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Some Constants of the Linearized Motion of Vlasov Plasmas*

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A new class of nonlocal constants for the linearized Vlasov equations is presented. These are constants which, in general, are not expressible as simple phase-space integrals of a locally defined integrand. The relevance of these constants to stability considerations is indicated.

I. INTRODUCTION

IT is our purpose here to demonstrate some new constants of the linearized motion of Vlasov plasmas. The search for such constants is strongly motivated since knowledge of them is of great value in determining questions of stability,[1-3] but we do not address ourselves, in the main, to such stability questions in this paper.

The constants we seek are quadratic forms in the first-order perturbations of the field quantities from their equilibrium values. We give two derivations, both different from that employed in Ref. 2 in that we here deal only with the equations of motion for first-order perturbations rather than, as there, eliminate explicitly second-order perturbations of the field quantities f, $\mathbf{E}$, $\mathbf{B}$ between the energy of the system written to second order and the general constant of the full nonlinear motion

$$C = \iint d^3x\, d^3v\, G[f(\mathbf{x}, \mathbf{v}, t)]$$

written to second order. Here G is an arbitrary functional of f, the distribution function. The use of the latter constant required that the equilibrium distribution function be a monotonic function of the particle energy. No such restriction is imposed in the present derivations.

We consider chiefly in this paper only perturbations from a spatially uniform equilibrium of an unbounded plasma. We treat only electronic motions with the ions regarded as a background of uniform density (the multispecies situation is of course a trivial generalization). However we also show that we can find at least one constant associated with the perturbations of the unidimensional nonlinear static solutions exhibited by Bernstein, Greene, and Kruskal.[4] Future papers shall deal with the generalization to nonuniform equilibria, formation of energy-type principles involving these constants, and a generalization of the energy principle of Ref. 2 achieved by now removing the monotonicity condition on the energy dependence of the equilibrium distribution function per tube.

II. FIRST DERIVATION

This first method of derivation is less straightforward than the second and was discovered later,

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[1] See, e.g., I. Bernstein, Phys. Rev. 109, 10 (1958), Appendix I.
[2] M. Kruskal and C. Oberman, Phys. Fluids 1, 275 (1958). See also T. Fowler, J. Math. Phys. 4, 559 (1963).
[3] C. Oberman and J. Dawson, Phys. Fluids 7, 773 (1964).
[4] I. Bernstein, J. Greene, and M. Kruskal, Phys. Rev. 108, 546 (1957).

but it leads to the final results much more quickly, as well as having the advantage of not requiring Fourier transformation of the space variables. This last feature is desirable when one seeks the generalization to spatially inhomogeneous equilibria. The second, more straightforward, derivation is reserved for the Appendix.

We begin by writing down the equations governing the perturbed field quantities, $f(\mathbf{x}, \mathbf{v}, t)$, $\mathbf{E}(\mathbf{x}, t)$, $\mathbf{B}(\mathbf{x}, t)$

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}} + \frac{e}{m}\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)\cdot\frac{\partial g}{\partial \mathbf{v}} = 0, \tag{1}$$

$$(\partial/\partial\mathbf{x})\cdot\mathbf{E} = 4\pi\sigma, \tag{2a}$$

$$(\partial/\partial\mathbf{x})\cdot\mathbf{B} = 0, \tag{2b}$$

$$\partial\mathbf{B}/\partial t = -c(\partial/\partial\mathbf{x})\times\mathbf{E}, \tag{2c}$$

$$\partial\mathbf{E}/\partial t = c(\partial/\partial\mathbf{x})\times\mathbf{B} - 4\pi\mathbf{j}. \tag{2d}$$

Here

$$\sigma(\mathbf{x}, t) = e\int d^3v f, \tag{3a}$$

$$\mathbf{j}(\mathbf{x}, t) = e\int d^3v\, \mathbf{v} f, \tag{3b}$$

and $g(\mathbf{v})$ is the equilibrium distribution function with $\int d^3v\, g = n_0$. We envisage either an infinite domain, in which case all perturbations of physical quantities are taken to die away sufficiently rapidly at infinity, or else a periodic system with all perturbations having zero spatial mean.

