathbf{k}_2}\rangle_t = O(1/V) + O(r^2). \tag{43}$$

We can now generalize the ordering process and prove

Theorem 2: For any two functions g, h of occupation numbers, matrix elements, and energy δ functions with upper bounds of the order of $(N/V)^r (r \geq 0)$,

$$\lim_{N/V} \Big[\sum_{\{n\mathbf{k}''\}} \Omega_{\{n\mathbf{k}'\}\{n\mathbf{k}''\}} g(\{n''_\kappa\}) h(\{n''_{\mathbf{K}}\}) - g(\{n'_\kappa\}) \sum_{\{n\mathbf{k}''\}} \Omega_{\{n\mathbf{k}'\}\{n\mathbf{k}''\}} h(\{n''_{\mathbf{K}}\}) - h(\{n'_{\mathbf{K}}\}) \sum_{\{n\mathbf{k}''\}} \Omega_{\{n\mathbf{k}'\}\{n\mathbf{k}''\}} g(\{n''_\kappa\}) \Big] = 0 \tag{44}$$

provided that if g depends on the occupation numbers over the set of states $\{\kappa\}$ and h on $\{\mathbf{K}\}$ then the elements of the set $\{\kappa, \mathbf{K}\}$ are all distinct.

Remark on Interpretation: In the abbreviated notation, $\{n'_\kappa\} = \alpha'$, a term like $\sum_{\alpha''} \Omega_{\alpha'\alpha''} h(\alpha'')$ has an upper bound of the order of $(N/V)^r (r \geq 0)$, because $h(\alpha'')$ is bounded above by $(N/V)^r$ and when $\Omega_{\alpha'\alpha''}$, which is symbolically of the form $V\delta(\ )$, operates on h, one or more summations must be contracted. From the conditions of the theorem, $g(\alpha')$ also has an upper bound of the same form so that

$$g(\alpha') \sum_{\alpha''} \Omega_{\alpha'\alpha''} h(\alpha'') \lesssim \text{const} \left(\frac{N}{V}\right)^s; \qquad s \geq 0.$$

Although, by definition, g and h have no common states, terms like $\sum_{\mathbf{p},\mathbf{q}} |v_\mathbf{q}|^2 n'(\mathbf{p}, \mathbf{q}) h'$ are obtained from $\sum_{\alpha''} \Omega_{\alpha'\alpha''} h(\alpha'')$ so $g(\alpha')$ and $\sum_{\alpha''} \Omega_{\alpha'\alpha''} h(\alpha'')$ may have common states when particular parts of the $\mathbf{p}$, $\mathbf{q}$ summations are selected. However, as these are finite in number and for each contraction a summation disappears, the contracted terms have upper bounds like $(1/V)(N/V)^s$ and are negligible in the (N/V) limit. Therefore, in the (N/V) limit, $g(\alpha')$ and $\sum_{\alpha''} \Omega_{\alpha'\alpha''} h(\alpha'')$ have no common states.

Proof: Consider, again in abbreviated notation,

$$J = \sum_{\alpha''} \Omega_{\alpha'\alpha''} g(\alpha'') h(\alpha'') - g(\alpha') \sum_{\alpha''} \Omega_{\alpha'\alpha''} h(\alpha'') - h(\alpha') \sum_{\alpha''} \Omega_{\alpha'\alpha''} g(\alpha'').$$

From the definitions (17) and (28), this becomes

$$\begin{aligned} J &= \sum_{\alpha''} W_{\alpha'\alpha''} [\{g(\alpha'') - g(\alpha')\}\{h(\alpha'') - h(\alpha')\}] \\ &= \frac{1}{V^2} \sum_{\mathbf{p},\mathbf{q},\mathbf{r}} |v_\mathbf{q}|^2 \, \delta(\epsilon_\mathbf{p} + \epsilon_\mathbf{r}; \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{r}-\mathbf{q}}) \\ &\qquad \times n'_\mathbf{p}(1 - n'_{\mathbf{p}+\mathbf{q}}) n'_\mathbf{r}(1 - n'_{\mathbf{r}-\mathbf{q}}) \\ &\qquad \times [g(\{n'_\kappa - \delta_{\kappa,\mathbf{p}} - \delta_{\kappa,\mathbf{r}} + \delta_{\kappa,\mathbf{p}+\mathbf{q}} + \delta_{\kappa,\mathbf{r}-\mathbf{q}}) - g(\{n'_\kappa\})] \\ &\qquad \times [h(\{n'_\mathbf{K} - \delta_{\mathbf{K},\mathbf{p}} - \delta_{\mathbf{K},\mathbf{r}} + \delta_{\mathbf{K},\mathbf{p}+\mathbf{q}} + \delta_{\mathbf{K},\mathbf{r}-\mathbf{q}}) - h(\{n'_\mathbf{K}\})]. \end{aligned}$$

For the first bracket not to be zero, the sets $\{\kappa\}$, $\{\mathbf{p}, \mathbf{r}, \mathbf{p}+\mathbf{q}, \mathbf{r}-\mathbf{q}\}$ must have at least one element in common. For the second bracket not to be zero at least one of the remaining elements in $\{\mathbf{p}, \mathbf{r}, \mathbf{p}+\mathbf{q}, \mathbf{r}-\mathbf{q}\}$ must belong to $\{\mathbf{K}\}$, since the elements of $\{\kappa, \mathbf{K}\}$ are all distinct. Therefore, at least two summations must be contracted for J to be nonzero. The number of possible contractions is finite and each contracted term has upper and lower bounds like $\pm(1/V)(N/V)^r$, $r \geq 0$, which in the (N/V) limit become zero. Therefore,

$$J = 0[(1/V)(N/V)^r]; \qquad r \geq 0.$$

This completes the proof of Theorem 2.

In particular, for $\{n'_\mathbf{k}\} = \{n_\mathbf{k}\}$,

$$\sum_{\alpha''} \Omega_{\alpha\alpha'} n''_{\mathbf{k}_1} n_{\mathbf{k}_2}{}'' = n_{\mathbf{k}_1} \sum_{\alpha''} \Omega_{\alpha\alpha'} n''_{\mathbf{k}_2} + n_{\mathbf{k}_2} \sum_{\alpha''} \Omega_{\alpha\alpha'} n''_{\mathbf{k}_1} + O\left(\frac{1}{V}\right), \tag{45}$$

and, for example, $n_{\mathbf{k}_1} \sum_{\alpha''} \Omega_{\alpha\alpha'} n''_{\mathbf{k}_2}$ is interpreted with the remark after Theorem 2. The above expression is equivalent to Eq. (43).

Using a symbolic notation, the previous result can be written as

$$\Omega(n_{\mathbf{k}_1} n_{\mathbf{k}_2}) = n_{\mathbf{k}_1} \Omega(n_{\mathbf{k}_2}) + n_{\mathbf{k}_2} \Omega(n_{\mathbf{k}_1}) + O(1/V). \tag{46}$$

We now generate $\Omega^{(2)}(n_{\mathbf{k}_1} n_{\mathbf{k}_2})$ by operating with Ω on this equation.

Lemma 2:

$$\Omega[n_{\mathbf{k}_2} \Omega(n_{\mathbf{k}_1})] = n_{\mathbf{k}_2} \Omega^{(2)}(n_{\mathbf{k}_1}) + \Omega(n_{\mathbf{k}_2}) \Omega(n_{\mathbf{k}_1}) + O(1/V). \tag{47}$$

Proof: Consider the first part of the summand in $\Omega(n_{\mathbf{k}_1})$, Eq. (30). Put

$$g(\{n_\kappa\}) = n_{\mathbf{k}_2};$$

$$h(\{n_\mathbf{K}\}) = |v_\mathbf{q}|^2\, \delta(\epsilon_{\mathbf{k}_1} + \epsilon_\mathbf{p} : \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{k}_1-\mathbf{q}}) \times n_{\mathbf{k}_1-\mathbf{q}}(1 - n_{\mathbf{k}_1})n_{\mathbf{p}+\mathbf{q}}(1 - n_\mathbf{p}).$$

Then g and h are (i) non-negative, (ii) bounded above like $(N/V)^r (r \geq 0)$, (iii) without any state in common. Therefore all conditions of Theorem 2 are satisfied and likewise with the second part of $\Omega(n_{\mathbf{k}_1})$.

The two parts of $\Omega(n_{\mathbf{k}_1})$ can now be resummed over $(1/V^2)\sum_{\mathbf{p},\mathbf{q}}$ and the lemma proved.

The indices of (47) can be interchanged to give

$$\Omega[n_{\mathbf{k}_1}\Omega(n_{\mathbf{k}_2})] = n_{\mathbf{k}_1}\Omega^{(2)}(n_{\mathbf{k}_2}) + \Omega(n_{\mathbf{k}_1})\Omega(n_{\mathbf{k}_2}) + O(1/V). \quad (48)$$

From Eqs. (47) and (48),

$$\begin{aligned}\Omega^{(2)}(n_{\mathbf{k}_1}n_{\mathbf{k}_2}) &= \Omega[\Omega(n_{\mathbf{k}_1}n_{\mathbf{k}_2})] \\ &= \Omega\{n_{\mathbf{k}_1}\Omega(n_{\mathbf{k}_2}) + n_{\mathbf{k}_2}\Omega(n_{\mathbf{k}_1}) + O(1/V)\} \\ &= n_{\mathbf{k}_1}\Omega^{(2)}(n_{\mathbf{k}_2}) + 2\Omega(n_{\mathbf{k}_1})\Omega(n_{\mathbf{k}_2}) + n_{\mathbf{k}_2}\Omega^{(2)}(n_{\mathbf{k}_1}) + O(1/V), \quad (49)\end{aligned}$$

since

$$\Omega[O(1/V)] = O(1/V).$$

Proof by Induction of Lemma 1:

(a) $G(n' : \{\kappa\}) = n'_{\mathbf{k}_1}; \qquad H(n' : \{\mathbf{K}\}) = n'_{\mathbf{k}_2}.$

We have already shown that the lemma is true for $m = 1$ and 2, and we know from Eq. (21) that it is true for $m = 0$.

Assume the lemma holds for $m = M$. Take each term of the right-hand side of Eq. (36) in turn:

$$\frac{1}{s!}\,\Omega^{(s)}(n_{\mathbf{k}_1})\cdot\frac{1}{(M-s)!}\,\Omega^{(M-s)}(n_{\mathbf{k}_2}).$$

Put

$$g = \frac{1}{s!}\,\Omega^{(s)}(n_{\mathbf{k}_1}) \quad \text{and} \quad h = \frac{1}{(M-s)!}\,\Omega^{(M-s)}(n_{\mathbf{k}_2})$$

and use Theorem 2 and the remark. Then in the (N/V) limit

$$\Omega\left\{\frac{1}{s!}\,\Omega^{(s)}(n_{\mathbf{k}_1})\cdot\frac{1}{(M-s)!}\,\Omega^{(M-s)}(n_{\mathbf{k}_2})\right\} = \frac{1}{s!}\,\Omega^{(s+1)}(n_{\mathbf{k}_1})\cdot\frac{1}{(M-s)!}\,\Omega^{(M-s)}(n_{\mathbf{k}_2}) + \frac{1}{s!}\,\Omega^{(s)}(n_{\mathbf{k}_1})\cdot\frac{1}{(M-s)!}\,\Omega^{(M-s+1)}(n_{\mathbf{k}_2}).$$

From the terms

$$\Omega\left\{\frac{1}{s!}\,\Omega^{(s)}(n_{\mathbf{k}_1})\cdot\frac{1}{(M-s)!}\,\Omega^{(M-s)}(n_{\mathbf{k}_2})\right\} + \Omega\left\{\frac{1}{(s+1)!}\,\Omega^{(s+1)}(n_{\mathbf{k}_1})\cdot\frac{\Omega^{(M-s-1)}}{(M-s-1)!}(n_{\mathbf{k}_2})\right\},$$

we obtain the two terms of the form

$$\Omega^{(s+1)}(n_{\mathbf{k}_1})\cdot\Omega^{(M-s)}(n_{\mathbf{k}_2}):$$

$$\begin{aligned}&\Omega^{(s+1)}(n_{\mathbf{k}_1})\cdot\Omega^{(M-s)}(n_{\mathbf{k}_2}) \times\left\{\frac{1}{s!\,(M-s)!} + \frac{1}{(s+1)!\,(M-s-1)!}\right\} \\ &= (M+1)\,\frac{1}{(s+1)!}\,\Omega^{(s+1)}(n_{\mathbf{k}_1})\cdot\frac{1}{(M-s)!}\,\Omega^{(M-s)}(n_{\mathbf{k}_2}).\end{aligned}$$

Sum over s and divide throughout by $(M+1)$. Equation (36) then results with $m = M + 1$.

Therefore, if the lemma is true for $m = M$, it is also true for $m = M + 1$. But we know the lemma to be true for $m = 0$, 1, and 2. Therefore, it is true for all m.

(b) Since Theorem 2 is valid for arbitrary functions g and h of occupation numbers, the above proof by induction can be repeated exactly with $n_{\mathbf{k}_1}$, $n_{\mathbf{k}_2}$ replaced by G, H as defined in Theorem 1.

We now use Theorem 1 to establish the following theorem.

Theorem 3: If for all possible sets of states $\{\kappa\}$ and $\{\mathbf{K}\}$, containing i and j elements, respectively, and such that all states of the set $\{\kappa, \mathbf{K}\}$ are distinct

$$f_{i+j}(\{\kappa\}, \{\mathbf{K}\}; 0) = f_i(\{\kappa\}; 0)\cdot f_j(\{\mathbf{K}\}; 0) \quad \text{for} \quad i, j = 1, 2, 3 \cdots, \quad (50)$$

then in the (N/V) limit

$$f_2(\mathbf{k}_1, \mathbf{k}_2; t) = f_1(\mathbf{k}_1; t)\cdot f_1(\mathbf{k}_2; t). \quad (51)$$

Proof: From Eq. (33), the condition (50) can be written as

$$\begin{aligned}&f_{i+j}(\{\kappa\}, \{\mathbf{K}\}; 0) \\ &= \sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2 \langle(n_{\kappa_1}\cdots n_{\kappa_i})(n_{\mathbf{K}_1}\cdots n_{\mathbf{K}_j})\rangle_{t=0} \\ &= \sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2\,(n_{\kappa_1}\cdots n_{\kappa_i})(n_{\mathbf{K}_1}\cdots n_{\mathbf{K}_j}) \\ &\equiv \Big[\sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2\,(n_{\kappa_1}\cdots n_{\kappa_i})\Big] \times \Big[\sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2\,(n_{\mathbf{K}_1}\cdots n_{\mathbf{K}_j})\Big]. \quad (52)\end{aligned}$$

Now, from Theorem 1, in the (N/V) limit

$$f_2(\mathbf{k}_1, \mathbf{k}_2; t) = \sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2 \langle n_{\mathbf{k}_1} n_{\mathbf{k}_2}\rangle_t = \sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2 \langle n_{\mathbf{k}_1}\rangle_t \langle n_{\mathbf{k}_2}\rangle_t .$$

$\langle n_{\mathbf{k}_1}\rangle_t$ can be expanded in powers of τ, each term in the expansion being a summation over matrix elements, energy δ functions and products of occupation numbers. Symbolically,

$$\langle n_{\mathbf{k}_1}\rangle_t = \sum_l \tau^l [\sum_{\{\varkappa\}} F_l(v, \epsilon; \{\varkappa\}) n_{\varkappa_1} \cdots n_{\varkappa_l}].$$

Similarly,

$$\langle n_{\mathbf{k}_2}\rangle_t = \sum_m \tau^m [\sum_{\{\mathbf{K}\}} F_m(v, \epsilon; \{\mathbf{K}\}) n_{\mathbf{K}_1} \cdots n_{\mathbf{K}_l}]. \quad (53)$$

In the product $\langle n_{\mathbf{k}_1}\rangle_t \langle n_{\mathbf{k}_2}\rangle_t$, the leading-order terms, bounded by $(N/V)^r$ are those terms of the form

$$\sum_{\{\varkappa\}} F_l(v, \epsilon; \{\varkappa\}) n_{\varkappa_1} \cdots n_{\varkappa_l} \times \sum_{\{\mathbf{K}\}} F_m(v, \epsilon; \{\mathbf{K}\}) n_{\mathbf{K}_1} \cdots n_{\mathbf{K}_j} \quad (54)$$

in which all elements of the set $\{\varkappa_1 \cdots \varkappa_l \mathbf{K}_1 \cdots \mathbf{K}_j\}$ are distinct. The condition (52) can then be applied to each product of the form (54) and the products summed to give

$$f_2(\mathbf{k}_1, \mathbf{k}_2; t) = [\sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2 \langle n_{\mathbf{k}_1}\rangle_t][\sum_{\{n\mathbf{k}\}} |c(\{n_\mathbf{k}\})|^2 \langle n_{\mathbf{k}_2}\rangle_t] = f_1(\mathbf{k}_1; t) \cdot f_1(\mathbf{k}_2; t).$$

Lemma 3: Because Theorem 1 is valid for arbitrary, distinct products G and H of occupation numbers, all factorization theorems

$$f_{i+j}(\varkappa_1 \cdots \varkappa_i, \mathbf{K}_1 \cdots \mathbf{K}_j; t) = f_i(\varkappa_1 \cdots \varkappa_i; t) \cdot f_j(\mathbf{K}_1 \cdots \mathbf{K}_j; t)$$

can be proved by the same method, in the (N/V) limit. Therefore, if *all* the momentum correlation functions factorize at some particular time, then they factorize at later times.

5. RANGE OF VALIDITY

While assuming the system satisfies all those requirements necessary for the derivation of the Pauli master equation, we must also include the further condition that V_1 and V_2 converge. Furthermore, the range of t must be restricted to ensure the convergence of expectation values.

Consider $\langle n_{\mathbf{k}_1}\rangle_t$ in the (N/V) limit:

$$\langle n_{\mathbf{k}_1}\rangle_t = n_{\mathbf{k}_1} + 2\tau \Big[\sum_{\mathbf{p},\mathbf{q}} \frac{|v_\mathbf{q}|^2}{V^2} \delta(\epsilon_{\mathbf{k}_1} + \epsilon_{\mathbf{p}+\mathbf{q}}; \epsilon_\mathbf{p} + \epsilon_{\mathbf{k}_1+\mathbf{q}}) \times \{n_\mathbf{p}(1 - n_{\mathbf{p}+\mathbf{q}}) n_{\mathbf{k}_1+\mathbf{q}}(1 - n_{\mathbf{k}_1}) - (1 - n_\mathbf{p}) n_{\mathbf{p}+\mathbf{q}}(1 - n_{\mathbf{k}_1+\mathbf{q}}) n_{\mathbf{k}_1}\}\Big] + O(\tau^2).$$

Then,

$$|\langle n_{\mathbf{k}_1}\rangle_t| \lesssim 1 + 2\frac{N}{V}\frac{V_2}{E}\tau + \cdots + u_n \left(\frac{N}{V}\right)^n \left(\frac{V_2}{E}\right)^n \tau^n + \cdots , \quad (55)$$

where u_n is a numerical factor. By considering in more detail the expansion and the way in which contractions can be made, we find $u_0 = 1$; $u_1 = 2$; $u_n = u_{n-1} \cdot 4(3n - 2)$ for $n = 2, 3, \cdots$. Thus,

$$u_n \leq u_{n-1} \cdot 4 \cdot 4n \leq (16)^n \cdot n! \quad \text{for all } n.$$

Therefore, $\langle n_{\mathbf{k}_1}\rangle_t$ converges for

$$\tau < [16(V_2/E)(N/V)]^{-1}. \quad (56)$$

On the natural time scale, $t = \tau/2\pi\lambda^2$,

$$t < (1/\lambda^2)(1/\Delta E) \equiv \tau_1,$$

where

$$\Delta E = 32\pi(N/V)(V_2/E).$$

On the other hand, the Pauli master equation only applies for times t such that

$$\tau_c \ll t,$$

where τ_c is the duration of a collision.

Hence, the factorization theorem is valid when

$$\tau_c \ll t < \tau_1. \quad (57)$$

However, we can now start at time t_0, where

$$\tau_c \ll t_0 \leq \tau_1 - \tau_c,$$

and by repeating the arguments extend the proof to the range

$$t_0 + \tau_c < t < t_0 + \tau_1.$$

Then the theorem is true for

$$\tau_c \ll t < t_0 + \tau_1.$$

Proceeding this way, the time range

$$\tau_c \ll t < \infty \quad (58)$$

can be covered.

6. GENERALIZATION

The proof of the factorization theorem can be generalized for weakly interacting systems for which the Pauli master equation can be derived.

Consider a weakly interacting system of N fermions and $\mathfrak{N}$ bosons. The factorization theorem can be proved in the double limiting process $N \to \infty$, $\mathfrak{N} \to \infty$, $V \to \infty$ with $N^r \mathfrak{N}^{s-r}/V^s$ constant by the same method, provided:

(i) The Pauli master equation is valid.

(ii) The transition operator Ω_{f-b} has a similar structure to Ω given by (17) and (28) with the correct volume factors to balance the summations.

(iii) The matrix elements $|v_q|^2_{f-b}$ converge like $|v_q|^2$.

(iv) The Bose occupation numbers are bounded above by a number η which is independent of the total number of bosons. The last condition excludes the possibility of a Bose–Einstein condensate.

The double limiting process implies a simple relationship between N and $\mathfrak{N}$. For a system of electrons and phonons in a metal of volume V containing n atoms,

$$N = nr,$$

where r is the number of valence electrons per atom. If $N_{\mathbf{K}}$ is the phonon occupation number for the state $\mathbf{K}$, from condition (iv)

$$\mathfrak{N} = \sum_{\mathbf{K}} N_{\mathbf{K}} \leq \eta \cdot \sum_{\mathbf{K}\,\text{allowed}} 1.$$

Furthermore, if there is one atom per unit cell, then

$$\sum_{\mathbf{K}\,\text{allowed}} 1 = 3n$$

so that

$$\mathfrak{N} \leq 3n\eta = (3/r)\eta N.$$

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Relationship between Linear Response Theory and the Boltzmann Equation for a Weakly Interacting System of Electrons and Phonons

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Van Hove's weak coupling master equation and the factorization theorem of Kac are used to show that the transport coefficients derived from linear response theory are equivalent to those derived from the Boltzmann equation for a weakly interacting system of electrons and phonons.

INTRODUCTION

IT has been possible to demonstrate for some simple models that linear response theory is equivalent to the use of the Boltzmann equation. Chester and Thellung[1] and Verboven[2] have calculated the electrical conductivity resulting from randomly distributed scattering centers in a one-electron model of a metal. In order to extend their calculations to a more realistic system, a factorization theorem is required to decouple expectation values of products of operators which occur in linear response theory and in the derivation of the Boltzmann equation.

McLennan and Swenson[3] have discussed a dilute, nondegenerate, monatomic gas with short-range interactions, and have been able to establish the equivalence between linear response theory and the Boltzmann equation approach by proving the factorization theorem of Kac[4] for their system. We wish to generalize this result by using the factorization theorems derived in a previous paper.[5]

We discuss a weakly interacting system of electrons and phonons in a metal because this system is sufficiently general to illustrate all the points in the treatment of a weakly interacting system of fermions or bosons. We assume that the system satisfies all those requirements necessary for the derivation of Van Hove's weak coupling master equation[6] and the establishment of the factorization theorems.[5]

The procedure is then straightforward. The master function is used to describe the time evolution of the current operators in the Kubo formulas of linear response theory.[7] These formulas are then "contracted" by using the equilibrium properties of the currents and the factorization theorems. The resulting expressions for the transport coefficients can then be rewritten in a form identical to that derived from the coupled Boltzmann equations.

REPRESENTATION

The Hamiltonian for a system of interacting electrons and phonons in a metal of volume $\mathcal{V}$ with one atom per unit cell can be written in the form

$$H = H_0 + \lambda H_1, \tag{1}$$

where the unperturbed Hamiltonian H_0 is given by

$$H_0 = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}} + \sum_{\mathbf{q}} w_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} \tag{2}$$

and the interaction H_1 by[8]

$$\begin{aligned} H_1 &= \frac{1}{\mathcal{V}^{\frac{1}{2}}} \sum_{\mathbf{pq}} v_{\mathbf{q}} c_{\mathbf{p}+\mathbf{q}}^{\dagger} c_{\mathbf{p}} \{ b_{\mathbf{q}} + b_{-\mathbf{q}}^{\dagger} \} \\ &= \frac{1}{\mathcal{V}^{\frac{1}{2}}} \sum_{\mathbf{pq}} \{ v_{\mathbf{q}} c_{\mathbf{p}+\mathbf{q}}^{\dagger} c_{\mathbf{p}} b_{\mathbf{q}} + v_{-\mathbf{q}} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}+\mathbf{q}} b_{\mathbf{q}}^{\dagger} \}. \end{aligned} \tag{3}$$

$c^{\dagger}$, c and $b^{\dagger}$, b are creation, annihilation operators for electrons and phonons, respectively. The spin indices have been suppressed and we assume the electrons interact only with longitudinal phonons. λ is the coupling constant. Since $v_{\mathbf{q}}$ is the Fourier transform of a real potential,

$$v_{\mathbf{q}}^{*} = v_{-\mathbf{q}}. \tag{4}$$

In the interaction term H_1, the summations over $\mathbf{p}$ and $\mathbf{q}$ are taken to be in the extended zone scheme

* Part of a thesis submitted by J. Sykes in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mathematical Physics at Birmingham University, England, (1964).

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[8] H_1 has been simplified by assuming that the system is isotropic.

to allow for umklapp processes (Peierls[9]) and the terms with $\mathbf{q} = 0$ have been included in H_0.

If $\mathcal{V}_0$ is the volume of a unit cell or the atomic volume, then

$$\mathcal{V} = \mathfrak{N}\mathcal{V}_0, \tag{5}$$

where $\mathfrak{N}$ is the number of atoms or electrons, since we assume one valence electron per atom.

The normalized eigenstates $|\alpha\rangle$ of H_0 are of the form

$$|\alpha\rangle = |\{n_\mathbf{k}\}\{N_\mathbf{K}\}\rangle, \tag{6}$$

where $n_\mathbf{k}$ and $N_\mathbf{K}$ are the electron Bloch state and phonon normal-mode occupation numbers. Therefore, if

$$H_0|\alpha\rangle = |\alpha\rangle E(\alpha),$$
$$E(\alpha) = \sum_\mathbf{p} \epsilon_\mathbf{p} n_\mathbf{p} + \sum_\mathbf{q} w_\mathbf{q} N_\mathbf{q}.$$

The transition probability W is defined by

$$\begin{aligned} W_{\alpha\alpha'} &= |\langle\alpha|H_1|\alpha'\rangle|^2 \delta[E(\alpha) - E(\alpha')] \\ &= \frac{1}{\mathcal{V}} \sum_{\mathbf{pq}} |v_\mathbf{q}|^2 \delta(\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_\mathbf{p} - w_\mathbf{q}) \\ &\times [n_\mathbf{p}(1 - n_{\mathbf{p}+\mathbf{q}}) N_\mathbf{q} \\ &\quad \times \delta\{n'_\mathbf{k}; n_\mathbf{k} - \delta_{\mathbf{k},\mathbf{p}} + \delta_{\mathbf{k},\mathbf{p}+\mathbf{q}}\} \\ &\quad \times \delta\{N'_\mathbf{K}; N_\mathbf{K} - \delta_{\mathbf{K},\mathbf{q}}\} \\ &\quad + (1 - n_\mathbf{p}) n_{\mathbf{p}+\mathbf{q}} (1 + N_\mathbf{q}) \\ &\quad \times \delta\{n'_\mathbf{k}; n_\mathbf{k} - \delta_{\mathbf{k},\mathbf{p}+\mathbf{q}} + \delta_{\mathbf{k},\mathbf{p}}\} \\ &\quad \times \delta\{N'_\mathbf{K}; N_\mathbf{K} + \delta_{\mathbf{K},\mathbf{q}}\}] \end{aligned} \tag{7}$$

so that

$$\begin{aligned} \Omega_{\alpha\alpha'} &= W_{\alpha\alpha'} - \sum_{\alpha''} W_{\alpha\alpha''} \delta_{\alpha,\alpha'} \\ &= \frac{1}{\mathcal{V}} \sum_{\mathbf{pq}} |v_\mathbf{q}|^2 \delta(\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_\mathbf{p} - w_\mathbf{q}) \\ &\times [n_\mathbf{p}(1 - n_{\mathbf{p}+\mathbf{q}}) N_\mathbf{q} (\delta\{n'_\mathbf{k}; n_\mathbf{k} - \delta_{\mathbf{k},\mathbf{p}} + \delta_{\mathbf{k},\mathbf{p}+\mathbf{q}}\} \\ &\quad \times \delta\{N'_\mathbf{K}; N_\mathbf{K} - \delta_{\mathbf{K},\mathbf{q}}\} \\ &\quad - \delta\{n'_\mathbf{k}; n_\mathbf{k}\}\ \delta\{N'_\mathbf{K}; N_\mathbf{K}\}) \\ &\quad + (1 - n_\mathbf{p}) n_{\mathbf{p}+\mathbf{q}} (1 + N_\mathbf{q}) \\ &\quad \times (\delta\{n'_\mathbf{k}; n_\mathbf{k} - \delta_{\mathbf{k},\mathbf{p}+\mathbf{q}} + \delta_{\mathbf{k},\mathbf{p}}\} \\ &\quad \times \delta\{N'_\mathbf{K}; N_\mathbf{K} + \delta_{\mathbf{K},\mathbf{q}}\} \\ &\quad - \delta\{n'_\mathbf{k}; n_\mathbf{k}\}\ \delta\{N'_\mathbf{K}; N_\mathbf{K}\})]. \end{aligned} \tag{8}$$

We assume that the time evolution of this system in the limit $\mathcal{V} \to \infty$, $\mathfrak{N} \to \infty$ with $\mathcal{V}_0$ constant can be described by Van Hove's weak coupling master equation[6]:

$$\begin{aligned} \frac{d}{d\tau} P_{\alpha\alpha'}(t) &= \sum_{\alpha''} \Omega_{\alpha\alpha''} P_{\alpha''\alpha'}(t) \\ &= \sum_{\alpha''} P_{\alpha\alpha''}(t) \Omega_{\alpha''\alpha'} \end{aligned} \tag{9}$$

with the initial condition

$$P_{\alpha\alpha'}(0) = \delta_{\alpha,\alpha'}, \tag{10}$$

where

$$\tau = 2\pi\lambda^2 t. \tag{11}$$

This equation has the formal solution

$$P_{\alpha\alpha'}(t) = \sum_{m=0}^{\infty} \frac{\tau^m}{m!} \Omega^{(m)}_{\alpha\alpha'}, \tag{12}$$

where

$$\Omega^{(m)}_{\alpha\alpha'} = \sum_{\alpha_1} \cdots \sum_{\alpha_{m-1}} \Omega_{\alpha\alpha_1} \cdots \Omega_{\alpha_{m-1}\alpha'}; \tag{13}$$

$\Omega_{\alpha\alpha'}$ is defined in Eq. (8) and

$$\Omega^{(0)}_{\alpha\alpha'} = \delta_{\alpha,\alpha'}. \tag{14}$$

We start with a discrete representation and later when the $\mathcal{V}$ limit is taken put

$$\sum_{\mathbf{k}''} \to \frac{\mathcal{V}}{(2\pi)^3} \cdot \int d\mathbf{k}'' \tag{15}$$

and

$$\frac{\mathcal{V}}{(2\pi)^3} \delta_{\mathbf{k},\mathbf{k}''} \to \delta(\mathbf{k} - \mathbf{k}''), \tag{16}$$

where the integral is over one band for electrons and over the basic cell of the reciprocal lattice for phonons.

The expectation values of the occupation numbers $n_{\mathbf{k}_1}$ and $N_{\mathbf{K}_1}$ at time t are

$$\langle n_{\mathbf{k}_1}\rangle_t = \sum_{\{n\mathbf{k}''\}\{N\mathbf{k}''\}} P_{\{n\mathbf{k}\}\{N\mathbf{k}\};\{n\mathbf{k}''\}\{N\mathbf{k}''\}}(t) n''_{\mathbf{k}_1} \tag{17}$$

and

$$\langle N_{\mathbf{K}_1}\rangle_t = \sum_{\{n\mathbf{k}''\}\{N\mathbf{k}''\}} P_{\{n\mathbf{k}\}\{N\mathbf{k}\};\{n\mathbf{k}''\}\{N\mathbf{k}''\}}(t) N''_{\mathbf{K}_1}.$$

Then, in the limit of an infinite system, provided that for all $\mathbf{K}$

$$N_\mathbf{k} \leq \eta,$$

where η is independent of $\mathfrak{N}$ or $\mathcal{V}$, the factorization theorems are[5]

$$\begin{aligned} \langle n_{\mathbf{k}_i} n_{\mathbf{k}_j}\rangle_t &= \langle n_{\mathbf{k}_i}\rangle_t \cdot \langle n_{\mathbf{k}_j}\rangle_t, \\ \langle n_{\mathbf{k}_i} N_{\mathbf{K}_j}\rangle_t &= \langle n_{\mathbf{k}_i}\rangle_t \cdot \langle N_{\mathbf{K}_j}\rangle_t, \\ \langle N_{\mathbf{K}_i} N_{\mathbf{K}_j}\rangle_t &= \langle N_{\mathbf{K}_i}\rangle_t \langle N_{\mathbf{K}_j}\rangle_t, \text{ etc.}, \end{aligned} \tag{18}$$

[9] R. E. Peierls, *Quantum Theory of Solids* (Clarendon Press, Oxford, England, 1955).

or, more fundamentally,

$$\sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}_1} n'_{\mathbf{k}_2} = n_{\mathbf{k}_1} \cdot \sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}_2} + n_{\mathbf{k}_2} \cdot \sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}_1} + O\left(\frac{1}{\mathcal{V}}\right), \tag{19}$$

with similar expressions holding for $n_{\mathbf{k}_1}$ and/or $n_{\mathbf{k}_2}$ replaced by $N_{\mathbf{K}_1}$ and/or $N_{\mathbf{K}_2}$. We have used the abbreviated notation α for the eigenstate (6).

Two further relations are required:

$$\sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}_1} = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} |v_{\mathbf{q}}|^2 [\delta(\epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_1} - w_{\mathbf{q}}) \times \{(1 - n_{\mathbf{k}_1}) n_{\mathbf{k}_1+\mathbf{q}} (1 + N_{\mathbf{q}}) - n_{\mathbf{k}_1}(1 - n_{\mathbf{k}_1+\mathbf{q}}) N_{\mathbf{q}}\} + \delta(\epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_1+\mathbf{q}} - w_{-\mathbf{q}}) \{(1 - n_{\mathbf{k}_1}) n_{\mathbf{k}_1+\mathbf{q}} N_{-\mathbf{q}} - n_{\mathbf{k}_1}(1 - n_{\mathbf{k}_1+\mathbf{q}})(1 + N_{-\mathbf{q}})\}] \tag{20}$$

and

$$\sum_{\alpha'} \Omega_{\alpha\alpha'} N'_{\mathbf{K}_1} = \frac{1}{\mathcal{V}} \sum_{\mathbf{p}} |v_{\mathbf{K}_1}|^2 \, \delta(\epsilon_{\mathbf{K}_1+\mathbf{p}} - \epsilon_{\mathbf{p}} - w_{\mathbf{K}_1}) \times \{(1 - n_{\mathbf{p}}) n_{\mathbf{K}_1+\mathbf{p}} (1 + N_{\mathbf{K}_1}) - n_{\mathbf{p}}(1 - n_{\mathbf{K}_1+\mathbf{p}}) N_{\mathbf{K}_1}\}. \tag{21}$$

LINEAR RESPONSE THEORY

We assume that the electrical ($\bar{\mathbf{J}}$) and thermal ($\bar{\mathbf{Q}}$) currents are linear functions of the electric field $\mathbf{E}$ and temperature gradient ∇T. Then

$$\begin{aligned} \bar{\mathbf{J}} &= L(J, J)\mathbf{E} - L(J, Q)(\nabla T/T), \\ \bar{\mathbf{Q}} &= L(Q, J)\mathbf{E} - L(Q, Q)(\nabla T/T). \end{aligned} \tag{22}$$

Since the phonons are uncharged, the electric current is entirely electronic, whereas the heat current is a sum of an electronic and a lattice (phonon) heat current. Thus,

$$\mathbf{J} = \mathbf{J}_e, \tag{23}$$

where, neglecting spin,[10]

$$\mathbf{J}_e = -\sum_{\mathbf{p}} e v(\mathbf{p}) n_{\mathbf{p}} \tag{24}$$

and

$$\mathbf{Q} = \mathbf{Q}_e + \mathbf{Q}_{ph}, \tag{25}$$

where

$$\begin{aligned} \mathbf{Q}_e &= \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} v(\mathbf{p}) n_{\mathbf{p}}, \\ \mathbf{Q}_{ph} &= \sum_{\mathbf{q}} w_{\mathbf{q}} u(\mathbf{p}) N_{\mathbf{q}}. \end{aligned} \tag{26}$$

$v(\mathbf{p})$ and $u(\mathbf{p})$ are the group velocities of the electrons and phonons, respectively. The summations $\mathbf{p}$, $\mathbf{q}$ are taken over the extended-zone scheme. Equations (22) can then be rewritten as

$$\begin{aligned} \bar{\mathbf{J}} &= L(J_e, J_e)\mathbf{E} - \{L(J_e, Q_e) + L(J_e, Q_{ph})\}(\nabla T/T), \\ \bar{\mathbf{Q}} &= \{L(Q_e, J_e) + L(Q_{ph}, J_e)\}\mathbf{E} - \{L(Q_e, Q_e) + L(Q_e, Q_{ph}) + L(Q_{ph}, Q_e) + L(Q_{ph}, Q_{ph})\}(\nabla T/T). \end{aligned} \tag{27}$$

The Kubo formula for the (ν, μ) component of the electrical conductivity, $L(J_e, J_e)$, is[2]

$$L^{\nu\mu}(J_e, J_e) = \lim_{\theta' \to 0} \frac{\beta}{\mathcal{V}} \operatorname{Re} \int_0^{T \to \infty} dt \, e^{-\theta' t} \operatorname{Tr} \rho J_e^{\mu}(t) J_e^{\nu}(0), \tag{28}$$

where Re means that the real part of the expression is required and ρ is the density matrix.

Since $\mathbf{J}_e$ is diagonal in the $|\alpha\rangle$ representation,

$$J_e^{\nu}(0) \, |\alpha\rangle = |\alpha\rangle \, J_e^{\nu}(\alpha), \tag{29}$$

the master function $P(t)$ can be used to express the time evolution of $J_e^{\mu}(t)$, because from the definition of $P(t)$ in the weak coupling limit,[5]

$$\langle\alpha''| \, J_e^{\mu}(t) \, |\alpha\rangle = \sum_{\alpha_1} P_{\alpha\alpha_1}(t) J_e^{\mu}(\alpha_1) \, \delta_{\alpha,\alpha''}. \tag{30}$$

Thus,

$$\operatorname{Tr} \rho J_e^{\mu}(t) J_e^{\nu}(0) = \sum_{\alpha\alpha_1} \rho(\alpha) J_e^{\nu}(\alpha) P_{\alpha\alpha_1}(t) J_e^{\mu}(\alpha_1), \tag{31}$$

where

$$\rho(\alpha) = \langle\alpha| \, \rho \, |\alpha\rangle. \tag{32}$$

The integration in Eq. (28) can be transformed from the t time scale to the τ scale by Eq. (11). From (31) and (12), (28) becomes

$$L^{\nu\mu}(J_e, J_e) = \lim_{\theta \to 0} \frac{\beta}{\mathcal{V}} \int_0^{\bar{T}} \frac{d\tau}{2\pi\lambda^2} e^{-\theta\tau} \sum_{\alpha\alpha'} \rho(\alpha) J_e^{\nu}(\alpha) \times \sum_{m=0}^{\infty} \frac{\tau^m}{m!} \Omega_{\alpha\alpha'}^{(m)} J_e^{\mu}(\alpha'), \tag{33}$$

in which we have assumed (i) $\lambda^2 \to 0$ such that

$$\lim_{\substack{T \to \infty \\ \lambda^2 \to 0}} \lambda^2 T = \text{const} = \frac{\bar{T}}{2\pi},$$

and (ii) $\theta' \to 0$ "faster" than $\lambda^2 \to 0$ so that if $\theta = \theta'/2\pi\lambda^2$, then $\theta \to 0$. As we are concerned with the static transport coefficients, we now let $\bar{T} \to \infty$. The other transport coefficients are defined by analogy with (33).

The Kubo formulas are subject to the supple-

[10] We can assume that the master function $P(t)$ describes the time evolution of current operators referring to electrons with spin ↑ and to electrons with spin ↓. The arguments can then be reworked and the spin included.

mentary condition that in equilibrium there is no net current flow in any direction. Hence,

$$\text{Tr}\ \rho J_e^\nu \equiv \text{Tr}\ \rho Q_e^\nu \equiv \text{Tr}\ \rho Q_{ph}^\nu = 0. \tag{34}$$

When the explicit form of $J_e^\nu(\alpha)\Omega_{\alpha\alpha'}^{(m)}J_e^\mu(\alpha')$ is used in Eq. (33) and the trace taken over ρ, many of the resulting terms are zero because of the above conditions. Furthermore, as we are only concerned with the limit of an infinite system, we can use the factorization theorem[5] and retain only the terms of leading order in $\mathcal{V}$ and $\mathfrak{N}$. The resulting expressions are thus called "contracted."

We make one further approximation. An approximate density matrix[11] $\rho_0(\alpha)$ obtained from $\rho(\alpha)$ by replacing H by H_0 is used. Then

$$\text{Tr}\ \rho_0 n_\mathbf{k} = f_\mathbf{k} \qquad \text{and} \qquad \text{Tr}\ \rho_0 N_\mathbf{K} = F_\mathbf{K}, \tag{35}$$

where $f_\mathbf{k}$ and $F_\mathbf{K}$ are the Fermi and Bose equilibrium distribution functions, respectively.

CONTRACTED KUBO FORMULAS

The procedure for contracting a generalized set of transport coefficients, currents and driving forces is given in an Appendix. The resulting contracted formulas are used here to derive equations for the transport coefficients defined in Eqs. (22)–(33).

From (27),

$$\bar{\mathbf{Q}} = \bar{\mathbf{Q}}^e + \bar{\mathbf{Q}}^{ph}, \tag{36}$$

where

$$\begin{aligned}\bar{Q}^e &= \{L(Q_e, J_e)\mathbf{E} - L(Q_e, Q_e)(\nabla T/T)\} \\ &\qquad - L(Q_e, Q_{ph})(\nabla T/T), \\ \bar{Q}^{ph} &= \{L(Q_{ph}, J_e)\mathbf{E} - L(Q_{ph}, Q_e)(\nabla T/T)\} \\ &\qquad - L(Q_{ph}, Q_{ph})(\nabla T/T).\end{aligned} \tag{37}$$

Hence, $\bar{\mathbf{J}}$, $\bar{\mathbf{Q}}$ can be constructed from $\bar{\mathbf{C}}$, $\bar{\mathbf{D}}$, Eq. (A1), by putting

$$\bar{\mathbf{C}} = \bar{\mathbf{J}} + \bar{\mathbf{Q}}^e, \qquad \bar{\mathbf{D}} = \bar{\mathbf{Q}}^{ph}, \tag{38}$$

and, from Eqs. (22)–(33), and (A2),

$$\begin{aligned}R(\mathbf{p}) &= -ev(\mathbf{p}) + \epsilon_\mathbf{p} v(\mathbf{p}), \\ P(\mathbf{p}) &= w_\mathbf{p} u(\mathbf{p}), \\ S(\mathbf{p})X &= -ev(\mathbf{p})\mathbf{E} - \epsilon_\mathbf{p} v(\mathbf{p})(\nabla T/T), \\ T(\mathbf{p})Y &= -w_\mathbf{p} u(\mathbf{p})(\nabla T/T).\end{aligned} \tag{39}$$

Therefore, from (A44) and (A45), and explicitly introducing the components ν, μ,

$$\begin{aligned}\bar{J}_\nu &= \frac{e}{\mathcal{V}} \sum_{\mathbf{k}_1} v_\nu(\mathbf{k}_1)\ \Phi_C(\mathbf{k}_1)\ \frac{df_{\mathbf{k}_1}}{d\epsilon_{\mathbf{k}_1}}, \\ \bar{Q}_\nu &= -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} \epsilon_{\mathbf{k}_1} v_\nu(\mathbf{k}_1)\ \Phi_C(\mathbf{k}_1)\ \frac{df_{\mathbf{k}_1}}{d\epsilon_{\mathbf{k}_1}}, \\ &\qquad - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} w_{\mathbf{k}_1} u_\nu(\mathbf{k}_1)\ \Phi_D(\mathbf{k}_1)\ \frac{dF_{\mathbf{k}_1}}{dw_{\mathbf{k}_1}},\end{aligned} \tag{40}$$

where the deviations from equilibrium Φ_C, Φ_D are solutions of the coupled operator equations

$$\begin{aligned}&J[\Phi_C(\mathbf{k}_1)] + K[\Phi_D(\mathbf{k}_1)] \\ &\quad = (1/2\pi\lambda^2)\{v_\mu(\mathbf{k}_1)eE_\mu + v_\mu(\mathbf{k}_1)\epsilon_{\mathbf{k}_1}(\nabla_\mu T/T)\},\end{aligned} \tag{41}$$

and

$$L[\Phi_C(\mathbf{k}_1)] + M[\Phi_D(\mathbf{k}_1)] = \frac{1}{2\pi\lambda^2}\, u_\mu(\mathbf{k}_1) w_{\mathbf{k}_1}(\nabla_\mu T/T).$$

We now show that the same equations can be derived from the coupled Boltzmann equations.

BOLTZMANN EQUATIONS

The collision integrals for the coupled Boltzmann equations of the electron–phonon system can be derived from the master equation by using the factorization theorem.[5]

Differentiate Eq. (17) with respect to t. Then, from (12)

$$\frac{d}{dt}\langle n_{\mathbf{k}_1}\rangle_t = 2\pi\lambda^2\langle \sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}_1}\rangle_t \tag{42}$$

and

$$\frac{d}{dt}\langle N_{\mathbf{K}_1}\rangle_t = 2\pi\lambda^2\langle \sum_{\alpha'} \Omega_{\alpha\alpha'} N'_{\mathbf{K}_1}\rangle_t.$$

The quantities on the right-hand sides of these equations have already been defined in Eqs. (20) and (21). Therefore, from the factorization theorems,

$$\begin{aligned}\frac{d}{dt}\langle n_{\mathbf{k}_1}\rangle_t = \frac{2\pi\lambda^2}{\mathcal{V}} \sum_\mathbf{q} |v_\mathbf{q}|^2\ [&\delta(\epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_1} - w_\mathbf{q}) \\ &\times \{\langle(1 - n_{\mathbf{k}_1})\rangle_t \langle n_{\mathbf{k}_1+\mathbf{q}}\rangle_t \langle(1 + N_\mathbf{q})\rangle_t \\ &- \langle n_{\mathbf{k}_1}\rangle_t \langle(1 - n_{\mathbf{k}_1+\mathbf{q}})\rangle_t \langle N_\mathbf{q}\rangle_t\} \\ &+ \delta(\epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_1+\mathbf{q}} - w_{-\mathbf{q}}) \\ &\times \{\langle(1 - n_{\mathbf{k}_1})\rangle_t \langle n_{\mathbf{k}_1+\mathbf{q}}\rangle_t \langle N_{-\mathbf{q}}\rangle_t \\ &- \langle n_{\mathbf{k}_1}\rangle_t \langle(1 - n_{\mathbf{k}_1+\mathbf{q}})\rangle_t \langle(1 + N_{-\mathbf{q}})\rangle_t\}]\end{aligned} \tag{43}$$

and

$$\begin{aligned}\frac{d}{dt}\langle N_{\mathbf{K}_1}\rangle_t = \frac{2\pi\lambda^2}{\mathcal{V}} \sum_\mathbf{p} |v_{\mathbf{K}_1}|^2\ &\delta(\epsilon_{\mathbf{K}_1+\mathbf{p}} - \epsilon_\mathbf{p} - w_{\mathbf{K}_1}) \\ &\times \{\langle(1 - n_\mathbf{p})\rangle_t \langle n_{\mathbf{K}_1+\mathbf{p}}\rangle_t \langle(1 + N_{\mathbf{K}_1})\rangle_t \\ &- \langle n_\mathbf{p}\rangle_t \langle(1 - n_{\mathbf{K}_1+\mathbf{p}})\rangle_t \langle N_{\mathbf{K}_1}\rangle_t\}.\end{aligned} \tag{44}$$

[11] This is exact in the weak coupling limit.

For a constant external electric field and a temperature gradient, the distribution functions g and G of the electrons and phonons, respectively, are the solutions of the steady-state coupled Boltzmann equations

$$v_\mu(\mathbf{k})\frac{d}{d\epsilon_\mathbf{K}}g_\mathbf{k}\{-eE_\mu\}+v_\mu(\mathbf{k})\frac{d}{dT}g_\mathbf{k}\nabla_\mu T=\frac{d}{dt}g_\mathbf{k}\Big|_{\text{collision}} \tag{45}$$

and

$$u_\mu(\mathbf{k})\frac{d}{dT}G_\mathbf{k}\nabla_\mu T=\frac{d}{dt}G_\mathbf{k}\Big|_{\text{collision}}.$$

The collision integrals are obtained from (43) and (44) by replacing $\langle n_\mathbf{k}\rangle_t$ and $\langle N_\mathbf{k}\rangle_t$ by $g_\mathbf{k}$ and $G_\mathbf{k}$, respectively.

The electric and thermal currents are given by

$$\begin{aligned}\mathbf{J}&=-\frac{e}{\mathcal{V}}\sum_\mathbf{k}v(\mathbf{k})g_\mathbf{k},\\ \mathbf{Q}&=\frac{1}{\mathcal{V}}\sum_\mathbf{k}\epsilon_\mathbf{k}v(\mathbf{k})g_\mathbf{k}+\frac{1}{\mathcal{V}}\sum_\mathbf{k}w_\mathbf{k}u(\mathbf{k})G_\mathbf{k},\end{aligned} \tag{46}$$

in which we have again neglected spin.[10]

The procedure for deriving the transport equations is standard; see, for example, Sondheimer.[12] Substitute

$$\begin{aligned}g_\mathbf{k}&=f_\mathbf{k}-\Phi_1(\mathbf{k})\frac{d}{d\epsilon_\mathbf{k}}f_\mathbf{k},\\ G_\mathbf{k}&=F_\mathbf{k}-\Phi_2(\mathbf{k})\frac{d}{dw_\mathbf{k}}F_\mathbf{k}\end{aligned} \tag{47}$$

into (45) and neglect terms of order Φ^2. This linear approximation is consistent with the linear response theory. Then, to lowest order in Φ,

$$v_\mu(\mathbf{k})f_\mathbf{k}(1-f_\mathbf{k})\beta\left\{eE_\mu+\epsilon_\mathbf{k}\frac{\nabla_\mu T}{T}\right\}=\frac{d}{dt}g_\mathbf{k}\Big|_{\text{collision}} \tag{48}$$

and

$$u_\mu(\mathbf{k})F_\mathbf{k}(1+F_\mathbf{k})\beta w_\mathbf{k}\frac{\nabla_\mu T}{T}=\frac{d}{dt}G_\mathbf{k}\Big|_{\text{collision}}.$$

[Although

$$\frac{d}{dT}f_\mathbf{k}=-\frac{d}{d\epsilon_\mathbf{K}}f_\mathbf{k}\left\{\frac{\epsilon_\mathbf{K}}{T}+T\frac{d}{dT}\left(\frac{\mu}{T}\right)\right\},$$

where μ is the chemical potential, we have neglected the last term and put

$$\frac{d}{dT}f_\mathbf{k}=-\frac{d}{d\epsilon_\mathbf{K}}f_\mathbf{k}\frac{\epsilon_\mathbf{K}}{T}.$$

This is consistent with our definition of the Kubo formulas (37).

The effect of the chemical potential can be included by making the transformation

$$e\mathbf{E}\rightarrow e\mathbf{E}+T(d/dT)(\mu/T)\cdot\nabla T.]$$

Since the distribution functions f, F satisfy the collision integral equations

$$(d/dt)f_\mathbf{k}\,|_{\text{collision}}\equiv(d/dt)F_\mathbf{k}\,|_{\text{collision}}=0, \tag{49}$$

to lowest order in Φ

$$\begin{aligned}\frac{d}{dt}g_\mathbf{k}\Big|_{\text{collision}}=2\pi\lambda^2\frac{\beta}{\mathcal{V}}\sum_\mathbf{q}|v_\mathbf{q}|^2\,[&\delta(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_\mathbf{k}-w_\mathbf{q})\\ &\times(1-f_\mathbf{k})f_{\mathbf{k}+\mathbf{q}}(1+F_\mathbf{q})\\ &\times\{\Phi_1(\mathbf{k}+\mathbf{q})-\Phi_1(\mathbf{k})-\Phi_2(\mathbf{q})\}\\ &+\delta(\epsilon_\mathbf{k}-\epsilon_{\mathbf{k}+\mathbf{q}}-w_{-\mathbf{q}})(1-f_\mathbf{k})f_{\mathbf{k}+\mathbf{q}}F_{-\mathbf{q}}\\ &\times\{\Phi_1(\mathbf{k}+\mathbf{q})-\Phi_1(\mathbf{k})+\Phi_2(-\mathbf{q})\}]\end{aligned} \tag{50}$$

and

$$\begin{aligned}\frac{d}{dt}G_\mathbf{k}\Big|_{\text{collision}}=2\pi\lambda^2\frac{\beta}{\mathcal{V}}\sum_\mathbf{p}|v_\mathbf{k}|^2\,&\delta(\epsilon_{\mathbf{k}+\mathbf{p}}-\epsilon_\mathbf{p}-w_\mathbf{k})\\ &\times(1-f_\mathbf{p})f_{\mathbf{k}+\mathbf{p}}(1+F_\mathbf{k})\\ &\times\{\Phi_1(\mathbf{k}+\mathbf{p})-\Phi_1(\mathbf{p})-\Phi_2(\mathbf{k})\}.\end{aligned}$$

The explicit forms of f and F can now be used to show that

$$\begin{aligned}&\frac{d}{dt}g_\mathbf{k}\Big|_{\text{collision}}\\ &\quad=2\pi\lambda^2\beta f_\mathbf{k}(1-f_\mathbf{k})\{J[\Phi_1(\mathbf{k})]+K[\Phi_2(\mathbf{k})]\},\\ &\frac{d}{dt}G_\mathbf{k}\Big|_{\text{collision}}\\ &\quad=2\pi\lambda^2\beta F_\mathbf{k}(1+F_\mathbf{k})\{L[\Phi_1(\mathbf{k})]+M[\Phi_2(\mathbf{k})]\},\end{aligned} \tag{51}$$

where J, K, L, and M are the operators defined in (A17). Therefore,

$$\begin{aligned}v_\mu(\mathbf{k})\left\{eE_\mu+\epsilon_\mathbf{k}\frac{\nabla_\mu T}{T}\right\}&=2\pi\lambda^2\{J[\Phi_1(\mathbf{k})]+K[\Phi_2(\mathbf{k})]\},\\ u_\mu(\mathbf{k})w_\mathbf{k}\frac{\nabla_\mu T}{T}&=2\pi\lambda^2\{L[\Phi_1(\mathbf{k})]+M[\Phi_2(\mathbf{k})]\}.\end{aligned} \tag{52}$$

From (46) and (47)

$$\begin{aligned}\mathbf{J}_\nu&=\frac{e}{\mathcal{V}}\sum_\mathbf{k}v_\nu(\mathbf{k})\Phi_1(\mathbf{k})\frac{d}{d\epsilon_\mathbf{k}}f_\mathbf{k},\\ \mathbf{Q}_\nu&=-\frac{1}{\mathcal{V}}\sum_\mathbf{k}\epsilon_\mathbf{k}v_\nu(\mathbf{k})\Phi_1(\mathbf{k})\frac{d}{d\epsilon_\mathbf{K}}f_\mathbf{k},\\ &\quad-\frac{1}{\mathcal{V}}\sum_\mathbf{k}w_\mathbf{k}u_\nu(\mathbf{k})\Phi_2(\mathbf{k})\frac{d}{dw_\mathbf{k}}F_\mathbf{k}.\end{aligned} \tag{53}$$

[12] E. H. Sondheimer, Proc. Roy. Soc. (London) **A234**, 391 (1956).

Therefore, in the $\mathcal{V}$ limit, the transport coefficients derived from the Kubo formulas (40) and (41) are identical to those derived from the Boltzmann equations (52) and (53) when we put

$$\Phi_C = \Phi_1 \quad \text{and} \quad \Phi_D = \Phi_2.$$

The two methods are thus equivalent.

Finally, as we mentioned in the Introduction, all the formulas are now available for the treatment of an infinite system of weakly interacting fermions or bosons. The contraction process is simpler because only one type of occupation number is involved. The 2×2 matrix operator a reduces to a single operator which can be connected with the usual collision operator by the same methods as those used above.

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APPENDIX. CONTRACTION OF THE KUBO FORMULAS

Instead of considering Eqs. (24), (26), (27), (33), and (34), we introduce generalized currents $\bar{C}$, $\bar{D}$, transport coefficients L, and driving forces X, Y defined by

$$\begin{aligned} \bar{C}_\nu &= L'^{\mu}(R, S)X_\mu + L'^{\mu}(R, T)Y_\mu, \\ \bar{D}_\nu &= L'^{\mu}(P, S)X_\mu + L'^{\mu}(P, T)Y_\mu, \end{aligned} \tag{A1}$$

where

$$\begin{aligned} L'^{\mu}(R, S) &= \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2}\frac{\beta}{\mathcal{V}} \\ &\times \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{\alpha\alpha'} \rho_0(\alpha) \sum_{\mathbf{p}} R_\nu(\mathbf{p})n_{\mathbf{p}} \\ &\times \sum_{m=0}^{\infty} \frac{\tau^m}{m!}\, \Omega^{(m)}_{\alpha\alpha'}[\sum_{\mathbf{r}} S_\mu(\mathbf{r})n'_{\mathbf{r}}], \\ L'^{\mu}(R, T) &= \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2}\frac{\beta}{\mathcal{V}} \\ &\times \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{\alpha\alpha'} \rho_0(\alpha) \sum_{\mathbf{p}} R_\nu(\mathbf{p})n_{\mathbf{p}} \\ &\times \sum_{m=0}^{\infty} \frac{\tau^m}{m!}\, \Omega^{(m)}_{\alpha\alpha'}[\sum_{\mathbf{r}} T_\mu(\mathbf{r})N'_{\mathbf{r}}], \end{aligned} \tag{A2}$$

$$\begin{aligned} L'^{\mu}(P, S) &= \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2}\frac{\beta}{\mathcal{V}} \\ &\times \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{\alpha\alpha'} \rho_0(\alpha) \sum_{\mathbf{p}} P_\nu(\mathbf{p})N_{\mathbf{p}} \\ &\times \sum_{m=0}^{\infty} \frac{\tau^m}{m!}\, \Omega^{(m)}_{\alpha\alpha'}[\sum_{\mathbf{r}} S_\mu(\mathbf{r})n'_{\mathbf{r}}], \end{aligned}$$

and

$$\begin{aligned} L'^{\mu}(P, T) &= \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2}\frac{\beta}{\mathcal{V}} \\ &\times \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{\alpha\alpha'} \rho_0(\alpha) \sum_{\mathbf{p}} P_\nu(\mathbf{p})N_{\mathbf{p}} \\ &\times \sum_{m=0}^{\infty} \frac{\tau^m}{m!}\, \Omega^{(m)}_{\alpha\alpha'}[\sum_{\mathbf{r}} T_\mu(\mathbf{r})N'_{\mathbf{r}}]. \end{aligned}$$

The current fluxes P, R, S, and T are assumed to have the equilibrium properties

$$\begin{aligned} &\mathrm{Tr}\ \rho_0 \sum_{\mathbf{p}} P_\nu(\mathbf{p})N_{\mathbf{p}} \equiv \mathrm{Tr}\ \rho_0 \sum_{\mathbf{p}} R_\nu(\mathbf{p})n_{\mathbf{p}} \\ &\equiv \mathrm{Tr}\ \rho_0 \sum_{\mathbf{r}} S_\mu(\mathbf{r})n_{\mathbf{r}} \equiv \mathrm{Tr}\ \rho_0 \sum_{\mathbf{r}} T_\mu(\mathbf{r})N_{\mathbf{r}} = 0. \end{aligned} \tag{A3}$$

The currents $\mathbf{J}$ and $\bar{\mathbf{Q}}$ can be constructed by taking the corresponding particular forms of P, R, S, T and X, Y.

The general rules for contracting the linear-response formulas can be derived by considering some simple examples.

Consider

$$I_1 = \mathrm{Tr}\ \rho_0 \sum_{\mathbf{k}_1} S(\mathbf{k}_1)n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)n_{\mathbf{k}_2} \tag{A4}$$

subject to the conditions

$$\sum_{\mathbf{k}_1} S(\mathbf{k}_1)f_{\mathbf{k}_1} \equiv \sum_{\mathbf{k}_2} R(\mathbf{k}_2)f_{\mathbf{k}_2} = 0. \tag{A5}$$

In order to make the procedure clear, suppose there are only three possible states (1, 2, 3). Then

$$\begin{aligned} &I_1(1, 2, 3) \\ &= \mathrm{Tr}\ \rho_0[\{n_1S_1 + n_2S_2 + n_3S_3\}\{n_1R_1 + n_2R_2 + n_3R_3\}] \\ &= \{f_1S_1 + f_2S_2 + f_3S_3\}\{f_1R_1 + f_2R_2 + f_3R_3\} \\ &\quad + S_1R_1f_1(1 - f_1) + S_2R_2f_2(1 - f_2) + S_3R_3f_3(1 - f_3) \\ &= S_1R_1f_1(1 - f_1) + S_2R_2f_2(1 - f_2) + S_3R_3f_3(1 - f_3). \end{aligned}$$

This can be generalized immediately to give

$$I_1 = \sum_{\mathbf{k}_1} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}). \tag{A6}$$

Similarly,

$$\begin{aligned} I_2 &= \mathrm{Tr}\ \rho_0 \sum_{\mathbf{k}_1} S(\mathbf{k}_1)n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)(1 - n_{\mathbf{k}_2}) \\ &= -\sum_{\mathbf{k}_1} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}). \end{aligned} \tag{A7}$$

An example trivially related to I_1 since $\sum_{\mathbf{p}} n_{\mathbf{p}} = \mathfrak{N}$ is

$$\begin{aligned} I_3 &= \mathrm{Tr}\,\rho_0 \sum_{\mathbf{k}_1} S(\mathbf{k}_1)n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)n_{\mathbf{k}_2} \sum_{\mathbf{p}} n_{\mathbf{p}} \\ &= \sum_{\mathbf{k}_1} S(\mathbf{k}_1)f_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)f_{\mathbf{k}_2} \sum_{\mathbf{p}} f_{\mathbf{p}} \\ &\quad + \sum_{\mathbf{k}_2} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}) \sum_{\mathbf{p}} f_{\mathbf{p}} \\ &\quad + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}) \sum_{\mathbf{k}_2} R(\mathbf{k}_2)f_{\mathbf{k}_2} \\ &\quad + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)f_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)f_{\mathbf{k}_2}(1 - f_{\mathbf{k}_2}) \\ &\quad + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1})(1 - 2f_{\mathbf{k}_1}) \\ &= \sum_{\mathbf{k}_1} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}) \sum_{\mathbf{p}} f_{\mathbf{p}} \\ &\quad + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1})(1 - 2f_{\mathbf{k}_1}). \end{aligned} \tag{A8}$$

But the second term on the right-hand side of the last equation is a factor of $\mathcal{V}$ less than the first in the limit of an infinite system, when the summations are replaced by integrals. Thus

$$I_3 = \sum_{\mathbf{k}_1} S(\mathbf{k}_1)R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}) \sum_{\mathbf{p}} f_{\mathbf{p}}$$

to leading order, as required.

We anticipate one of the later results by noting here that each contracted term in a particular Kubo formula, which by definition is the leading-order term in $\mathcal{V}$, is of the same order as all the other contracted terms, so that the above procedure of keeping only the highest-order terms in $\mathcal{V}$ is a consistent approximation.

We indicate the occupation numbers involved in the contraction process by means of a left-superscript con. For example,

$$\begin{aligned} I_1 = \sum_{\mathbf{k}_1} S(\mathbf{k}_1)n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)n_{\mathbf{k}_2} \\ + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)\,{}^{\mathrm{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)\,{}^{\mathrm{con}}n_{\mathbf{k}_2}, \end{aligned}$$

where the first term means that $\mathbf{k}_1 \neq \mathbf{k}_2$ and the second term means that $\mathbf{k}_1 = \mathbf{k}_2$. Similarly,

$$\begin{aligned} I_3 = \sum_{\mathbf{k}_1} S(\mathbf{k}_1)n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)n_{\mathbf{k}_2} \sum_{\mathbf{p}} n_{\mathbf{p}} \\ + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)\,{}^{\mathrm{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)\,{}^{\mathrm{con}}n_{\mathbf{k}_2} \sum_{\mathbf{p}} n_{\mathbf{p}} \\ + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)\,{}^{\mathrm{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)n_{\mathbf{k}_2} \sum_{\mathbf{p}} {}^{\mathrm{con}}n_{\mathbf{p}} \\ + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)\,{}^{\mathrm{con}}n_{\mathbf{k}_2} \sum_{\mathbf{p}} {}^{\mathrm{con}}n_{\mathbf{p}} \\ + \sum_{\mathbf{k}_1} S(\mathbf{k}_1)\,{}^{\mathrm{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} R(\mathbf{k}_2)\,{}^{\mathrm{con}}n_{\mathbf{k}_2} \sum_{\mathbf{p}} {}^{\mathrm{con}}n_{\mathbf{p}}. \end{aligned}$$

We now propose the general rules.

(a) Write down explicitly all possible single contractions.

(b) If the contraction is of the form

(i) ${}^{\mathrm{con}}n_{\mathbf{k}_1}\,{}^{\mathrm{con}}n_{\mathbf{k}_2}$, replace it by $f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1})$; $\mathbf{k}_1 = \mathbf{k}_2$.

(ii) ${}^{\mathrm{con}}n_{\mathbf{k}_1}(1 - {}^{\mathrm{con}}n_{\mathbf{k}_2})$ replace it by $-f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1})$; $\mathbf{k}_1 = \mathbf{k}_2$.

The resulting expression is the total contribution in the $\mathcal{V}$ limit. For the reconstructed original summation with n replaced by f (for example, the first term in I_3), is zero by the equilibrium properties. All those terms resulting from two or more contractions are at least a factor $1/\mathcal{V}$ less in order, and are therefore negligible.

So far, we have confined our attention to fermion occupation numbers. The same arguments can be applied to bosons and the rules are the same except that (b) becomes

$$\begin{aligned} {}^{\mathrm{con}}N_{\mathbf{K}_1}\,{}^{\mathrm{con}}N_{\mathbf{K}_2} &\equiv {}^{\mathrm{con}}N_{\mathbf{K}_1}(1 + {}^{\mathrm{con}}N_{\mathbf{K}_2}) \\ &= F_{\mathbf{K}_1}(1 + F_{\mathbf{K}_1}); \qquad \mathbf{K}_1 = \mathbf{K}_2. \end{aligned}$$

These rules must now be used to contract expressions of the form

$$I_m^{AB} = \frac{1}{\mathcal{V}} \sum_{\alpha} \rho_0(\alpha)A(\alpha) \sum_{\alpha'} \Omega_{\alpha\alpha'}^{(m)}B(\alpha'), \tag{A9}$$

where A and B are particular currents P, R, S, and T.

When A and B are fermion currents, we know from previous work[5]

$$\Omega^{(m)}(n) \approx Q_0(n) + (1/\mathcal{V})Q_1(n) + O(1/\mathcal{V})^2,$$

where Q_0, Q_1 are independent of $\mathcal{V}$ and functions of distinct occupation numbers. A factor $\mathcal{V}^2$ is introduced when the two summations over states α and α' in I_m^{AB} are replaced by integrals. Thus,

$$I_m^{AB} \approx \mathcal{V}\left\{{}^{\mathrm{con}}n\,{}^{\mathrm{con}}Q_0(n) + \frac{1}{\mathcal{V}}\,{}^{\mathrm{con}}n\,{}^{\mathrm{con}}Q_1(n) + O(1/\mathcal{V})^2\right\}.$$

Each contraction reduces a term by a factor $1/\mathcal{V}$ so that

$$I_m^{AB} \approx \mathcal{V}\,{}^{\mathrm{con}}n\,{}^{\mathrm{con}}Q_0(n) + O(1/\mathcal{V}),$$

which is valid for all m.

Since the same arguments can be applied for bosons, the contraction process is consistent in the $\mathcal{V}$ limit.

Consider

$$\begin{aligned} I_m^R &= I_m^{RS}X + I_m^{RT}Y \\ &= \frac{1}{\mathcal{V}} \sum_{\alpha} \rho_0(\alpha) \sum_{\mathbf{p}} R(\mathbf{p})n_{\mathbf{p}} \sum_{\alpha'} \Omega_{\alpha\alpha'}^{(m)}[\sum_{\mathbf{r}} S(\mathbf{r})n_{\mathbf{r}}']X \\ &\quad + \frac{1}{\mathcal{V}} \sum_{\alpha} \rho_0(\alpha) \sum_{\mathbf{p}} R(\mathbf{p})n_{\mathbf{p}} \sum_{\alpha'} \Omega_{\alpha\alpha'}^{(m)}[\sum_{\mathbf{r}} T(\mathbf{r})N_{\mathbf{r}}']Y. \end{aligned} \tag{A10}$$

For $m = 0$, from (14)

$$I_0^R = \frac{1}{\mathcal{V}} \sum_\alpha \rho_0(\alpha) \sum_{\mathbf{p}} R(\mathbf{p})\, {}^{\mathrm{con}}n_{\mathbf{p}} \sum_{\mathbf{r}} S(\mathbf{r})\, {}^{\mathrm{con}}n_{\mathbf{r}} X + \frac{1}{\mathcal{V}} \sum_\alpha \rho_0(\alpha) \sum_{\mathbf{p}} R(\mathbf{p})\, {}^{\mathrm{con}}n_{\mathbf{p}} \sum_{\mathbf{r}} T(\mathbf{r})\, {}^{\mathrm{con}}N_{\mathbf{r}} Y = \frac{1}{\mathcal{V}} \sum_{\mathbf{p}} R(\mathbf{p}) S(\mathbf{p}) f_{\mathbf{p}}(1 - f_{\mathbf{p}}) X \tag{A11}$$

since ${}^{\mathrm{con}}n\,{}^{\mathrm{con}}N = fF$.

Now put $m = 1$. From Eqs. (20) and (21)

$$\sum_{\mathbf{k}} S(\mathbf{k}) \sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}} X + \sum_{\mathbf{q}} T(\mathbf{q}) \sum_{\alpha'} \Omega_{\alpha\alpha'} N'_{\mathbf{q}} Y = \frac{1}{\mathcal{V}} \sum_{\mathbf{kq}} |v_{\mathbf{q}}|^2 n_{\mathbf{k}}(1 - n_{\mathbf{k}+\mathbf{q}}) [\delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) \times \{S(\mathbf{k}+\mathbf{q})X - S(\mathbf{k})X - T(\mathbf{q})Y\} N_{\mathbf{q}} + \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} - w_{-\mathbf{q}}) \times \{S(\mathbf{k}+\mathbf{q})X - S(\mathbf{k})X + T(-\mathbf{q})Y\}(1 + N_{-\mathbf{q}})] \tag{A12}$$

by rearranging the summations. There are two nonzero contributions to the contraction of I_1^R: ${}^{\mathrm{con}}n_{\mathbf{p}}\,{}^{\mathrm{con}}n_{\mathbf{k}}(1 - n_{\mathbf{k}+\mathbf{q}})$ and ${}^{\mathrm{con}}n_{\mathbf{p}} n_{\mathbf{k}}(1 - {}^{\mathrm{con}}n_{\mathbf{k}+\mathbf{q}})$.

Define the operators $\mathcal{J}$, $\mathcal{K}$, $\mathcal{L}$, and $\mathfrak{M}$ by the equations

$$\mathcal{J}[A(\mathbf{k})] = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} |v_{\mathbf{q}}|^2 \{A(\mathbf{k}+\mathbf{q}) - A(\mathbf{k})\} \times [\delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) \times \{(1 - n_{\mathbf{k}+\mathbf{q}})N_{\mathbf{q}} + n_{\mathbf{k}+\mathbf{q}}(1 + N_{\mathbf{q}})\} + \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} - w_{-\mathbf{q}}) \times \{(1 - n_{\mathbf{k}+\mathbf{q}})(1 + N_{-\mathbf{q}}) + n_{\mathbf{k}+\mathbf{q}}N_{-\mathbf{q}}\}], \tag{A13}$$

$$\mathcal{K}[A(\mathbf{k})] = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} |v_{\mathbf{q}}|^2 [\delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} - w_{-\mathbf{q}}) A(-\mathbf{q}) \times \{(1 - n_{\mathbf{k}+\mathbf{q}})(1 + N_{-\mathbf{q}}) + n_{\mathbf{k}+\mathbf{q}}N_{-\mathbf{q}}\} - \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) \times \{(1 - n_{\mathbf{k}+\mathbf{q}})N_{\mathbf{q}} + n_{\mathbf{k}+\mathbf{q}}(1 + N_{\mathbf{q}})\} A(\mathbf{q})], \tag{A14}$$

$$\mathcal{L}[A(\mathbf{q})] = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} |v_{\mathbf{q}}|^2 \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) \times \{A(\mathbf{k}+\mathbf{q}) - A(\mathbf{k})\} \times \{n_{\mathbf{k}}(1 - n_{\mathbf{k}+\mathbf{q}}) - (1 - n_{\mathbf{k}})n_{\mathbf{k}+\mathbf{q}}\}, \tag{A15}$$

$$\mathfrak{M}[A(\mathbf{q})] = -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} |v_{\mathbf{q}}|^2 \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) \times A(\mathbf{q}) \{n_{\mathbf{k}}(1 - n_{\mathbf{k}+\mathbf{q}}) - (1 - n_{\mathbf{k}})n_{\mathbf{k}+\mathbf{q}}\} \tag{A16}$$

and the operators J, K, L, and M by the equations

$$\mathrm{Tr}\, \rho_0 \mathcal{J}(A) = J(A), \text{ etc.} \tag{A17}$$

Then the two terms in the contraction of I_1^R can be arranged to give

$$I_1^R = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} R(\mathbf{k}_1) f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}) \times \{J[S(\mathbf{k}_1)]X + K[T(\mathbf{k}_1)]Y\}. \tag{A18}$$

It is convenient to introduce two more operators G and H by

$$G[A(\mathbf{k})] = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} |v_{\mathbf{q}}|^2 (1 - n_{\mathbf{k}+\mathbf{q}}) \times \{A(\mathbf{k}+\mathbf{q}) - A(\mathbf{k})\} [\delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) N_{\mathbf{q}} + \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} - w_{-\mathbf{q}})(1 + N_{-\mathbf{q}})] \tag{A19}$$

and

$$H[A(\mathbf{k})] = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} |v_{\mathbf{q}}|^2 (1 - n_{\mathbf{k}+\mathbf{q}}) \times [\delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} - w_{-\mathbf{q}})(1 + N_{-\mathbf{q}}) A(-\mathbf{q}) - \delta(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - w_{\mathbf{q}}) N_{\mathbf{q}} A(\mathbf{q})]. \tag{A20}$$

Then, from (A12),

$$\sum_{\mathbf{k}} S(\mathbf{k}) \sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}} X + \sum_{\mathbf{q}} T(\mathbf{q}) \sum_{\alpha'} \Omega_{\alpha\alpha'} N'_{\mathbf{q}} Y = \sum_{\mathbf{k}} n_{\mathbf{k}} \{G[S(\mathbf{k})]X + H[T(\mathbf{k})]Y\}$$

and the contraction of I_1^R can be written as

$$I_1^R = \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\mathrm{con}}n_{\mathbf{k}_1} \times \sum_{\mathbf{k}_2} {}^{\mathrm{con}}n_{\mathbf{k}_2} \{G[S(\mathbf{k}_2)]X + H[T(\mathbf{k}_2)]Y\} + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\mathrm{con}}n_{\mathbf{k}_1} \times \sum_{\mathbf{k}_2} n_{\mathbf{k}_2} \{{}^{\mathrm{con}}G[S(\mathbf{k}_2)]X + {}^{\mathrm{con}}H[T(\mathbf{k}_2)]Y\}. \tag{A21}$$

Alternatively, I_1^R can be written in its original form as

$$I_1^R = \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\mathrm{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} S(\mathbf{k}_2) \sum_{\alpha'} {}^{\mathrm{con}}\Omega_{\alpha\alpha'} n'_{\mathbf{k}_2} X + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\mathrm{con}}n_{\mathbf{k}_1} \sum_{\mathbf{q}} T(\mathbf{q}) \sum_{\alpha'} {}^{\mathrm{con}}\Omega_{\alpha\alpha'} N'_{\mathbf{q}} Y, \tag{A22}$$

since T and S have no occupation number dependence. However, even if S and T had (n, N) dependence, the result would still be (A22), since

$$({}^{\mathrm{con}}n, N)({}^{\mathrm{con}}n, N) \sum_{\alpha'} \Omega^{(m)}_{\alpha\alpha'}(n', N') = 0; \quad m > 0 \tag{A23}$$

because

$$\mathrm{Tr}\, \rho_0 \Omega^{(m)}(n, N) = 0; \qquad m > 0.$$

Now consider $m = 2$.

$$\sum_{\mathbf{k}_2} S(\mathbf{k}_2) \sum_{\alpha''} \Omega^{(2)}_{\alpha\alpha'',} n''_{\mathbf{k}_2} = \sum_{\alpha'} \Omega_{\alpha\alpha'} \{ \sum_{\mathbf{k}_2} n'_{\mathbf{k}_2} G'[S(\mathbf{k}_2)] \} = \sum_{\mathbf{k}_2} \{ n_{\mathbf{k}_2} \sum_{\alpha'} \Omega_{\alpha\alpha'} G'[S(\mathbf{k}_2)] + G[S(\mathbf{k}_2)] \sum_{\alpha'} \Omega_{\alpha\alpha'} n'_{\mathbf{k}_2} \} \quad \text{(A24)}$$

in the $\mathcal{V}$ limit. A similar expression holds for H and T. Therefore, using (A23),

$$\begin{aligned} I_2^R = & \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} n_{\mathbf{k}_2} \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, G'[S(\mathbf{k}_2)]X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} G[S(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, n'_{\mathbf{k}_2} X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} n_{\mathbf{k}_2} \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, H'[T(\mathbf{k}_2)]Y \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} H[T(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, n'_{\mathbf{k}_2} Y. \end{aligned} \quad \text{(A25)}$$

From the definition of G, (A19), and the factorization property of Ω, (19),

$$\begin{aligned} & \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} n_{\mathbf{k}_2} \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, G'[S(\mathbf{k}_2)] \\ & = -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}_2\mathbf{q}} |v_{\mathbf{q}}|^2 \{ S(\mathbf{k}_2 + \mathbf{q}) - S(\mathbf{k}_2) \} \\ & \quad \times [\delta(\epsilon_{\mathbf{k}_2+\mathbf{q}} - \epsilon_{\mathbf{k}_2} - w_{\mathbf{q}}) N_{\mathbf{q}} \\ & \quad + \delta(\epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_2+\mathbf{q}} - w_{-\mathbf{q}})(1 + N_{-\mathbf{q}})] \\ & \quad \times n_{\mathbf{k}_2} \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, n'_{\mathbf{k}_2+\mathbf{q}} \\ & \quad + \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_2\mathbf{q}} |v_{\mathbf{q}}|^2 \{ S(\mathbf{k}_2 + \mathbf{q}) - S(\mathbf{k}_2) \} \\ & \quad \times \delta(\epsilon_{\mathbf{k}_2+\mathbf{q}} - \epsilon_{\mathbf{k}_2} - w_{\mathbf{q}}) \\ & \quad \times \{ n_{\mathbf{k}_2}(1 - n_{\mathbf{k}_2+\mathbf{q}}) - (1 - n_{\mathbf{k}_2}) n_{\mathbf{k}_2+\mathbf{q}} \} \\ & \quad \times \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, N'_{\mathbf{q}}. \end{aligned} \quad \text{(A26)}$$

A similar expression can be derived for the third term on the right-hand side of (A25). When (A26) and the corresponding equation involving $H(T)$ are substituted into (A25), the summations can be rearranged to give

$$\begin{aligned} I_2^R = & \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \mathcal{J}[S(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, n'_{\mathbf{k}_2} X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{q}} \mathcal{L}[S(\mathbf{q})] \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, N'_{\mathbf{q}} X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \mathcal{K}[T(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, n'_{\mathbf{k}_2} Y \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{q}} \mathfrak{M}[T(\mathbf{q})] \sum_{\alpha'} {}^{\text{con}}\Omega_{\alpha\alpha'}\, N'_{\mathbf{q}} Y. \end{aligned} \quad \text{(A27)}$$

Therefore, by analogy with (A18), (A22), and using (A23),

$$\begin{aligned} I_2^R = & \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} R(\mathbf{k}_1) f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}) \\ & \times [(J\{J[S(\mathbf{k}_1)]\} + K\{L[S(\mathbf{k}_1)]\})X \\ & + (J\{K[T(\mathbf{k}_1)]\} + K\{M[T(\mathbf{k}_1)]\})Y]. \end{aligned} \quad \text{(A28)}$$

We can easily construct a recurrence formula for I_m^R. For, in the $\mathcal{V}$ limit

$$\sum_{\mathbf{k}_2} S(\mathbf{k}_2) \sum_{\alpha''} \Omega^{(m+1)}_{\alpha\alpha'',} n''_{\mathbf{k}_2} = \sum_{\alpha'} \Omega^{(m)}_{\alpha\alpha'} \{ \sum_{\mathbf{k}_2} n'_{\mathbf{k}_2} G'[S(\mathbf{k}_2)] \}, \quad \text{(A29)}$$

so that

$$\begin{aligned} & \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} S(\mathbf{k}_2) \sum_{\alpha''} {}^{\text{con}}\Omega^{(m+1)}_{\alpha\alpha'',}\, n''_{\mathbf{k}_2} \\ & \equiv \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} G[S(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, n'_{\mathbf{k}_2} \\ & \quad + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} n_{\mathbf{k}_2} \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'} G'[S(\mathbf{k}_2)] \end{aligned} \quad \text{(A30)}$$

since terms like

$$\sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \sum_{\alpha'} {}^{\text{con}}\Omega^{(s)}_{\alpha\alpha'}\, n'_{\mathbf{k}_2} \times \sum_{\alpha''} \Omega^{(m-s)}_{\alpha\alpha'',} G''[S(\mathbf{k}_2)] \equiv 0 \quad \text{(A31)}$$

from (A23). Similar equations hold for the $H(T)$ term.

Using (A31), an equation analogous to (A26) can be obtained with $\Omega_{\alpha\alpha'}$ replaced by $\Omega^{(m)}_{\alpha\alpha'}$. Therefore, for $m \geq 1$,

$$\begin{aligned} I_{m+1}^R = & \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \mathcal{J}[S(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, n'_{\mathbf{k}_2} X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{q}} \mathcal{L}[S(\mathbf{q})] \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, N'_{\mathbf{q}} X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \mathcal{K}[T(\mathbf{k}_2)] \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, n'_{\mathbf{k}_2} Y \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{q}} \mathfrak{M}[T(\mathbf{q})] \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, N'_{\mathbf{q}} Y. \end{aligned} \quad \text{(A32)}$$

But by definition,

$$\begin{aligned} I_m^R = & \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{k}_2} S(\mathbf{k}_2) \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, n'_{\mathbf{k}_2} X \\ & + \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, {}^{\text{con}}n_{\mathbf{k}_1} \sum_{\mathbf{q}} T(\mathbf{q}) \sum_{\alpha'} {}^{\text{con}}\Omega^{(m)}_{\alpha\alpha'}\, N'_{\mathbf{q}} Y. \end{aligned} \quad \text{(A33)}$$

Therefore, I_{m+1}^R is related to I_m^R by the transformation

$$\begin{aligned} SX &\rightarrow J(S)X + K(T)Y, \\ TY &\rightarrow L(S)X + M(T)Y. \end{aligned} \quad \text{(A34)}$$

If all of the above procedure is repeated for

$$I_m^P = I_m^{PS}X + I_m^{PT}Y$$
$$= \frac{1}{\mathcal{V}} \sum_\alpha \rho_0(\alpha) \sum_{\mathbf{p}} P(\mathbf{p})N_{\mathbf{p}} \sum_{\alpha'} \Omega_{\alpha\alpha'}^{(m)}[\sum_{\mathbf{r}} S(\mathbf{r})n_{\mathbf{r}}']X$$
$$+ \frac{1}{\mathcal{V}} \sum_\alpha \rho_0(\alpha) \sum_{\mathbf{p}} P(\mathbf{p})N_{\mathbf{p}} \sum_{\alpha'} \Omega_{\alpha\alpha'}^{(m)}[\sum_{\mathbf{r}} T(\mathbf{r})N_{\mathbf{r}}']Y, \tag{A35}$$

then

$$I_0^P = \frac{1}{\mathcal{V}} \sum_{\mathbf{p}} P(\mathbf{p})F_{\mathbf{p}}(1 + F_{\mathbf{p}})T(\mathbf{p})Y. \tag{A36}$$

Furthermore, I_{m+1}^P can be obtained from I_m^P in exactly the same way as I_{m+1}^R is obtained from I_m^R, the only difference being in the starting values I_0^P and I_0^R.

Define

$$\bar{C} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\beta f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1})\Phi_C(\mathbf{k}_1),$$
$$\bar{D} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} P(\mathbf{k}_1)\beta F_{\mathbf{k}_1}(1 + F_{\mathbf{k}_1})\Phi_D(\mathbf{k}_1), \tag{A37}$$

where

$$\Phi_C(\mathbf{k}_1) = \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2} \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{m=0}^\infty \frac{\tau^m}{m!} \bar{I}_m^R(\mathbf{k}_1),$$
$$\Phi_D(\mathbf{k}_1) = \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2} \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{m=0}^\infty \frac{\tau^m}{m!} \bar{I}_m^P(\mathbf{k}_1). \tag{A38}$$

$\bar{I}_m^R$, $\bar{I}_m^P$ are obtained by removing the factors

$$\frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} R(\mathbf{k}_1)f_{\mathbf{k}_1}(1 - f_{\mathbf{k}_1}); \quad \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} P(\mathbf{k}_1)F_{\mathbf{k}_1}(1 + F_{\mathbf{k}_1})$$

from I_m^R, I_m^P, respectively. Then, in matrix notation,

$$\begin{bmatrix} \bar{I}_0^R(\mathbf{k}_1) \\ \bar{I}_0^P(\mathbf{k}_1) \end{bmatrix} = \begin{bmatrix} S(\mathbf{k}_1)X \\ T(\mathbf{k}_1)Y \end{bmatrix}, \tag{A39}$$

and from the recurrence transformation (A34),

$$\begin{bmatrix} \bar{I}_m^R(\mathbf{k}_1) \\ \bar{I}_m^P(\mathbf{k}_1) \end{bmatrix} = a^m \begin{bmatrix} S(\mathbf{k}_1)X \\ T(\mathbf{k}_1)Y \end{bmatrix}, \tag{A40}$$

where a is the matrix

$$a = \begin{bmatrix} J & K \\ L & M \end{bmatrix}. \tag{A41}$$

Equation (A38) becomes

$$\begin{bmatrix} \Phi_C(\mathbf{k}_1) \\ \Phi_D(\mathbf{k}_1) \end{bmatrix} = \lim_{\theta\to 0} \frac{1}{2\pi\lambda^2} \int_0^\infty d\tau\, e^{-\theta\tau} \sum_{m=0}^\infty \frac{\tau^m}{m!}\, a^m \begin{bmatrix} S(\mathbf{k}_1)X \\ T(\mathbf{k}_1)Y \end{bmatrix} \tag{A42}$$

so that

$$a \begin{bmatrix} \Phi_C(\mathbf{k}_1) \\ \Phi_D(\mathbf{k}_1) \end{bmatrix} = -\frac{1}{2\pi\lambda^2} \begin{bmatrix} S(\mathbf{k}_1)X \\ T(\mathbf{k}_1)Y \end{bmatrix} \tag{A43}$$

provided $e^{a\tau}$ increases slower than $e^{-\theta\tau}$ decreases as $\tau \to \infty$.

Therefore, in the limit of an infinite system, the contracted formulas are

$$\bar{C} = -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} R(\mathbf{k}_1)\, \Phi_C(\mathbf{k}_1) \frac{df_{\mathbf{k}_1}}{d\epsilon_{\mathbf{k}_1}},$$
$$\bar{D} = -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} P(\mathbf{k}_1)\, \Phi_D(\mathbf{k}_1) \frac{dF_{\mathbf{k}_1}}{dw_{\mathbf{k}_1}}, \tag{A44}$$

where $\Phi_C(\mathbf{k}_1)$, $\Phi_D(\mathbf{k}_1)$ are the solutions of the coupled equations

$$J[\Phi_C(\mathbf{k}_1)] + K[\Phi_D(\mathbf{k}_1)] = -(1/2\pi\lambda^2)S(\mathbf{k}_1)X,$$
$$L[\Phi_C(\mathbf{k}_1)] + M[\Phi_D(\mathbf{k}_1)] = -(1/2\pi\lambda^2)T(\mathbf{k}_1)Y. \tag{A45}$$

Statistical Mechanics of Finite Systems: Asymptotic Expansions. I. Two Petit Canonical Ensembles—(N, V, T) and (N, p, T) Systems*

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The statistical mechanics of a finite system differs from that of an infinite system in details of calculation, possession of additional variables and modification of fundamental relations, i.e., altered thermodynamics. Results become size-dependent, and ensemble-dependent. As examples of the general situation for finite systems, two petit canonical ensembles are examined here in relation to the grand canonical ensemble. The full asymptotic expansion is obtained for a one-phase region of one-component systems for each ensemble; all terms can be calculated within a grand canonical ensemble formalism. An analysis is made of both size dependence and the modified thermodynamics resulting from various approximations. The method presented represents both an approach to the study the general problems of the statical mechanical treatment of finite systems as well as a practical device for calculation in particular problems of small systems.

1. INTRODUCTION

MACROSCOPIC statistical mechanics and thermodynamics are disciplines generally defined for systems of unbounded size; statistical mechanics can also be formulated for finite systems but definite changes are involved including a modified thermodynamics. Assuming the same basic foundations relating ensemble averaging to observable quantities (ergodicity or *a priori* weighting of states), there are size-dependent corrections as well as modifications of concepts and relations as compared with the macroscopic results. The thermodynamics of finite systems has been examined extensively in a monograph of Hill.[1] The statistical mechanics of specific finite systems has been studied by Hill and others.[2] An extensive literature exists using statistical mechanical methods in application to many-particle systems[3] including application to finite systems such as atoms and nuclei. This work is the first of several in which we investigate some general aspects of the statistical mechanics of finite systems.

In this and a subsequent paper we have studied the ensemble dependence of finite system statistical mechanics by means of a full asymptotic expansion for the partition functions. In this work we consider general systems under assumptions which would macroscopically correspond to a one-phase region and would be expected to break down under conditions leading to a phase transition. With these assumptions, an asymptotic expansion is determined which is the basis for the analysis both of the size-dependent corrections as well as the modification of the thermodynamic relations. A general examination has not been made of the conditions of the breakdown of the asymptotic series which lead to a phase transition. However, in a following paper treating some applications of the method especially to a perfect gas obeying Bose–Einstein statistics, a modified contour leading to a valid asymptotic expansion through the region of the phase transition is found.

For a finite system the statistical mechanics becomes size-dependent and ensemble-dependent; results calculated using, for example, the grand canonical ensemble (GCE) differ from those using a petit canonical ensemble with constant volume (CVE) or the less common ensemble with pressure[4] (CPE). The ensemble used should correspond to the actual constraints of the system, fixed (z, V, T), (N, V, T), or (N, p, T) corresponding, respectively, to GCE, CVE, and CPE with N the number of particles, V the volume, p the pressure, and z the fugacity of a one-component system. Our approach is to present results for the finite system petit ensembles calculated via a GCE formalism, which latter is most convenient for calculation especially for quantum systems.

Under what conditions does statistical mechanics become ensemble-dependent, under what conditions size-dependent? If the systems are sufficiently small, the resulting statistical mechanics is both size-de-

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[1] T. L. Hill, *Thermodynamics of Small Systems, Parts 1 & 2* (W. A. Benjamin, New York, 1963 and 1964).

[2] T. L. Hill, J. Chem. Phys. **36**, 153 (1962); C. Domb, Proc. Phys. Soc. (London) **86**, 933 (1965).

[3] For review and other references see, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

[4] R. A. Sack, Mol. Phys. **2**, 8 (1959); T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), Chap. 3.

pendent and ensemble-dependent. In fact, if it is too small, statistical mechanics may not be useful. Even macroscopic systems under special conditions such as at critical points may become ensemble-dependent; the special conditions corresponding to extra-large fluctuations or cases of very long-range correlations. On the other hand, many of the treatments of finite size effects are in a range of smallness where fluctuations are negligible, but effects like surface, boundary condition, and inhomogeneity corrections, as well as effects of discreteness of parameters, etc. are used with ordinary macroscopic formalism. There can still be some significant ensemble-dependent effects, and in particular certain thermodynamic relations are changed from the macroscopic case. This case corresponds in our framework to the saddle-point approximation of the asymptotic expansion, retaining only the saddle-point contribution. The differences from the macroscopic case here are in addition to the size effects enumerated above, the sensitivity of relations involving the fluctuations in contrast to the insensitivity of the average quantities such as the energy and finally the breakdown of validity of certain relations like the identification of the Gibbs free energy per particle with the chemical potential (the difference vanishing, of course, in the macroscopic limit).

Comparison is repeatedly made then not only between results for different ensembles but with the above discussed level of approximation which is most accessible to macroscopic methods. Employing the CVE partition function $Z(N, V, T)$, we find the Helmholtz free energy F; the saddle-point value of this we denote F^*. Similarly, for the CPE partition function $W(N, p, T)$, we find the Gibbs free energy G; G^* represents its value at the maximum of the integrand; W being determined from Z as a Laplace transform; hence the integrand is real. An important point of emphasis is to observe the differences of F, F^*, G, and G^* from the macroscopic results and from each other. We do not strive for completeness in this analysis, merely indicating some of the differences made evident from our general results.

Although in this work we consider only the general derivation of the asymptotic expansion and some thermodynamic consequences thereof, we wish to indicate some applications which we have in mind. Some of these we hope to examine in detail in future publications. These results should have direct application to computer experiments on classical and quantum imperfect gases which necessarily involve a finite number of particles. Lebowitz and Percus[5] have developed a $1/N$ expansion for the classical gas with a finite range interaction. Only classical systems have been studied by these methods so far, but it is expected in the near future to extend the computer experiments to quantum systems.

An interesting and potentially important application of these methods should be to the study of such small quantum systems such as nuclei. Statistical mechanics methods are of interest to this problem for several purposes including:

(1) Problems involving nuclear reactions which can be regarded as finite-temperature situations.

(2) Certain kinds of nonanalytic results available directly with statistical mechanics perturbation theory and not with ordinary (zero-temperature) perturbation theory such as effects involving the shift of the Fermi surface[6]

(3) Finite-system analogs of phase transitions such as the connection of pairing effects to the superfluidity of nuclear matter.

GCE formalism represents the most straightforward finite-temperature extension of many-body perturbation theory as well as of Green's function methods. The GCE is certainly not the most appropriate ensemble for such finite systems; the question is how big and what types of errors are introduced by its use. Balian[7] has investigated some aspects of this problem in a particular case. We have here discussed a formulation which should allow results to be calculated with the GCE and then transposed into a more appropriate ensemble.

A most interesting application of this type of analysis of which we have barely scratched the surface, is to the question of phase transitions. Although this paper is limited to conditions remote from a phase transition, in our work on the Bose–Einstein condensation we have been able to extend

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[5] J. L. Lebowitz and J. K. Percus, Phys. Rev. **124**, 1673 (1961). Lebowitz and Percus obtained a $1/N$ expansion by inverting an expression for F^* in terms of F. The application is to classical systems with a finite range potential, but the method could be applied to quantum systems. They have a general expansion for pressure calculated from GCE as a functional of pressure calculated from CVE, but not a general expression of the inverse relation. The present work has an explicit expansion for the CVE results expressed in terms of GCE. This approach is likely to be more useful for treatment of quantum systems and appears to permit a more general analysis.

[6] (a) W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 41 (1960); (b) J. M. Luttinger and J. Ward, *ibid.* **118**, 1452 (1960); (c) R. Brout and F. Englert, *ibid.* **120**, 1519 (1960); (d) G. Horwitz, F. Englert, and R. Brout, *ibid.* **130**, 409 (1963); (e) R. Balian, C. Bloch, and C. de De Dominicis, Nucl. Phys. **25**, 529 (1961).

[7] R. Balian, Nucl. Phys. **13**, 594 (1959).

the method to include a phase transition. There are two types of problems of general interest. The first is relevant even for macroscopic systems and relates to the modifications which must be made in the statistical mechanics–thermodynamics analysis under conditions of a phase transition. The key factor is the influence of large fluctuations and/or long-range correlations. An example of such effect is the error in calculation of density fluctuations of a portion (even of macroscopic size) of a larger system for a critical region with the subsystem as a GCE the rest of the system treated as a reservoir. Klein and Tisza[8] have analyzed this question and we also deal with this in the treatment of the Bose–Einstein condensation. A second question of both theoretical and practical interest relates to the character of phase transitions for finite systems. Strictly, phase transitions are only sharply defined for infinite systems. The basic phenomena which they represent persists, however, for finite systems. Since all of the abrupt changes are rounded off, it becomes more difficult to define a transition temperature, the nature of a "discontinuity," etc. The questions as to what is the analogous behavior which becomes a phase transition for an infinite system and how the actual phase transition is approached as the system becomes larger are problems of interest.

The principal result of this work is a full asymptotic expansion for the CVE partition function $Z(N, V, T)$ and for the CPE partition function $W(N, p, T)$ for a general quantum system whose assumed properties are discussed below. A reference GCE is introduced whose partition function $\mathcal{Q}(z, V, T)$ appears in the contour integral for Z, where ζ is a (complex) variable whose real value corresponds to the fugacity. Assuming $\mathcal{Q}$ is an analytic function of ζ and that the fluctuations are normal, i.e., that the mean-square fluctuations in N are of order N, it follows that the asymptotic expansion exists. The analyticity of $\mathcal{Q}$ excludes a phase transition (cf. Yang and Lee[9]).

The asymptotic expansion for Z is obtained beginning with the usual saddle-point method. Then using $\log \zeta$ as the variable of integration rather than ζ we take a contour tangent to the steepest descent path at the saddle-point rather than the steepest descent path; for the conditions assumed the two contours yield the same asymptotic expansion. The asymptotic expansion involves two types of size dependence which it is convenient to separate. With $M_n\{N\}$ denoting the nth semi-invariant of particle number, M_2 is the mean-square fluctuations. Then assuming $M_2 = O(N)$ and $M_n/M_2 = o(N)$ along with the analyticity of $\mathcal{Q}$ in ζ, the asymptotic expansion exists. The expansion becomes an asymptotic power series in $1/N$ or $1/V$ if we further approximate the M_n by their infinite limiting values. However, it suffices that our order-of-magnitude assumptions are maintained for the two effects to be treated separately. A similar analysis can be made for the evaluation of the asymptotic expansion for W except that there we are dealing with a real integral.

In Sec. 2 we discuss some of the elementary ideas relating to the application of statistical mechanics to finite systems. In Sec. 3 the asymptotic expansion for Z is given. Appendix A is devoted to an evaluation of the integrals in the terms of the asymptotic expansion for Z. The expansion for W is obtained in Sec. 4 with some of the details worked out in Appendix B. Some further thermodynamic analysis is considered in Sec. 5.

2. THE PETIT CANONICAL ENSEMBLE WITH CONSTANT VOLUME: (N,V,T) SYSTEM

For a quantum system of N particles in thermodynamic equilibrium in a fixed volume V (we may wish to consider periodic boundary conditions instead) in contact with a heat bath at temperature T, the Helmholtz free energy $F(N, V, T)$ contains all relevant equilibrium information. The CVE partition function is

$$\begin{aligned} Z(N, V, T) &= \mathrm{Tr}^{(N)} \exp(-\beta H) \\ &= \sum_s \exp[-\beta E_s(N, V)], \end{aligned} \tag{1}$$

where the notation $\mathrm{Tr}^{(N)}$ means the trace in any convenient representation spanning the Hilbert space of eigenfunctions of the N-particle Hamiltonian, the index s labels the states, while the energies are functions of V (and any other extensive parameters) and depend on N.

For many-particle systems one can much more readily calculate with the GCE than with the canonical ensemble [except see Ref. 5(c) and 5(d)]. Linked cluster expansions, Green's functions, etc., are all more straightforward for the GCE. We introduce the GCE here only as an auxiliary device. For a Hamiltonian H which commutes with the number operator N_{op}, we can relate the grand partition function to the CVE partition function by

$$\mathcal{Q}(z, V, T) = \sum_{N=0}^{\infty} z^N Z(N, V, T). \tag{2}$$

[8] M. J. Klein and L. Tisza, Phys. Rev. **76**, 1861 (1949).
[9] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952); *ibid* **87**, 410 (1952).

Introducing Eq. (1) for Z and noting that the summation removes the restriction on N, we obtain

$$\mathcal{Q}(z, V, T) = \mathrm{Tr} \exp(-\beta H + \alpha N_{op}), \quad (3)$$

where

$$\alpha = \ln z \quad (4)$$

and the Tr is now an unrestricted trace. Z being the coefficient of z^N, we can obtain Z by the contour integral

$$Z(N, V, T) = \frac{1}{2\pi i} \int_c \frac{d\zeta}{\zeta^{N+1}} \mathcal{Q}(\zeta, V, T). \quad (5)$$

The contour C in the complex ζ plane encloses the pole at $\zeta = 0$ but no poles for $\mathcal{Q}$. This integral can be evaluated by the method of steepest descents determining an asymptotic expansion for Z.

In the steepest descents method one evaluates integrals of the form

$$\int_a^b dt\, h(t) e^{zg(t)}$$

for $g(t)$, $h(t)$ analytic and z large to be developed in an asymptotic series in $1/z$. Points were $g'(t) = 0$ determine the saddle points; since g is analytic, for Re $g(t)$ at point where $g'(t) = 0$ there are two perpendicular directions along one of which Re $g(t)$ has a maximum while along the other it has a minimum. The contour is chosen so that near the saddle point the contour goes along the path having for Im $g(t)$ constant and Re $g(t)$ going through its maximum at the saddle point. For z large enough the contribution of the integral comes principally from the neighborhood of the largest saddle point. The full asymptotic series is obtained if the steepest-descents path is followed from one limit to the other (provided limits lie on the steepest-descent path passing through saddle point). For many cases the full asymptotic series can be obtained by merely choosing a convenient contour passing through the saddle point tangent to the steepest descents curve; that is the method which we employ. That does in fact lead to correct results for the simple case involved here; provided there are no singular points too close to the chosen contour, such procedure should be perfectly satisfactory. In the usual application of the steepest-descent integrals one uses the procedure only to justify the usual macroscopic results with the significant contribution being that of the saddle point except near phase transitions. We extend the results here to a complete asymptotic expansion.

To put results into a convenient form for evaluating the integral we write Eq. (5) in the form

$$Z(N, V, T) = \frac{1}{2\pi i} \int_c \frac{d\zeta}{\zeta} \exp[Nf(\zeta)], \quad (6)$$

where

$$f(\zeta) = N^{-1} \log \mathcal{Q}(\zeta, V, T) - \log \zeta. \quad (7)$$

The function is analytic in the ζ-plane cut from the branch point at $\zeta = 0$ along the negative real axis. Thus the contour must be chosen so that $-\pi < \arg \zeta < \pi$. Under conditions where only a single stable phase exists in the thermodynamic limit, $f(\zeta)$ is an analytic function of ζ in that portion of the cut ζ-plane enclosed by C.[10] The contour C then crosses the real axis at a saddle point with the steepest-descents path perpendicular to the real axis. The contour by definition excludes poles of $\mathcal{Q}$, but it is necessary that the contour C stay within the radius of convergence of $f(\zeta)$ for the simple evaluation of the integrals. It is this feature which is violated when a pole in $\mathcal{Q}$ is too close to the saddle point. (Cf. the discussion of the steepest-descents evaluation for the Bose–Einstein condensation of Berlin and Ford.[11] Let us take

$$\zeta = e^y \quad (8)$$

for real u and v

$$y = u + iv, \qquad -\pi \leq v \leq \pi. \quad (8')$$

The saddle point is determined by

$$\left.\frac{\partial f}{\partial y}\right|_{\substack{u=\alpha_0 \\ u=0}} = \left(\frac{1}{N} \frac{\partial \log \mathcal{Q}}{\partial y} - 1\right) = 0, \quad (9)$$

where

$$\mu_0 = \alpha_0/\beta \quad (10)$$

corresponds to the chemical potential of the reference GCE such that

$$\frac{\partial \log \mathcal{Q}(e^{\alpha_0}, V, T)}{\partial \alpha_0} = \langle N \rangle = N. \quad (11)$$

This makes the usual macroscopic correspondence of GCE with the CVCE with N particles satisfying Eq. (11): as the defining equation for α_0. For a finite system the saddle-point parameter is not the chemical potential of the CVE. The second derivative verifies this path as a maximum direction for Re f.

$$\left.\frac{\partial^2 f}{\partial v^2}\right|_{u=\alpha_0} = i^2 \left[\frac{1}{N} \frac{\partial^2}{\partial \alpha_0^2} \log \mathcal{Q}(e^{\alpha_0}, V, T)\right] \quad (12)$$

$$= -\left[\frac{\langle N^2 \rangle - \langle N^3 \rangle}{N}\right]. \quad (13)$$

This quantity is negative-semidefinite; macroscop-

[10] The conditions of definition of the countour integral imply that C encloses no poles of $\mathcal{Q}$. If it also encloses no zero of $\mathcal{Q}$, $f(z)$ is analytic in the region of the cut plane enclosed by C.

[11] J. Ford and T. Berlin, J. Chem. Phys. **27**, 931 (1957). See also S. Katsura, Progr. Theoret. Phys. (Kyoto) **16**, 589 (1956).

ically this is proportional to the compressibility. Equation (13) follows on comparison with Eq. (1) if we regard $\mathcal{Q}(e^{\alpha_0}, V, T)$ the reference GCE corresponding to $z = e^{\alpha_0}$. The saddle point is sharply peaked if fluctuations in N are normal, i.e., proportional to N. We can then write Eq. (6) in the form

$$Z_N = \frac{1}{2\pi}\int_{-\pi}^{\pi} dv \exp\left[Nf_0 - \frac{N}{2}f_0''v^2 + R(v)\right], \quad (14)$$

where

$$f_0 = f(e^{\alpha_0}) \quad (15)$$

and

$$f_0'' = f''(e^{\alpha_0}), \quad (16)$$

and the remainder is

$$R(v) = N[f(e^{\alpha_0+iv}) - f_0 - f_0''], \quad (17)$$

which is expanded in view of the analyticity of f,

$$= N\sum_{r=1}^{\infty} A_{r+2}(iv)^{r+2}, \quad (18)$$

where

$$A_r = (1/r!)(\partial^r f_0/\partial\alpha_0^r). \quad (19)$$

The quantities

$$NA_r r! = M_r\{N_{op}\} \quad (20)$$

are the semi-invariants of the number operator

$$M_2 = \langle N_{op}^2\rangle - \langle N_{op}\rangle^2,$$
$$M_3 = \langle N_{op}^3\rangle - 3\langle N_{op}^2\rangle\langle N_{op}\rangle + 2\langle N_{op}\rangle^3, \quad \text{etc.} \quad (21)$$

the average $\langle\ \rangle$ being the average in the reference GCE. These results follow from Eqs. (3), (7), and (9).

The usual procedure is to argue that for f_0'' of order 1, the remainder term is small and can be neglected. The integral can then be evaluated introducing the change of variables

$$y = v(\tfrac{1}{2}f_0''N)^{\frac{1}{2}}. \quad (22)$$

The limits of the integral can then be taken to be infinity and this gives

$$Z(N, V, T) \approx (2\pi Nf_0'')^{-\frac{1}{2}}e^{Nf_0}. \quad (23)$$

The correction terms to F are then of $O(\log N)$ for $f_0'' = O(1)$. Let us now, instead of dropping $R(v)$, include it, in which case using Eqs. (14) and (22) we obtain

$$Z(N, V, T) = e^{Nf_0}(2\pi Nf_0'')^{-\frac{1}{2}}\frac{1}{\pi^{\frac{1}{2}}}\int_{-y_0(N)}^{y_0(N)} \exp[-y^2 + S(y)] \quad (24)$$

with

$$y_0(N) = (\tfrac{1}{2}Nf_0'')^{\frac{1}{2}}\pi \quad (25)$$

and

$$S(y) = \sum_{r=1}^{\infty}\left(\frac{A_{r+2}}{A_2}\right)\left(\frac{1}{NA_2}\right)^{\frac{1}{2}r}(iy)^{r+2}. \quad (26)$$

Expanding $\exp[S(y)]$ in y, regrouping the terms in powers of $1/N$ and carrying out the integrals term by term, we obtain the asymptotic expansion

$$Z(N, V, T) = (2\pi f_0''N)^{-\frac{1}{2}}e^{Nf_0}\sum_{n=0}^{\infty}\left(-\frac{1}{NA}\right)^n \times \sum_{\{m_r\}}\prod_r \frac{1}{m_r!}\left(-\frac{A_{r+2}}{A_2}\right)\frac{\Gamma(n + \sum m_r + \frac{1}{2})}{\Gamma(\frac{1}{2})}, \quad (27)$$
$$\sum rm_r = 2n.$$

For the details see Appendix A. In view of our assumptions that $2A_2 = M_2/N = O(1)$ and $A_r/A_2 \sim M_r/M_2 = o(N)$, we see that this satisfies the condition for an asymptotic expansion

$$\lim_{N\to\infty} N[Z(N, V, T) - S_\nu(N, V, T)] < \epsilon, \quad (28)$$

where

$$S_\nu(N, V, T) = (2\pi Nf_0'')^{-\frac{1}{2}}e^{Nf_0}\sum_{\nu=0}^{\nu}\left(\frac{-1}{NA_2}\right)^n \times \sum_{\{m_r\}}\prod_\gamma \frac{1}{m_r!}\left(\frac{-A_{r+2}}{A_2}\right)^{m_r}\frac{\Gamma(\nu + \sum m_r th)}{\Gamma(\frac{1}{2})}. \quad (29)$$

The expansion is not an asymptotic power series as the coefficients depend on N. In writing the asymptotic expansion we have dropped contributions to the integral of the order $\exp(-NA_2)$, which of course do not belong in an asymptotic expansion. In the limit of $N \to \infty$ the error is less than the magnitude of the first term not included in [Eq. (29)]; the best approximation is generally the one cut off at the smallest term.

This asymptotic expansion breaks down under two extreme conditions. Macroscopically if there is no phase transition f_0'' goes to zero as $T \to 0$; we cannot then use this asymptotic expansion. Referring back to Eq. (14), one could then simply expand the exponential, including now, in addition to $R(v)$ the term quadratic in v, an integrate over v. The asymptotic expansion also breaks down if the A_r are too large. This latter is macroscopically associated with a phase transition.

The Helmholtz free energy $F(N, V, T)$ is then

$$-\beta F = \ln Z(N, V, T), \quad (30)$$

which can be conveniently written

$$F = F^* + kT\log(2\pi)^{\frac{1}{2}} + \tfrac{1}{2}kT\log Nf_0'' - kT\log\left[1 + \sum_{n=1}^{\infty}\alpha_n\left(-\frac{1}{N}\right)^n\right], \quad (31)$$

where F^* corresponds to the Legendre transform of the grand potential

$$\Omega(\alpha_0, V, T) = -kT \log \mathcal{Q}(e^{\alpha_0}, V, T) \tag{32}$$

obtained from the reference GCE.

Thus

$$F^* = \Omega(\alpha_0, V, T) + kT\alpha_0 N \tag{33}$$

with

$$(\partial F^*/\partial \alpha_0)_N = 0 \tag{34}$$

and

$$\alpha_n = \left(\frac{1}{A_2}\right)^n \sum_{\{m_r\}} \prod_r \left(\frac{-A_{r+2}}{A_2}\right)^{m_r} \times \frac{1}{m_r!} \frac{\Gamma(n + \sum m_r + \frac{1}{2})}{\Gamma(\frac{1}{2})}. \tag{35}$$

From this expression for F we can derive all of the equilibrium properties of the system including the distribution function and higher moments or semi-invariants. As we have indicated it is convenient to examine separately F^* and $F - F^*$, since the latter involves much more radical departures from macroscopic character than the former.

3. THE PETIT CANONICAL ENSEMBLE WITH CONSTANT PRESSURE: (N, p, T) SYSTEM

We now consider an ensemble with constant pressure, a system of N particles in contact with a heat reservoir at temperature T in mechanical equilibrium with an external pressure p which may be zero for a self-bound system. The CPE partition function $W(N, p, T)$ is given by a Laplace transform of $Z(N, V, T)$. There are various ways of defining the normalization of the integral to make it dimensionless as discussed by Sack.[4] Sack suggests

$$W'(N, p, T) = \beta p \int_0^\infty dV \, \mathrm{Tr}^{(N,V)} \exp[-(\beta H + \beta p V)], \tag{36}$$

which corresponds to including the walls exerting the pressure and then dividing out the effect of the walls. For a self-bound system Hill's[4] definition is probably better where

$$W(N, p, T) = \frac{1}{v^*} \int_0^\infty dV \, \mathrm{Tr}^{(N,V)} \exp[-(\beta H + \beta p V)], \tag{37}$$

and a convenient choice of v^* would probably be $1/N$ times the zero-temperature value of V which maximizes the integrand. The symbol $\mathrm{Tr}^{(N,V)}$ is used to indicate explicitly that the representation refers to one with N particles normalized to a volume V. The Gibbs free energy is related to this by

$$e^{-\beta G} = W(N, p, T). \tag{38}$$

$W(N, p, T)$ can be expressed in the form

$$W(N, p, T) = \frac{1}{v^*} \int_0^\infty dV \, Z(N, V, T) e^{-\beta p V} \tag{39}$$

in which form we develop our asymptotic expansion. This integral can be rewritten in the form

$$W(N, p, T) = \frac{1}{v^*} \int_0^\infty dV \exp[Ng(V)] \tag{40}$$

with

$$g(V) = (1/N) \log Z(N, V, T) - \beta p V/N. \tag{41}$$

We now expand about the maximum point of the exponent.

$$g'(V_0) = \frac{1}{N}\left(\frac{\partial \log \mathcal{Q}}{\partial V} + \beta p\right) = 0 \tag{42}$$

and

$$g''(V_0) = \frac{1}{N} \frac{\partial^2 \log Z}{\partial V^2}\bigg|_{V=V_0}. \tag{43}$$

Equation (42) corresponds to the macroscopic relation between external pressure and $-\partial F/\partial V$ at the equilibrium volume. The condition of Eq. (43) corresponds macroscopically to the relation

$$\frac{1}{N}\frac{\partial p}{\partial V} \sim \frac{V}{N}\frac{1}{K_T} < 0, \tag{44}$$

where K_T is the isothermal compressibility. For the finite system the CVE here is not a real one but a reference ensemble. Equations (43) and (44) are obvious mechanical stability conditions for the reference CVE. That this is a sufficient condition to treat the CPE becomes clear; that it is necessary is less obvious. We assume Eq. (43) in any case.

Returning to the macroscopic situation K_T becomes anomolously large as a critical point is approached and the expansion breaks down for that case. Let us define

$$B_2 = -\tfrac{1}{2} g''(V_0) V_0^2, \tag{45}$$

a quantity which by assumption is positive and $O(1)$. The expansion of $g(V)$ and V_0 can then be written

$$g(V) = g(V_0) - B_2[(V - V_0)/V_0]^2 + T(V), \tag{46}$$

where $T(V)$ is the remainder term. Then

$$W(N, p, T) = \frac{1}{v^*} \int_0^\infty dV \times \exp\{N[g(V_0) - B_2(v - 1)^2 + T(v)]\}. \tag{47}$$

Assuming we can neglect the remainder for a large enough system we have with $v = V/V_0$, $g(V_0) = g_0$, $V^* = Nv^*$

$$W(N, p, T) = N\frac{V_0}{V^*}\int_0^\infty dv \exp\{N[g_0 - B_2(v-1)^2]\} \quad (48)$$

$$= \frac{V_0}{V^*}N\left(\frac{NB_2}{2}\right)^{\frac{1}{2}}e^{Ng_0}\int_{-(\frac{1}{2}NB_2)^{\frac{1}{2}}}^\infty dv\, e^{-\frac{1}{2}u^2}, \quad (49)$$

and taking the limit as infinity we obtain

$$= [(2\pi)^{\frac{1}{2}}/NB_2]N(V_0/V^*)e^{Ng_0}. \quad (50)$$

Introducing the corresponding approximation for Z,

$$X(N, V, T) = e^{-\beta F^*}(2\pi N f_0'')^{-\frac{1}{2}}. \quad (51)$$

We then have

$$W(N, p, T) = e^{-\beta(F^*+pV_0)}(V_0/V^*)(f_0''B_2)^{-\frac{1}{2}}. \quad (52)$$

Let us evaluate the coefficient of the exponent using the macroscopically valid relations

$$f_0'' = (\langle N^2\rangle - \langle N\rangle^2)/N \quad (53)$$

and

$$\langle N^2\rangle - \langle N\rangle^2 = (N/V_0)NkTK_T, \quad (54)$$

$$B_2 = \frac{V_0 2}{kT}\frac{1}{N}\left(\frac{\partial p}{\partial V}\right)_N = \frac{V_0}{N}\frac{1}{K_T}kT. \quad (55)$$

From these equations we find

$$W(N, p, T) = e^{-\beta G^*}(V_0/V^*) \quad (56)$$

with

$$G^*(N, p, T) = F^*(N, V_0, T) + pV_0. \quad (57)$$

If we are near a phase transition it is not correct generally to compound the separate asymptotic expansions; one must expand simultaneously in both variables and find negative-definite conditions for the quadratic form. As we are assuming in this work that we are far from a phase transition, that should not be significant in this case.

We have indicated the development of a full asymptotic expansion for the CPE in Appendix B. This has been left to the Appendix since the conditions of validity of such expansion are less clearly understood by us than for the CVE.

4. THERMODYNAMIC CONSEQUENCES

Resuming the discussion of the thermodynamics of finite systems, we compare the thermodynamic consequences of different ensembles and different approximations to them. The respective thermodynamic potentials contain all relevant information for calculation of all thermodynamic quantities including fluctuations, provided the ensemble is matched to the constraints. This discussion is completely in the context of equilibrium only.

The discussion proceeds from the reference GCE whose average particle number and volume are the same as the fixed parameters of the CVE. We first discuss results derived from the grand potential $-\beta\Omega(\alpha, V, B)$ and F^* and G^*, the saddle-point values of F and G corresponding to the respective Legendre transforms of

$$-\beta F^*(N, V, T) = -\beta\Omega(\alpha, V, B) - \alpha[\partial(-\beta\Omega)/\partial\alpha]_{V,B}, \quad (58)$$

$$[\partial(-\beta\Omega)/\partial\alpha]_{V,B} = N,$$

and

$$-\beta G^*(N, p, B) = -\beta\Omega(\alpha, V, B) - \alpha[\partial(-\beta\Omega)/\partial\alpha]_{V,B} + V[\partial(-\beta\Omega)/\partial V]_{\alpha,B}, \quad (59)$$

$$[\partial(-\beta\Omega)/\partial\alpha]_{V,B} = N, \qquad [\partial(-\beta\Omega)/\partial V]_{\alpha,\beta} = +\beta p.$$

The thermodynamic fundmental equation for the GCE is given by

$$-\beta\Omega(\alpha, V, B) = \log \mathrm{Tr}\exp(-\beta H + \alpha N_{op}), \quad (60)$$

where we assume we are able to evaluate the right side of the equation by statistical mechanical calculation. The variables canonical to α, V, B are given by differentiating the average energy

$$U = \langle H\rangle_{\mathrm{GCE}} = (\partial\beta\Omega/\partial\beta)_{V,\alpha}. \quad (61)$$

The pressure is given by

$$+\beta p = [\partial(-\beta\Omega)/\partial V]_{\alpha,\beta} \quad (62)$$

and the average particle number

$$\langle N_{op}\rangle = [\partial(-\beta\Omega)/\partial\alpha]_{\beta,V}. \quad (63)$$

Introducing the eigenvalues of H: $E(s, N)$ and of N_{op}: N the density function

$$p(s, N) = \{\exp[-\beta E(s, N)] + \alpha N\}/\sum_s\sum_N \times \exp[-\beta E(s, N)] + \alpha N \quad (64)$$

leads to an entropy which corresponds to the relation

$$S = k\sum_s\sum_N p(s, N)\log p(s, N). \quad (65)$$

This is equivalent to

$$-\beta\Omega(\alpha, V, B) = -\beta U - ks + \alpha(N) = (\partial\Omega/\partial T)_{\mu,V}. \quad (66)$$

The fluctuations of energy, particle number, pressure can be calculated by further differentiation of $-\beta\Omega$ with respect to α, $-\beta$, and V. The above relations are identical with those of macroscopic

thermodynamics. For a finite system in contact with a particle reservoir at chemical potential $\mu = \alpha kT$ a heat bath at temperature $T = (k\beta)^{-1}$ in a fixed volume, the above results would lead to correct results.

Let us now proceed to some relations which are not satisfied by the finite system even though the constraints are the above. All thermodynamic extensive variables of order N: Ω, U, (N), S; in extreme cases they could in fact be even of order N^2. The result of retension of terms like surface and boundary condition corrections is that the identification of Ω with $-pV$ is no longer valid. We could define a quantity

$$p^* = -\Omega/V, \tag{67}$$

where $p - p^*$ is a quantity which vanishes in the macroscopic limit. p^* does not have the usual meaning of pressure for the system. Hill[1] discusses a sense in which this is a pressure in relation to a particular grand ensemble made up of duplicates of our small system. It is p^* rather than p whose leading order contribution to the quantity $\partial p^*/\partial V$ is proportional to fluctuations in N; on the other hand, the compressibility is related to $\partial p/\partial V$. Thus one of the relationships which is not valid for a finite system is the relation we have used in Eq. (54) relating compressibility and fluctuations in N.

According to our analysis the quantities F^* and G^* which we have introduced in this section via Legendre transforms are the leading contributions to F and G. There is a range where the kind of size corrections not ignored in calculation of F^* and G^* is significant even though further corrections are negligible. In that case the thermodynamic relations calculated from these thermodynamic potentials agree with those calculated from Ω. Thus

$$\begin{aligned} U &= \left[\frac{\partial(-\beta\Omega)}{\partial(-\beta)}\right]_{V,\alpha} \\ &= \left[\frac{\partial(-\beta F^*)}{\partial(-\beta)}\right]_{V,N} = \left[\frac{\partial(-\beta G^*)}{\partial(-\beta)}\right]_{p,N} \end{aligned} \tag{68}$$

and

$$\beta p = \left[\frac{\partial(-\beta\Omega)}{\partial B}\right]_{\beta,\alpha} = \left[\frac{\partial(-\beta F)}{\partial V}\right]_{\beta,N}. \tag{69}$$

Consequently in this approximation the specific heats and conpressibilities are also in agreement. To summarize: If the asymptotic expansion is valid and $1/N$ or $1/V$ terms are negligible but not surface contributions, effects of boundary conditions or discreteness of levels, most macroscopic thermodynamic relations hold. Even in this approximation one must note differences of some importance such as $p^* \neq p$, on the same basis

$$G^*/N \neq (\partial G^*/\partial N) = \mu \text{ the chemical potential.} \tag{70}$$

A second important difference is that one cannot really separate a small part of this system for independent analysis; this disturbs the system as a whole. This can hold even for macroscopic systems as we have mentioned in the Introduction. We treat this matter in some detail in relation to the Bose–Einstein condensation in a following paper.

Proceeding to higher-order corrections we return to the asymptotic expansions for F and G obtained in the previous sections. For an (N, V, T) system we obtain

$$U_1 = [\partial(-\beta F)/\partial(-\beta)] = U + \delta U_1 \tag{71}$$

and

$$\beta p_1 = \beta p + \delta(\beta p_1), \tag{72}$$

$$\beta\mu_1 = \alpha + \delta(\beta\mu), \tag{73}$$

where $\delta U_1/N$, δp, $\delta\beta\mu$ are given by derivatives of $F - F^*$ in the expression of Eq. (31); the leading order of these quantities is of order $1/N$. Similarly we have for an (N, p, T) system

$$U_2 = \partial(-\beta G)/\partial(-\beta) = U + \delta U_2, \tag{74}$$

$$V = \partial(-\beta G)/\partial(\beta p) = \partial(-\beta G^*)/\partial\beta p + \delta V, \tag{75}$$

$$\beta\mu_2 = \alpha + \delta(\beta\mu)_2. \tag{76}$$

Here again $\delta U_2/V$, $\delta V/V$, $\delta\beta U_2$ are derivatives of $G - G^*$ beginning with terms of order $1/N$.

The entropy is related to F and G just as for macroscopic system

$$-\beta F = -\beta U_1 + kS_1, \tag{77}$$

$$-\beta G = -\beta U_1 - \beta F\langle V\rangle + kS_2, \tag{78}$$

which are again equivalent to the definition of entropy by

$$S = k \operatorname{Tr} p \log p \tag{79}$$

with the appropriate density function.

With the $1/N$ terms significant the results for different ensembles are completely nonequivalent. With these terms significant, fluctuations can be expected to be large enough so that average values are not an adequate measure of the state of a system.

5. SUMMARY AND EXTENSION

In applying statistical mechanics to finite systems there are various modifications of the usual theory in addition to the existence of explicit corrections to the macroscopic theory. Let us review those factors within the scope of the analysis of this paper which treats only conditions of thermodynamically stable one-phase regions. The conditions imposed to guarantee the latter are the assumption of analyticity of the reference grand partition function in the complex fugacity within a domain containing the contour for the integral of $Z(N, V, T)$, and that the mean-square fluctuations in N are of order N. Then, for sufficiently large N and V, asymptotic expansions for both CVE and CPE are obtained.

It was convenient to separate the analysis into two steps: (i) $1/N$ terms negligible but surface terms, etc. retained; (ii) $1/N$ or smaller terms significant. In the first case most of the macroscopic thermodynamic relations hold. The principal exceptions are those related to the extensive property of the energy and thermodynamic potentials. Such relations as between compressibility and number fluctuations are violated by terms of the order of $V^{1/3}$. Subdivision of system thermodynamically becomes problematical. If $1/N$ terms become important the nature of the changes become much more radical.

In a subsequent paper we examine the extension to a finite system which macroscopically undergoes a Bose–Einstein condensation. The extension of the method used here involves the problem of finding a contour leading to an asymptotic expansion even when the saddle point approaches a pole in the grand partition function.

In the continuation of our study we deal first as already mentioned with the extension to system undergoing a phase transition. The interacting Bose gas has engaged our attention in this respect and this has been under study. Other applications which we contemplate examining are finite system, Fermi liquid theory, and the theory of imperfect quantum and classical gases. Furthermore, it is expected that an analysis of perturbation theory and Green's function methods be made with the view of their use in evaluating the terms of the expansion which we have derived here.

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APPENDIX A. INTEGRALS FOR CVE PARTITION FUNCTION

In Eq. (24) we have an integral expression for $Z(N, V, T)$ which we write here as

$$Z_N = [e^{Nf_0}/(2\pi N f_0'')^{\frac{1}{2}}]I(N). \tag{A1}$$

In this Appendix the purpose is to evaluate $I(N)$ as an asymptotic expansion, where

$$I(N) = \frac{1}{\pi^{\frac{1}{2}}} \int_{-y_0(N)}^{y_0(N)} dy\, e^{-y^2 + S(y)}. \tag{A2}$$

Using the relation

$$\exp\left[\sum_{n=1}^{\infty} a_n \left(\frac{1}{N}\right)^{\frac{1}{2}n}\right] = \sum_{n=1}^{\infty} b_n \left(\frac{1}{N}\right)^{\frac{1}{2}n}, \tag{A3}$$

$$b_n = \sum_{\{m_r\}}{}' \prod_r (a_r)^{m_r}/m_r! \tag{A4}$$

follows.

The sum over m_r is over all sets of m_r such that

$$\sum r m_r = n. \tag{A5}$$

With the form of $S(y)$ from Eq. (26) we have

$$a_r = (A_{r+2}/A_2)(iy)^{r+2}(1/A_2)^r, \tag{A6}$$

whence

$$b_r = \sum_{\{m_r\}}{}' \prod_r \left(\frac{A_{r+2}}{A_2}\right)^{m_r} \frac{1}{m_r!} (iy)^{r+2}. \tag{A7}$$

All odd terms in y vanish and we obtain

$$I(N) = \frac{1}{\pi^{\frac{1}{2}}} \int_{-y_0(N)}^{y_0} e^{-y^2} \sum_{n=0}^{\infty} \left(\frac{1}{NA_2}\right)^{\frac{1}{2}n} \sum_{\{m_r\}} \frac{1}{m_r!} \times \left(\frac{A_{r+2}}{A_2}\right)^{m_r} (iy)^{2(n+\sum m_r)} \left(\sum r m_r = 2n\right). \tag{A8}$$

Interchanging sum and integral and noting that

$$\int_{-y_0}^{y_0} y^{2\nu} e^{-y^2}\, dy = \gamma\{\nu, y_0^2\} \tag{A9}$$

are incomplete gamma functions where in Eq. (A8) the ν are half integral, thus

$$\nu = n + \sum m_r + \tfrac{1}{2}. \tag{A10}$$

Thus we obtain for $I(N)$

$$I(N) = \frac{1}{\pi^{\frac{1}{2}}} \sum_{n=0}^{\infty} \left(-\frac{1}{N}\right)^n \left(\frac{1}{A_2}\right)^n \sum_{\{m_r\}} \frac{1}{m_r!} \left(\frac{-A_{r+2}}{A_2}\right)^{m_r} \times \gamma(n + \sum m_r + \tfrac{1}{2}, y_0^2). \tag{A11}$$

Asymptotically for large y_0 the incomplete gamma function is related to the complete gamma function by

$$\gamma(\tau + \tfrac{1}{2}, y_0^2) = \Gamma(\tau + \tfrac{1}{2}) - y_0^{2\nu} e^{-y_0^2} \times \sum_{m=0}^{M-1} \frac{(-1)^m \Gamma(1 - \tau - \frac{1}{2} + m)}{y_0^{2m} \Gamma(\frac{1}{2})} + O(L^{-2M}). \tag{A12}$$

Thus the asymptotic form of the quantity Z is

$$Z_N \approx e^{Nf_0}(2\pi N f_0'')^{-\frac{1}{2}} \sum_{n=0}^{\infty} \alpha_n \left(\frac{-1}{NA_2}\right)^n, \quad \text{(A13)}$$

with

$$\alpha_n = \sum_{\{m_r\}} \frac{1}{m_r!} \left(\frac{A_{r+2}}{A_2}\right) \frac{\Gamma(n + \sum m_r + \frac{1}{2})}{(\Gamma')} \quad (\textstyle\sum r m_r = 2n). \quad \text{(A14)}$$

This asymptotic expansion can also be obtained by an alternative procedure to be found in Morse–Feshbach[12] in detail. A new real variable w is introduced with the steepest descents contour evaluated by evaluating the integral for Z in the form

$$Z_N = \frac{1}{2\pi} \int dw \frac{dz}{dw} e^{Nf_0 - Nw^2}, \quad \text{(A15)}$$

$$f = f_0 - w^2(z). \quad \text{(A16)}$$

Inverting Eq. (A16) we can evaluate the integral asymptotically. Morse–Feshbach gives a result which is equivalent to the form we have obtained although it is less explicitly evaluated.

APPENDIX B. FULL ASYMPTOTIC EXPANSION FOR CPE

In Eq. (48) we have an integral for the CPE partition function $W(N, p, T)$. The remainder term $T(V) = T(V_0 v)$ can then be expanded

$$NT(v) = N \sum_{n=3} \frac{V_0^n}{n!} \left(\frac{\partial^n \ln Z_N}{\partial V^n}\right)_{V=V_0} (v-1)^n. \quad \text{(B1)}$$

Introducing the variable

$$u = (v-1)(NB_2)^{\frac{1}{2}} \quad \text{(B2)}$$

we obtain the expansion

$$NV(u) = \sum_{n=1}^{\infty} \left(\frac{1}{NB_2}\right)^{\frac{1}{2}n} \frac{1}{(n+2)!} \frac{1}{B_2} \times V_0^{n+2} \left(\frac{\partial^{n+2} \ln Z}{\partial V^{n+2}}\right)_{V=V_0}. \quad \text{(B3)}$$

Inserting this in the integral we obtain in a manner similar to that of Appendix A with

$$B_n = \frac{V_0^n}{n!} \frac{\partial^n \ln Z_N}{\partial V^n}\bigg|_{V=V_0}, \quad \text{(B4)}$$

$$W(N, p, T) = \frac{e^{-\beta G^*} V_0}{v^*} \int_{-(NB_2)^{\frac{1}{2}}}^{\infty} du\, e^{-u^2} \sum_{n=0}^{\infty} \left(\frac{1}{NB_2}\right)^n \times \sum_{\{m_r\}}^{\infty} \prod \left(\frac{B_{r+2}}{B_2}\right)^{m_r} \frac{1}{m_r!} u^{n+\sum m_r 2} (\textstyle\sum r m_r = n) \quad \text{(B5)}$$

and asymptotically

$$\cong e^{-\beta G^*} \frac{V_0}{v^*} \sum_n \left(\frac{1}{NB_2}\right)^n \times \sum_{\{m_r\}}{}' \prod \left(\frac{B_{r+2}}{B_2}\right)^{m_r} \frac{1}{m_r!} \frac{\Gamma(n + \sum m_r + \frac{1}{2})}{\Gamma(\frac{1}{2})} \quad \text{(B6)}$$

since

$$\int_{-\infty}^{-(NB)^{\frac{1}{2}}} du\, e^{-u^2} u^{n+2\sum m_r} \sim e^{-N}, \quad \text{(B7)}$$

which is asymptotically zero.

[12] See, for example, P. M. Morse, and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1963), Sec. 4.6; E. T. Copson, *Asymptotic Expansions* (Cambridge University Press, Cambridge, England, 1965).

A Class of Sum Rules with Application to Nondegenerate Perturbation Theory

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The main results of this paper are: (1) The derivation of a class of sum rules. These rules are then applied to operators $H(\alpha)$, which depend on a parameter α and have eigenvalues $E_n(\alpha)$. Writing $A_n(\alpha) \equiv H(\alpha) - E_n(\alpha)$, these rules give the matrix elements of $\partial^N A_n(\alpha)/\partial\alpha^N$ with respect to the eigenfunctions of $H(\alpha)$ in terms of matrix elements of lower derivatives and the eigenvalues $E_n(\alpha)$. (2) An explicit series expression for the Nth-order eigenvalue correction, due to a perturbation, directly in terms of the unperturbed eigenfunctions and eigenvalues. This expression seems a convenient one to use, since it does not involve eigenfunction corrections. An expression is also obtained for the eigenfunction corrections, but this is in less convenient form.

1. INTRODUCTION

IN an earlier paper,[1] we considered the eigenvalue equation

$$A_m(\alpha)\Psi_{ml}(\alpha) = 0, \qquad A_m(\alpha) \equiv H(\alpha) - E_m(\alpha), \quad (1.1)$$

where m labels the eigenvalues $E_m(\alpha)$ of a Hermitian operator $H(\alpha)$ and l distinguishes between eigenfunctions belonging to the same eigenvalue. Completeness and orthonormality of these eigenfunctions are assumed. α is a vector whose components are the parameters of interest in the problem. By differentiation with respect to these components, it was shown how certain known results (virial theorem, hypervirial theorems, the effective mass sum rule in solid-state physics) could be derived very simply. In most cases it was in fact possible to extend the conventional results and obtain useful generalizations.

Some of the equations found have striking similarities with perturbation theory. For example, after two differentiations with respect to one parameter only, one finds[1] the "second sum rule"

$$\langle ml'| \frac{\partial^2 A_m(\alpha)}{\partial\alpha^2} |ml\rangle = 2 \sum_{\substack{m'',l'' \\ (m''\neq m)}} \frac{\langle ml'| \frac{\partial A_m(\alpha)}{\partial\alpha} |m''l''\rangle\langle m''l''| \frac{\partial A_m(\alpha)}{\partial\alpha} |ml\rangle}{E_{m''}(\alpha) - E_m(\alpha)}, \quad (1.2)$$

where it is understood that, if the eigenvalue spectrum contains a discrete part and a continuous part, the sums must include an integration over the continuum. In (1.2), α is not necessarily an expansion parameter, and matrix elements are taken with respect to the exact eigenfunctions of the full Hamiltonian. This second sum rule is, therefore, not a perturbation theory result, although it looks like one at first sight. It was remarked[1] that higher-order sum rules can be used to extend the work of Epstein[2] on the perturbation theory formalism. We are indebted to Professor S. T. Epstein for drawing our attention to Aizu's work[3] in which this is done in a limited way by using the first few sum rules. The more general formulation has proved more difficult than first anticipated, but the result is of interest in giving explicit general sum rules of the Nth order (i.e., obtained by N-fold differentiation). An explicit expression for the Nth-order correction to the energy in nondegenerate perturbation theory is then easily obtained. In fact, the method gives the energy corrections directly in terms of matrix elements of the perturbation between the unperturbed wavefunctions, thus eliminating the need for the intermediate calculation of corrections to the wavefunctions.[4,5] Expressions for the coefficients in the expansions of the corrections to the wavefunctions are, however, also obtained [Eq. (3.22)]. These results are given for completeness, but do not have the basically simple structure of our results for the energy corrections. We regard the Nth-order sum rule and the convenient series expression for the Nth-order energy correction [Eq. (3.4)] in terms of zero-order wavefunctions as the main results of this paper.

No doubt, the results obtained can be shown to be equivalent to the many alternative formulations of perturbation theory, e.g., in terms of propagators,[4] but we do not report on these relationships here. However, we can remark that the results appear

[1] D. J. Morgan and P. T. Landsberg, Proc. Phys. Soc., (London) 86, 261 (1965).

[2] S. T. Epstein, Am. J. Phys., 22, 613 (1954).

[3] K. Aizu, J. Math. Phys. 4, 762 (1963).

[4] A. Dalgarno, *Pure and Applied Physics, 1-1, Quantum Theory*, D. R. Bates, Ed. (Academic Press Inc., New York 1961), pp. 171-208.

[5] J. O. Hirschfelder, W. B. Brown, and S. T. Epstein, *Advances in Quantum Chemistry* (Academic Press Inc., New York, 1964), Vol. 1.

to be more convenient than those given in terms of commutator brackets,[6] or projection operators,[7] elegant though these are.

2. THE MAIN THEOREM

For simplicity, attention is confined to nondegenerate situations in the sense that the suffix l is omitted in equations like (1.2). Also, only one parameter is considered. Differentiating (1.1) N_0 times, one finds

$$(E_m - E_{n_0})\langle n_0|\, D^{N_0}\, |m\rangle = \sum_{N_1=0}^{N_0-1} \binom{N_0}{N_1} \sum_{n_1} \langle n_0|\, \frac{\partial^{N_0-N_1} A_m}{\partial\alpha^{N_0-N_1}}(\alpha)\, |n_1\rangle\langle n_1|\, D^{N_1}\, |m\rangle \tag{2.1}$$

with

$$D^N \equiv \partial^N/\partial\alpha^N. \tag{2.2}$$

Equation (2.1) is a recurrence relation for the nondiagonal matrix elements of D^r; if $n_1 \neq m$ one can substitute for $\langle n_1|\, D^{N_1}\, |m\rangle$ using equation (2.1) itself with N_0 and n_0 replaced by n_0 and n_1 respectively. The solution of this relation for the nondiagonal matrix elements of D^r in terms of the diagonal matrix elements of D^s $(s < r)$, the matrix elements of the $\partial^t A_m(\alpha)/\partial\alpha^t$, and the eigenvalues $E_n(\alpha)$ comprise the main mathematical content of this paper.

Theorem: With the notation (2.2) and for positive integral N_0,

$$(E_m - E_{n_0})\langle n_0|\, D^{N_0}\, |m\rangle = \sum_{i=0}^{N_0-1} \binom{N_0}{i} Y_{n_0 m}^{N_0-i} \langle m|\, D^i\, |m\rangle, \tag{2.3}$$

where

$$Y_{n_0 m}^{N_0} = \langle n_0|\, \frac{\partial^{N_0} A_m}{\partial\alpha^{N_0}}\, |m\rangle + \sum_{i=1}^{N_0-1} \sum_{N_1=i}^{N_0-1} \sum_{N_2=i-1}^{N_1-1} \cdots \sum_{N_i=1}^{N_{i-1}-1} \frac{N_0!}{N_i! \prod_{l=0}^{i-1} (N_l - N_{l+1})!} \times \cdots$$

$$\times \sum_{\substack{n_1,\cdots,n_i \\ (\neq m)}} \frac{\langle n_0|\, \frac{\partial^{N_0-N_1} A_m}{\partial\alpha^{N_0-N_1}}\, |n_1\rangle\langle n_1|\, \frac{\partial^{N_1-N_2} A_m}{\partial\alpha^{N_1-N_2}}\, |n_2\rangle \cdots \langle n_{i-1}|\, \frac{\partial^{N_{i-1}-N_i} A_m}{\partial\alpha^{N_{i-1}-N_i}}\, |n_i\rangle\langle n_i|\, \frac{\partial^{N_i} A_m}{\partial\alpha^{N_i}}\, |m\rangle}{(E_m - E_{n_1})(E_m - E_{n_2}) \cdots (E_m - E_{n_i})}. \tag{2.4}$$

Proof: To prove this theorem, it is convenient to introduce the notation

$$B_{ik}^{NM} \equiv \binom{N}{M} \langle i|\, \frac{\partial^{N-M} A_m}{\partial\alpha^{N-M}}\, |k\rangle,$$
$$C_{ik}^{NM} \equiv B_{ik}^{NM}/(E_m - E_k), \tag{2.5}$$

and to put

$$(E_m - E_{n_0})\langle n_0|\, D^{N_0}\, |m\rangle = X_{n_0 m}^{N_0} + Y_{n_0 m}^{N_0}, \tag{2.6}$$

where diagonal matrix elements of D^r $(r = 1, 2, \cdots, N_0)$ occur only in the X term.

A. Recurrence Relation for the Y's

Separate recurrence relations for the X's and the Y's are obtained by substituting (2.6) on both sides of (2.1). The recurrence relation for the Y's is then

$$Y_{n_0 m}^{N_0} = B_{n_0 m}^{N_0 0} + \sum_{N_1=1}^{N_0-1} \sum_{\substack{n_1 \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} Y_{n_1 m}^{N_1} \qquad (N_0 = 1, 2, \cdots). \tag{2.7}$$

Substituting for $Y_{n_1 m}^{N_1}$ in this equation, by using the equation itself, one finds

$$\begin{aligned} Y_{n_0 m}^{N_0} &= B_{n_0 m}^{N_0 0} + \sum_{N_1=1}^{N_0-1} \sum_{\substack{n_1 \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} B_{n_1 m}^{N_1 0} + \sum_{N_1=2}^{N_0-1} \sum_{N_2=1}^{N_1-1} \sum_{\substack{n_1, n_2 \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} C_{n_1 n_2}^{N_1 N_2} Y_{n_2 m}^{N_2} \\ &= B_{n_0 m}^{N_0 0} + \sum_{N_1=1}^{N_0-1} \sum_{\substack{n_1 \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} B_{n_1 m}^{N_1 0} + \sum_{N_1=2}^{N_0-1} \sum_{N_2=1}^{N_1-1} \sum_{\substack{n_1, n_2 \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} C_{n_1 n_2}^{N_1 N_2} B_{n_2 m}^{N_2 0} \\ &\quad + \sum_{N_1=3}^{N_0-1} \sum_{N_2=2}^{N_1-1} \sum_{N_3=1}^{N_2-1} \sum_{\substack{n_1, n_2, n_3 \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} C_{n_1 n_2}^{N_1 N_2} C_{n_2 n_3}^{N_2 N_3} Y_{n_3 m}^{N_3} \\ &= \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &= B_{n_0 m}^{N_0 0} + \sum_{j=1}^{N_0-1} \sum_{N_1=j}^{N_0-1} \sum_{N_2=j-1}^{N_1-1} \cdots \sum_{N_j=1}^{N_{j-1}-1} \sum_{\substack{n_1, n_2, \cdots, n_j \\ (\neq m)}} C_{n_0 n_1}^{N_0 N_1} C_{n_1 n_2}^{N_1 N_2} \cdots C_{n_{j-1} n_j}^{N_{j-1} N_j} B_{n_j m}^{N_j 0}. \end{aligned} \tag{2.8}$$

This is the required solution (2.4).

[6] G. L. Goodman, J. Chem. Phys. **43**, S 268 (1965).
[7] P. O. Löwdin, J. Math. Phys. **3**, 969 (1962).

B. Recurrence Relation for the X's

The recurrence relation for the X's [also obtainable from (2.1)] is

$$X^{N_0}_{n_0 m} = \sum_{N_1=1}^{N_0-1} B^{N_0 N_1}_{n_0 m} \langle m|\ D^{N_1}\ |m\rangle + \sum_{N_1=1}^{N_0-1} C^{N_0 N_1}_{n_0 n_1} X^{N_1}_{n_1 m}. \tag{2.9}$$

Generating the solution as before, one finds

$$X^{N_0}_{n_0 m} = \sum_{N_1=1}^{N_0-1} B^{N_0 N_1}_{n_0 m} \langle m|\ D^{N_1}\ |m\rangle + \sum_{j=2}^{N_0-1} \sum_{N_1=j}^{N_0-1} \sum_{N_2=j-1}^{N_1-1} \cdots \sum_{N_j=1}^{N_{j-1}-1} \sum_{\substack{n_1, n_2, \cdots, n_{j-1} \\ (\neq m)}} C^{N_0 N_1}_{n_0 n_1} C^{N_1 N_2}_{n_1 n_2} \cdots C^{N_{j-2} N_{j-1}}_{n_{j-2} n_{j-1}} B^{N_{j-1} N_j}_{n_{j-1} n_j} \langle m|\ D^{N_j}\ |m\rangle. \tag{2.10}$$

Now consider the coefficient of $\langle m|\ D^M\ |m\rangle$ in (2.10), where M is fixed. It is

$$B^{N_0 M}_{n_0 m} + \sum_{j=2}^{N_0-M} \sum_{N_1=j}^{N_0-1} \cdots \sum_{N_{j-1}=2}^{N_{j-2}-1} \sum_{\substack{n_1, n_2, \cdots, n_{j-1} \\ (\neq m)}} C^{N_0 N_1}_{n_0 n_1} C^{N_1 N_2}_{n_1 n_2} \cdots C^{N_{j-2} N_{j-1}}_{n_{j-2} n_{j-1}} B^{N_{j-1} M}_{n_{j-1} m}. \tag{2.11}$$

We have here replaced the first upper limit by $N_0 - M$. Since by (2.10) $N_q \geq N_{q+1} + 1$, the largest value of j (for given N_0 and M) is obtained when each N_q has the value $N_{q+1} + 1$. Then

$$N_{j-1} = N_0 - (j-1) = M + 1, \text{ i.e., } \quad j = N_0 - M. \tag{2.12}$$

Observe next that, for similar reasons, the sum over N_{j-1} can start only at $M + 1$, the sum over N_{j-2} at $M + 2$, $\cdots$, the sum over N_2 at $j + M - 2$, and the sum over N_1 at $j + M - 1$. Next, change to new dummy suffices,

$$N^1_q \equiv N_q - M \qquad (q = 1, 2, \cdots, j-1). \tag{2.13}$$

Equation (2.11) then becomes

$$B^{N_0 M}_{n_0 m} + \sum_{j=2}^{N_0-M} \sum_{N_1=j-1}^{N_0-M-1} \cdots \sum_{N_{j-1}=1}^{N_{j-2}-1} \sum_{\substack{n_1, \cdots, n_{j-1} \\ (\neq m)}} \binom{N_0}{M} C^{N_0-M N_1}_{n_0 n_1} C^{N_1 N_2}_{n_1 n_2} \cdots C^{N_{j-2} N_{j-1}}_{n_{j-2} n_{j-1}} B^{N_{j-1} 0}_{n_{j-1} m}, \tag{2.14}$$

where the primes have been dropped. The binomial coefficient $\binom{N_0}{M}$ arises from the fact that by (2.5)

$$C^{N_q N_{q+1}}_{ik} = \left\{ \binom{N_q}{N_{q+1}} \Big/ \binom{N_q - M}{N_{q+1} - M} \right\} C^{N_q - M\, N_{q+1} - M}_{ik}, \tag{2.15}$$

and the binomial ratios of this type which arise in (2.11), as a result of the change (2.13), reduce to $\binom{N_0}{M}$. Using (2.5) again, (2.14) with $t = j - 1$ becomes

$$B^{N_0 M}_{n_0 m} + \binom{N_0}{M} \sum_{t=1}^{N_0-M-1} \sum_{N_1=t}^{N_0-M-1} \sum_{N_2=t-1}^{N_1-1} \cdots \sum_{N_t=1}^{N_{t-1}-1} \sum_{\substack{n_1, \cdots, n_t \\ (\neq m)}} C^{N_0-M N_1}_{n_0 n_1} C^{N_1 N_2}_{n_1 n_2} \cdots C^{N_{t-1} N_t}_{n_{t-1} n_t} B^{N_t 0}_{n_t m} = \binom{N_0}{M} Y^{N_0-M}_{n_0 m}, \tag{2.16}$$

since by (2.5)

$$B^{N_0 M}_{n_0 m} = \binom{N_0}{M} B^{N_0-M\, 0}_{n_0 m}. \tag{2.17}$$

Equation (2.10) can therefore be written as

$$X^{N_0}_{n_0 m} = \sum_{M=1}^{N_0-1} \binom{N_0}{M} Y^{N_0-M}_{n_0 m} \langle m|\ D^M\ |m\rangle, \tag{2.18}$$

and this, with (2.6), completes the proof of the theorem.

Corollary:

$$Y^N_{mm} = 0 \qquad (N = 1, 2, 3, \cdots). \tag{2.19}$$

Proof: From (2.3) with $N_0 = 1$ one sees that $Y^1_{mm} = 0$. One can then prove in turn, by putting $N_0 = 2, 3$, etc., that $Y^2_{mm} = 0$, $Y^3_{mm} = 0$, etc., because the left-hand side of (2.3) vanishes when $n_0 = m$.

Special cases of (2.19)

$$N = 1$$

$$\langle m| \frac{\partial A_m}{\partial \alpha} |m\rangle = 0, \quad \text{i.e., } \quad \langle m| \frac{\partial H}{\partial \alpha} |m\rangle = \frac{\partial E_m}{\partial \alpha}. \tag{2.20}$$

This is essentially the so-called Hellmann–Feynman

theorem,[8,9] and is the simplest of the sum rules, as already observed.[1]

$$N = 2$$

$$\langle m|\frac{\partial^2 A_m}{\partial\alpha^2}|m\rangle = 2\sum_{\substack{n_1\\(\neq m)}}\frac{\langle m|\frac{\partial A_m}{\partial\alpha}|n_1\rangle\langle n_1|\frac{\partial A_m}{\partial\alpha}|m\rangle}{E_{n_1}-E_m}. \tag{2.21}$$

$$N = 3$$

$$\langle m|\frac{\partial^3 A_m}{\partial\alpha^3}|m\rangle = 3\sum_{\substack{n_1\\(\neq m)}}\frac{\langle m|\frac{\partial^2 A_m}{\partial\alpha^2}|n_1\rangle\langle n_1|\frac{\partial A_m}{\partial\alpha}|m\rangle + \langle m|\frac{\partial A_m}{\partial\alpha}|n_1\rangle\langle n_1|\frac{\partial^2 A_m}{\partial\alpha^2}|m\rangle}{E_{n_1}-E_m}$$

$$-6\sum_{\substack{n_1,n_2\\(\neq m)}}\frac{\langle m|\frac{\partial A_m}{\partial\alpha}|n_1\rangle\langle n_1|\frac{\partial A_m}{\partial\alpha}|n_2\rangle\langle n_2|\frac{\partial A_m}{\partial\alpha}|m\rangle}{(E_{n_1}-E_m)(E_{n_2}-E_m)}. \tag{2.22}$$

This is a special case of the "third sum rule".[1]

The "fourth sum rule" [$N = 4$, Eq. (2.16) of Ref. 1] is also obtainable in this way. Thus (2.19) is a compact expression of general-order sum rules.

The Nth-order sum rule (2.19) gives the diagonal matrix element of the Nth derivative of $A_m(\alpha) = H(\alpha) - E_m(\alpha)$ with respect to the exact eigenfunctions of $H(\alpha)$ in terms of the matrix elements of the lower derivatives and the eigenvalues of $H(\alpha)$. The combination of matrix elements $Y^{N_0}_{n_0 m}$ which occurs in the theorem and the sum rule is, of course, a function of α.

The extension of the above theorem to the case when the operator H depends on a number of parameters $\alpha_1, \alpha_2, \alpha_3, \cdots$, is fairly straightforward, and we do not discuss it here.

3. CONNECTION WITH NONDEGENERATE PERTURBATION THEORY

The Hamiltonian $H(\alpha)$ is now taken in the form

$$H(\alpha) = H^{(0)} + \alpha H^{(1)}, \tag{3.1}$$

where $H^{(0)}$ and $H^{(1)}$ are independent of α, and we assume the possibility of the expansions

$$E_m(\alpha) = \sum_{l=0} E_m^{(l)}\alpha^l, \qquad \Psi_m(\alpha) = \sum_{l=0}\Psi_m^{(l)}\alpha^l \tag{3.2}$$

with

$$H^{(0)}\Psi_m^{(0)} = E_m^{(0)}\Psi_m^{(0)}. \tag{3.3}$$

A. The Eigenvalue Corrections

Using (3.1) and (3.2) in (2.19) and letting $\alpha \to 0$,

$$E_m^{(N_0)} = (m|H^{(1)}|m)\,\delta_{N_0,1} + \sum_{i=1}^{N_0-1} I_i^{(N_0)}, \tag{3.4}$$

where

$$I_i^{(N_0)} \equiv \sum_{N_1=i}^{N_0-1}\sum_{N_2=i-1}^{N_1-1}\cdots\sum_{N_i=1}^{N_{i-1}-1}\sum_{\substack{n_1,\cdots,n_i\\(\neq m)}}\delta_{N_1,N_0-1}\,\delta_{N_i,1}(m|H^{(1)}|n_1)\frac{(n_1|H^{(1)}\,\delta_{N_2,N_1-1}-E_m^{(N_1-N_2)}|n_2)}{(E_m^{(0)}-E_{n_1}^{(0)})}\times\cdots$$

$$\times\frac{(n_2|H^{(1)}\,\delta_{N_3,N_2-1}-E_m^{(N_2-N_3)}|n_3)}{(E_m^{(0)}-E_{n_2}^{(0)})}\cdots\frac{(n_{i-1}|H^{(1)}\,\delta_{N_i,N_{i-1}-1}-E_m^{(N_{i-1}-N_i)}|n_i)}{(E_m^{(0)}-E_{n_{i-1}}^{(0)})}\frac{(n_i|H^{(1)}|m)}{(E_m^{(0)}-E_{n_i}^{(0)})}, \tag{3.5}$$

and the round brackets $(\,|\,|\,)$ indicate that the matrix elements are with respect to the zero-order eigenfunctions $\Psi_m^{(0)}$ of $H^{(0)}$. For example, (3.5) yields

$$I_1^{(2)} = \sum_{\substack{n_1\\(\neq m)}}\frac{(m|H^{(1)}|n_1)(n_1|H^{(1)}|m)}{E_m^{(0)}-E_{n_1}^{(0)}}, \tag{3.6}$$

$$I_1^{(3)} = 0, \tag{3.7}$$

$$I_2^{(3)} = \sum_{\substack{n_1,n_2\\(\neq m)}}\frac{(m|H^{(1)}|n_1)(n_1|H^{(1)}-E_m^{(1)}|n_2)(n_1|H^{(1)}|m)}{(E_m^{(0)}-E_{n_1}^{(0)})(E_m^{(0)}-E_{n_2}^{(0)})}, \tag{3.8}$$

$$I_1^{(4)} = 0, \tag{3.9}$$

[8] R. P. Feynman, Phys. Rev., 56, 340 (1939).
[9] H. Hellmann, *Einführung in die Quantenchemie* (Franz Denticke, Leipzig, 1937), p. 285.

$$I_2^{(4)} = -E_m^{(2)} \sum_{\substack{n_1 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})^2}, \tag{3.10}$$

$$I_3^{(4)} = \sum_{\substack{n_1, n_2, n_3 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)} - E_m^{(1)}\, |n_2)(n_2|\, H^{(1)} - E_m^{(1)}\, |n_3)(n_3|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})(E_m^{(0)} - E_{n_3}^{(0)})}, \tag{3.11}$$

and hence, using (3.4),

$$E_m^{(1)} = (m|\, H^{(1)}\, |m), \tag{3.12}$$

$$E_m^{(2)} = \sum_{\substack{n_1 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)}\, |m)}{E_m^{(0)} - E_{n_1}^{(0)}}, \tag{3.13}$$

$$E_m^{(3)} = \sum_{\substack{n_1, n_2 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)} - E_m^{(1)}\, |n_2)(n_2|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})}, \tag{3.14}$$

$$E_m^{(4)} = \sum_{\substack{n_1, n_2, n_3 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)} - E_m^{(1)}\, |n_2)(n_2|\, H^{(1)} - E_m^{(1)}\, |n_3)(n_3|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})(E_m^{(0)} - E_{n_3}^{(0)})} - E_m^{(2)} \sum_{\substack{n_1 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})^2}. \tag{3.15}$$

Equations (3.4) and (3.5) show how to calculate the N_0th-order correction to the energy in terms of the lower-order corrections and the matrix elements of $H^{(1)}$ (the perturbation) between the zero-order eigenfunctions. This illustrates the rather wide use to which the sum rules can be put.

An alternative form of (3.4) is

$$E_m^{(N_0)} = (m|\, H^{(1)}\, |m)\, \delta_{N_0,1} + \delta_{N_0,2} \sum_{\substack{n_1 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)}\, |m)}{E_m^{(0)} - E_{n_1}^{(0)}}$$

$$+ \sum_{j=1}^{N_0-2} \sum_{\substack{N_1, \cdots, N_j\, (\neq 0) \\ \{\sum_{l=1}^{j} N_l = N_0 - 2\}}} \sum_{\substack{n_1, \cdots, n_{j+1} \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)}\, \delta_{N_1,1} - E_m^{(N_1)}\, |n_2) \cdots (n_j|\, H^{(1)}\, \delta_{N_j,1} - E_m^{(N_j)}\, |n_{j+1})(n_{j+1}|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)}) \cdots (E_m^{(0)} - E_{n_{j+1}}^{(0)})}, \tag{3.16}$$

where the second summation is over all possible combinations of nonzero integers $N_1, N_2, \cdots, N_j$ whose sum is equal to $N_0 - 2$. This form suggests a simple prescription for finding the N_0th-order correction to the energy. Consider, for example, the fifth-order correction $E_m^{(5)}$. We write the integer $5 - 2 = 3$ as

$$3, \quad 1 + 2, \quad 2 + 1, \quad 1 + 1 + 1. \tag{3.17}$$

The energy correction $E_m^{(5)}$ is then simply

$$\sum_{\substack{n_1, n_2 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, - E_m^{(3)}\, |n_2)(n_2|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})}$$

$$+ \sum_{\substack{n_1, n_2, n_3 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)\{(n_1|\, H^{(1)} - E_m^{(1)}\, |n_2)(n_2|\, - E_m^{(2)}\, |n_3) + (n_1|\, - E_m^{(2)}\, |n_2)(n_2|\, H^{(1)} - E_m^{(1)}\, |n_3)\}(n_3|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})(E_m^{(0)} - E_{n_3}^{(0)})}$$

$$+ \sum_{\substack{n_1, n_2, n_3, n_4 \\ (\neq m)}} \frac{(m|\, H^{(1)}\, |n_1)(n_1|\, H^{(1)} - E_m^{(1)}\, |n_2)(n_2|\, H^{(1)} - E_m^{(1)}\, |n_3)(n_3|\, H^{(1)} - E_m^{(1)}\, |n_4)(n_4|\, H^{(1)}\, |m)}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})(E_m^{(0)} - E_{n_3}^{(0)})(E_m^{(0)} - E_{n_4}^{(0)})}. \tag{3.18}$$

B. The Eigenfunction Corrections

From (2.3)

$$D^{N_0}\Psi_m = \sum_{\substack{n_0 \\ (\neq m)}} \sum_{i=0}^{N_0-1} \binom{N_0}{i} Y_{n_0 m}^{N_0-i}(\alpha) \frac{\langle m|\, D^i\, |m\rangle}{E_m - E_{n_0}} \Psi_{n_0} + \langle m|\, D^{N_0}\, |m\rangle \Psi_m, \tag{3.19}$$

and letting $\alpha \to 0$ in this equation

$$\Psi_m^{(N_0)} = \sum_{\substack{n_0 \\ (\neq m)}} \sum_{i=0}^{N_0-1} \frac{Y_{n_0 m}^{N_0-i}(0)(\Psi_m^{(0)}, \Psi_m^{(i)})\Psi_{n_0}^{(0)}}{(N_0 - i)!\,(E_m^{(0)} - E_{n_0}^{(0)})} + (\Psi_m^{(0)}, \Psi_m^{(N_0)})\Psi_m^{(0)}. \tag{3.20}$$

We now write

$$\Psi_m^{(N_0)} = \sum_n a_{nm}^{(N_0)} \Psi_n^{(0)}, \tag{3.21}$$

and (3.20) then yields

$$a_{nm}^{(N_0)} = \sum_{i=0}^{N_0-1} \frac{Y_{nm}^{N_0-i}(0) a_{mm}^{(i)}}{(N_0 - i)!\,(E_m^{(0)} - E_n^{(0)})} + a_{mm}^{(N_0)}\, \delta_{nm}. \tag{3.22}$$

Equation (3.22) yields the off-diagonal coefficients $a_{nm}^{(N_0)}$ in the expansion of the N_0th-order correction to the eigenfunction in terms of the diagonal coefficients $a_{mm}^{(i)}$ in lower-order corrections. These diagonal coefficients can be found by imposing the condition that the eigenfunctions should be normalized up to any order in the perturbation, and by choosing the phases of the eigenfunctions so that these diagonal coefficients are real.[4,10] This procedure then yields

$$a_{mm}^{(0)} = 1, \qquad a_{mm}^{(1)} = 0, \tag{3.23}$$

and for $N \geq 2$

$$a_{mm}^{(N)} = -\tfrac{1}{2} \sum_n \{a_{nm}^{*(1)} a_{nm}^{(N-1)} + + \cdots \cdots + a_{nm}^{*(2)} a_{nm}^{(N-2)} + a_{nm}^{*(N-1)} a_{nm}^{(1)}\}. \tag{3.24}$$

Equations (3.22)–(3.24) enable one to calculate the eigenfunction corrections to any order in the perturbation. For example, (3.24) yields

$$a_{mm}^{(2)} = -\tfrac{1}{2} \sum_{\substack{n \\ (\neq m)}} a_{nm}^{*(1)} a_{nm}^{(1)}, \tag{3.25}$$

$$a_{mm}^{(3)} = -\tfrac{1}{2} \sum_{\substack{n \\ (\neq m)}} \{a_{nm}^{*(1)} a_{nm}^{(2)} + a_{nm}^{*(2)} a_{nm}^{(1)}\}, \tag{3.26}$$

and (3.22) with $n \neq m$ yields

$$(E_m^{(0)} - E_n^{(0)}) a_{nm}^{(1)} = Y_{nm}^1(0), \tag{3.27}$$

$$(E_m^{(0)} - E_n^{(0)}) a_{nm}^{(2)} = \tfrac{1}{2} Y_{nm}^2(0), \tag{3.28}$$

$$(E_m^{(0)} - E_n^{(0)}) a_{nm}^{(3)} = \tfrac{1}{6} Y_{nm}^3(0) + Y_{nm}^1(0) a_{mm}^{(2)}. \tag{3.29}$$

Combining these results and using the definition (2.4) of $Y_{n_0 m}^{N_0}$,

$$a_{mm}^{(1)} = 0, \qquad a_{nm}^{(1)} = \frac{\langle n|\, H^{(1)}\, |m\rangle}{E_m^{(0)} - E_n^{(0)}}, \tag{3.30}$$

$$a_{mm}^{(2)} = -\tfrac{1}{2} \sum_{\substack{n_1 \\ (\neq m)}} \frac{\langle m|\, H^{(1)}\, |n_1\rangle\langle n_1|\, H^{(1)}\, |m\rangle}{(E_m^{(0)} - E_{n_1}^{(0)})^2}, \tag{3.31}$$

$$a_{nm}^{(2)} = \frac{1}{(E_m^{(0)} - E_n^{(0)})} \sum_{\substack{n_1 \\ (\neq m)}} \frac{\langle n|\, H^{(1)} - E_m^{(1)}\, |n_1\rangle\langle n_1|\, H^{(1)}\, |m\rangle}{(E_m^{(0)} - E_{n_1}^{(0)})}, \tag{3.32}$$

$$a_{mm}^{(3)} = -\sum_{\substack{n_1, n_2 \\ (\neq m)}} \frac{\langle m|\, H^{(1)}\, |n_1\rangle\langle n_1|\, H^{(1)} - E_m^{(1)}\, |n_2\rangle\langle n_2|\, H^{(1)}\, |m\rangle}{(E_m^{(0)} - E_{n_1}^{(0)})^2 (E_m^{(0)} - E_{n_2}^{(0)})}, \tag{3.33}$$

$$a_{nm}^{(3)} = \frac{1}{(E_m^{(0)} - E_n^{(0)})} \sum_{\substack{n_1, n_2 \\ (\neq m)}} \frac{\langle n|\, H^{(1)} - E_m^{(1)}\, |n_1\rangle\langle n_1|\, H^{(1)} - E_m^{(1)}\, |n_2\rangle\langle n_2|\, H^{(1)}\, |m\rangle}{(E_m^{(0)} - E_{n_1}^{(0)})(E_m^{(0)} - E_{n_2}^{(0)})} - \frac{\langle n|\, H^{(1)}\, |m\rangle}{2(E_m^{(0)} - E_n^{(0)})} \sum_{\substack{n_1 \\ (\neq m)}} \frac{\langle m|\, H^{(1)}\, |n_1\rangle\langle n_1|\, H^{(1)}\, |m\rangle}{(E_m^{(0)} - E_{n_1}^{(0)})^2} - E_m^{(2)} \frac{\langle n|\, H^{(1)}\, |m\rangle}{(E_m^{(0)} - E_n^{(0)})^2}. \tag{3.34}$$

Equations (3.30)–(3.34) enable one to calculate the first three corrections to the eigenfunction. Higher-order corrections follow from (3.22)–(3.24) analogously.

4. MULTIPLICATION PROPERTIES OF $\partial/\partial\alpha$

We have not used the following equation:

$$\langle n|\, \frac{\partial^2}{\partial \alpha^2}\, |m\rangle = \sum_{n'} \langle n|\, \frac{\partial}{\partial \alpha}\, |n'\rangle\langle n'|\, \frac{\partial}{\partial \alpha}\, |m\rangle. \tag{4.1}$$

[10] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), p. 154.

In fact, (4.1) is not generally true, and if this is not realized, erroneous results may be obtained.

The reason for this situation is easily seen. Since the eigenfunctions $\Psi_n(\alpha)$ form a complete set, we can write

$$\frac{\partial \Psi_m(\alpha)}{\partial \alpha} = \sum_{n'} c_{n'm}(\alpha)\Psi_{n'}(\alpha). \tag{4.2}$$

It now follows that

$$\frac{\partial^2 \Psi_m(\alpha)}{\partial \alpha^2} = \sum_{n'} \left\{ \frac{\partial c_{n'm}}{\partial \alpha} \Psi_{n'} + c_{n'm} \frac{\partial \Psi_{n'}}{\partial \alpha} \right\}$$

$$= \sum_{n'} \frac{\partial c_{n'm}}{\partial \alpha} \Psi_{n'} + \sum_{n',n''} c_{n''n'} c_{n'm} \Psi_{n''}. \tag{4.3}$$

The matrix elements arising from (4.2) and (4.3) are

$$\langle n| \frac{\partial}{\partial \alpha} |m\rangle = c_{nm}(\alpha), \tag{4.4}$$

$$\langle n| \frac{\partial^2}{\partial \alpha^2} |m\rangle = \frac{\partial c_{nm}}{\partial \alpha} + \sum_{n'} c_{nn'} c_{n'm}, \tag{4.5}$$

and hence

$$\langle n| \frac{\partial^2}{\partial \alpha^2} |m\rangle = \frac{\partial}{\partial \alpha} \left\{ \langle n| \frac{\partial}{\partial \alpha} |m\rangle \right\}$$

$$+ \sum_{n'} \langle n| \frac{\partial}{\partial \alpha} |n'\rangle\langle n'| \frac{\partial}{\partial \alpha} |m\rangle. \tag{4.6}$$

The failure of (4.1) is seen to be due to the fact that, if α is a parameter in the eigenfunction, the expansion coefficients $c_{n'n}$ in general depend on α. This differs from the more usual type of superposition

$$\phi(x) = \sum_n a_n \Psi_n(x), \tag{4.7}$$

in which the expansion coefficients a_n do not depend on the variable of interest.

As an example, consider the harmonic oscillator, for which

$$H(\alpha) = \frac{\hbar^2}{2\mu} \left\{ -\frac{d^2}{dx^2} + \alpha^4 x^2 \right\}, \tag{4.8}$$

$$\Psi_n(\alpha) = \left[\frac{\alpha}{(\pi)^{\frac{1}{2}} 2^n n!} \right]^{\frac{1}{2}} H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}, \tag{4.9}$$

$$\frac{\partial \Psi_n(\alpha)}{\partial \alpha} = -\frac{1}{2\alpha} [(n+1)(n+2)]^{\frac{1}{2}} \Psi_{n+2}(\alpha)$$

$$+ \frac{1}{2\alpha} [n(n-1)]^{\frac{1}{2}} \Psi_{n-2}(\alpha), \tag{4.10}$$

and hence

$$\langle n+2| \frac{\partial^2}{\partial \alpha^2} |n\rangle = \frac{1}{2\alpha^2} [(n+1)(n+2)]^{\frac{1}{2}}$$

$$+ \sum_{n'} \langle n+2| \frac{\partial}{\partial \alpha} |n'\rangle\langle n'| \frac{\partial}{\partial \alpha} |n\rangle, \tag{4.11}$$

$$\langle n-2| \frac{\partial^2}{\partial \alpha^2} |n\rangle = -\frac{1}{2\alpha^2} [n(n-1)]^{\frac{1}{2}}$$

$$+ \sum_{n'} \langle n-2| \frac{\partial}{\partial \alpha} |n'\rangle\langle n'| \frac{\partial}{\partial \alpha} |n\rangle. \tag{4.12}$$

These equations give explicit examples of the general points made above.

ACKNOWLEDGMENT

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Minimal Potentials for Schrödinger Equation with Fixed Eigenvalue*

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It is shown that the potential

$$V(x) = -\frac{nE}{n-1}\operatorname{sech}^2\left[\frac{(-E)^{\frac{1}{2}}x}{n-1}\right]$$

solves the problem of minimizing $\int_{-\infty}^{\infty} V^n(x)dx$ $(n > 1)$, where V is such that the Schrödinger equation has an eigenvalue E, specified in advance, with a square-integrable eigenfunction.

IN connection with the determination of the density of states in the low-energy tail of a high-density impurity band by Lax and Halperin[1] and Zittartz and Langer,[2] we were led to investigate the following simple variational problem. We want to minimize the integral

$$I(V) = \int_{-\infty}^{\infty} V^n(x)\,dx, \tag{1}$$

where V is the potential of a one-dimensional Schrödinger equation so that it has a square-integrable eigensolution corresponding to a specified energy E. That is, with $u \epsilon L_2(-\infty, \infty)$ and fixed E, we have

$$u_{xx} + V(x)u + Eu = 0. \tag{2}$$

A few years ago a similar problem was considered by Keller.[3] He considered the problem of determining the lowest eigenvalue of the Schrödinger equation for potentials which satisfied the condition

$$\int_{-\infty}^{\infty} V^n(x)\,dx = k. \tag{3}$$

It is intuitively clear that, in our problem, the given energy E must be the lowest eigenvalue of the desired potential. Then, by the usual reciprocity of isoperimetric problems, we expect that the solution of our problem must depend on the equations Keller obtained. This is indeed true. The only remaining task is to prove that we do obtain a minimum for I for the potential we get from Keller's equation.

Let $V_0(x)$ be the desired minimal potential and $u_0(x)$ the corresponding eigenfunction with the eigenvalue E. We consider a family of functions $V(x, \epsilon)$ depending smoothly on a parameter ϵ, such that $V(x, 0) = V_0(x)$, and the integral I still exists. Clearly the eigenfunctions $u(x, \epsilon)$ of (2) are also smooth functions of ϵ, with $u(x, 0) = u_0(x)$. Consider a variation of V from V_0:

$$V(x, \epsilon) = V_0(x) + \epsilon V_1(x). \tag{4}$$

Since $V_0(x)$ minimizes (1),

$$\int_{-\infty}^{\infty} V_0^{n-1}(x)\,V_1(x)\,dx = 0. \tag{5}$$

Correspondingly,

$$u(x, \epsilon) = u_0(x) + \epsilon u_1(x), \tag{6}$$

and we obtain

$$u_{0xx} + (V_0 + E)u_0 = 0; \tag{7}$$

and for $u_1(x)$,

$$u_{1xx} + (V_0 + E)u_1 = -V_1 u_0. \tag{8}$$

In order that a nontrivial solution u_1 exists for (8), the right-hand side must be orthogonal to the solution of the homogeneous equation, and therefore to u_0,

$$\int_{-\infty}^{\infty} V_1(x)u_0^2(x)\,dx = 0. \tag{9}$$

But u_1 clearly exists, and, as V_1 is arbitrary this implies, from (5) and (9), that V_0^{n-1} is proportional to u_0^2. Since normalization of u_0 is arbitrary, we can always choose the constant of proportionality such that

$$V_0^{n-1} = u_0^2. \tag{10}$$

From Eqs. (7) and (10), one can determine the form of V_0 as

$$V_0(x) = -\frac{nE}{n-1}\operatorname{sech}^2\left[\frac{(-E)^{\frac{1}{2}}x}{n-1}\right]. \tag{11}$$

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† On leave from the Institute for Theoretical Physics, University of Köln, Köln, Germany.
[1] M. Lax and B. Halperin, Phys. Rev. 148, 722 (1966).
[2] J. Zittartz and J. S. Langer, Phys. Rev. 148, 741 (1966).
[3] J. B. Keller, J. Math. Phys. 2, 262 (1961).

Clearly, the translational invariance of the problem makes the choice of the origin arbitrary, and we have fixed it by making $V_0(0) = -nE/(n-1)$. Also E must be negative to have a meaningful value of Eq. (1). Since u_0 must vanish as $|x|$ becomes infinite, Eq. (10) implies that we restrict ourselves to $n > 1$

The corresponding wavefunction is

$$u_0(x) = \left\{-\frac{nE}{n-1}\operatorname{sech}^2\frac{(-E)^{\frac{1}{2}}x}{n-1}\right\}^{\frac{1}{2}(n-1)}. \tag{12}$$

Since it is nodeless, it follows that E is the lowest eigenvalue of the potential V_0. The minimum value of (1) immediately follows:

$$\begin{aligned} I_{\min} &= \int_{-\infty}^{\infty} V_0^n\,dx \\ &= \frac{\Gamma(n)\Gamma(\frac{1}{2})}{2\Gamma(n+\frac{1}{2})}\left(-\frac{nE}{n-1}\right)^n\frac{2(n-1)}{(-E)^{\frac{1}{2}}}. \end{aligned} \tag{13}$$

In particular, for $n = 2$, $I_{\min} = \frac{16}{3}(-E)^{\frac{3}{2}}$, which is the characteristic exponent found in Ref. 1. These results follow directly from Keller's considerations.

PROOF THAT V_0 IS THE MINIMAL POTENTIAL

We now turn to show that the minimum in (1) is actually attained by V_0. It is convenient to write Eq. (2) as an integral constraint,

$$-\int_{-\infty}^{\infty} u_x^2\,dx + \int_{-\infty}^{\infty} Vu^2\,dx + E\int_{-\infty}^{\infty} u^2\,dx = 0. \tag{14}$$

Combine (14) with (1) by means of a Lagrange multiplier λ, and consider the minimization of

$$\begin{aligned} J[V] = &\int_{-\infty}^{\infty} V^n\,dx \\ &+ \lambda\int_{-\infty}^{\infty}(E+V)u^2\,dx - \lambda\int_{-\infty}^{\infty} u_x^2\,dx. \end{aligned} \tag{15}$$

The Euler–Lagrange equations are

$$nV^{n-1} + \lambda u^2 = 0, \tag{16a}$$

$$u_{xx} + (E+V)u = 0; \tag{16b}$$

and the equation for the constraint together with (16a, b) imply Eq. (8) for the first variations of u and V. Notice that the magnitude of λ is arbitrary, since in (14) the normalization of u is freely chosen. However, the sign of λ is not arbitrary, and the correct sign is easily seen to be *negative*, which enables one to obtain Eq. (10) again.

Consider now the variations of u and V from the minimizing solutions u_0 and V_0 to be

$$\begin{aligned} u(x) &= u_0(x) + \epsilon u_1(x) + \epsilon^2 u_2(x), \\ V(x) &= V_0(x) + \epsilon V_1(x) + \epsilon^2 V_2(x), \end{aligned} \tag{17}$$

where ϵ is the smallness parameter. Then, collecting powers of ϵ, we have

$$\begin{aligned} J_0 &= \int_{-\infty}^{\infty} V_0^n\,dx + \lambda\int_{-\infty}^{\infty}[(E+V_0)u_0^2 - u_{0x}^2]\,dx \\ &\equiv \int_{-\infty}^{\infty} V_0^n\,dx, \\ J_1 &= \int_{-\infty}^{\infty} V_1[nV_0^{n-1} + \lambda u_0^2]\,dx \\ &\quad + 2\lambda\int_{-\infty}^{\infty} u_1[(E+V_0)u_0 + u_{0xx}]\,dx, \\ J_2 &= \int_{-\infty}^{\infty} dx\,\{V_2(\lambda u_0^2 + nV_0^{n-1}) \\ &\quad + 2u_2\lambda[(E+V_0)u_0 + u_{0xx}] + V_1^2V_0^{n-2}\frac{n(n-1)}{2!} \\ &\quad + 2\lambda V_1u_0u_1 + \lambda(E+V_0)u_1^2 - \lambda u_{1x}^2\}. \end{aligned} \tag{18}$$

The first variation identically vanishes by Eq. (16). The same holds for the first two terms of the second variation. The third term in the second variation is evidently positive. To handle the fourth term we utilize Eq. (8), and write

$$-\int_{-\infty}^{\infty} V_1u_0u_1\,dx = \int_{-\infty}^{\infty}[(E+V_0)u_1^2 - u_{1x}^2]\,dx, \tag{19}$$

so that we get

$$\begin{aligned} J_2 = &\int_{-\infty}^{\infty} V_1^2V_0^{n-2}\frac{n(n-1)}{2!}\,dx \\ &- \lambda\int_{-\infty}^{\infty}[(E+V_0)u_1^2 - u_{1x}^2]\,dx. \end{aligned} \tag{20}$$

However, E is the lowest eigenvalue of the potential V_0. Hence, by the Rayleigh–Ritz principle, we have.

$$\begin{aligned} E &= \frac{\int_{-\infty}^{\infty} u_{0x}^2\,dx - \int_{-\infty}^{\infty} V_0u_0^2\,dx}{\int_{-\infty}^{\infty} u_0^2\,dx} \\ &\le \frac{\int_{-\infty}^{\infty} u_{1x}^2\,dx - \int_{-\infty}^{\infty} V_0u_1^2}{\int_{-\infty}^{\infty} u_1^2\,dx}, \end{aligned} \tag{21}$$

so

$$\int_{-\infty}^{\infty}[(E+V_0)u_1^2 - u_{1x}^2]\,dx \le 0. \tag{22}$$

But we have already noted that the sign of λ must be negative. It follows that

$$J_2 \ge 0, \tag{23}$$

which shows that the minimum of $I(V)$ is actually attained for V_0.

Erratum: Applications of Gel'fand–Moshinsky Bases in Unitary Symmetry and its Breaking

J. A. Castilho Alcarás, V. C. Aguilera Navarro, and P. Leal Ferreira
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In Eq. (3.21m), t should read t^{-1}. Also, the definition of t, on page 213 should read $t^{-1} = t_1 t_2 t_3$.

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Erratum: Multipole Theory in the Time Domain

Kenneth D. Granzow
[J. Math. Phys. **7**, 634 (1966)]

On p. 640, next to last line, $-\frac{3}{2} \pm i\sqrt{3}$ should be $-\frac{3}{2} \pm \frac{1}{2}i\sqrt{3}$. The roots of $H^{(1)}_{l+\frac{1}{2}}(iz) = 0$ have been recomputed using two different numerical schemes in double precision on Dikewood's IBM system 360 and in single and double precision on the CDC 6600 at the Air Force Weapons Laboratory. Most of the roots given in Table I, p. 639, for order (l) ten through sixteen are in error; the correct values are given below.

Table I. Roots of $H_{l+\frac{1}{2}}{}^{(1)}(iz) = 0$.

Order (l)	Real part of z	Imaginary part of z	Order (l)	Real part of z	Imaginary part of z
10	−6.922045	0.867665	14	−9.583171	0.867711
10	−6.615291	2.611568	14	−9.363146	2.607553
10	−5.967528	4.384947	14	−8.911001	4.361604
10	−4.886220	6.224985	14	−8.198847	6.143041
10	−3.108916	8.232699	14	−7.172396	7.973217
			14	−5.720352	9.894708
11	−7.622340	0.	14	−3.551087	12.025738
11	−7.484230	1.737103			
11	−7.057892	3.489015	15	−10.273110	0.
11	−6.301337	5.276192	15	−10.170914	1.736389
11	−5.115648	7.137021	15	−9.859567	3.480671
11	−3.229722	9.177112	15	−9.323599	5.242259
			15	−8.532459	7.034394
12	−8.253422	0.867694	15	−7.429397	8.878983
12	−7.997271	2.609067	15	−5.900152	10.819999
12	−7.465571	4.370170	15	−3.647357	12.979501
12	−6.611004	6.171535			
12	−5.329709	8.052907	16	−10.911886	0.867723
12	−3.343023	10.124297	16	−10.718986	2.606567
			16	−10.325120	4.356163
13	−8.947710	0.	16	−9.712326	6.125761
13	−8.830252	1.736666	16	−8.847968	7.928773
13	−8.470592	3.483868	16	−7.673241	9.787697
13	−7.844380	5.254903	16	−6.071241	11.747875
13	−6.900373	7.070644	16	−3.739232	13.935028
13	−5.530681	8.972248			
13	−3.449867	11.073928			