Let us introduce the potentials $\mathbf{A}(\mathbf{x}, t)$ and $\phi(\mathbf{x}, t)$ with

$$\mathbf{E} = -\frac{\partial\phi}{\partial\mathbf{x}} - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}, \tag{4a}$$

$$\mathbf{B} = (\partial/\partial\mathbf{x})\times\mathbf{A}. \tag{4b}$$

Then (1) reads

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial\mathbf{x}} - \frac{e}{mc}\left(\frac{\partial\mathbf{A}}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial x}\mathbf{A}\right)\cdot\frac{\partial g}{\partial\mathbf{v}} + \frac{e}{m}\frac{\partial g}{\partial\mathbf{v}}\cdot\frac{\partial}{\partial\mathbf{x}}\left(-\phi + \frac{1}{c}\mathbf{A}\cdot\mathbf{v}\right) = 0. \tag{5}$$

Define

$$\bar{f} \equiv f - (e/mc)\mathbf{A}\cdot\partial g/\partial\mathbf{v} \tag{6}$$

and

$$x_\parallel \equiv \mathbf{x}\cdot\frac{\partial g}{\partial\mathbf{v}}\Big/\left|\frac{\partial g}{\partial\mathbf{v}}\right|. \tag{7}$$

Then (5) may be rewritten as

$$\frac{m}{|\partial g/\partial\mathbf{v}|}\left(\frac{\partial\bar{f}}{\partial t} + \mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}}\bar{f}\right) + e\frac{\partial}{\partial x_\parallel}\left(-\phi + \frac{1}{c}\mathbf{A}\cdot\mathbf{v}\right) = 0. \tag{8}$$

Now introduce a primitive F by

$$\bar{f} = \partial F/\partial x_\parallel. \tag{9}$$

The independence of the results to the arbitrariness in F is shown in Sec. III. A quadrature on (8) then gives

$$\frac{m}{|\partial g/\partial\mathbf{v}|}\left(\frac{\partial F}{\partial t} + \mathbf{v}\cdot\frac{\partial F}{\partial\mathbf{x}}\right) + e\left(-\phi + \frac{1}{c}\mathbf{A}\cdot\mathbf{v}\right) = 0. \tag{10}$$

Now multiply (8) by $\frac{1}{2}\mathbf{v}\cdot\partial F/\partial\mathbf{x}$, operate on (10) with $\frac{1}{2}\bar{f}\mathbf{v}\cdot\partial/\partial\mathbf{x}$, add the resulting equations together and integrate over the phase space. A simple integration by parts yields

$$\frac{\partial}{\partial t}\frac{m}{2}\iint d^3x\, d^3v\, \frac{\bar{f}\mathbf{v}\cdot\partial F/\partial\mathbf{x}}{|\partial g/\partial\mathbf{v}|} + e\iint d^3x\, d^3v\, \bar{f}\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}}\left(-\phi + \frac{1}{c}\mathbf{A}\cdot\mathbf{v}\right) = 0. \tag{11}$$

If we now employ (6) and (8) in the second term of (11), with K denoting $m/2$ times the first of the integrals we find,

$$\frac{\partial K}{\partial t} - e\iint d^3x\, d^3v\left(f - \frac{e}{mc}\mathbf{A}\cdot\frac{\partial g}{\partial\mathbf{v}}\right)\mathbf{v}\cdot\frac{\partial\phi}{\partial\mathbf{x}} + \frac{e}{c}\iint d^3x\, d^3v\left[\frac{\partial\bar{f}}{\partial t} + \frac{e}{m}\frac{\partial g}{\partial\mathbf{v}}\cdot\frac{\partial}{\partial\mathbf{x}} \times\left(-\phi + \frac{1}{c}\mathbf{A}\cdot\mathbf{v}\right)\right]\mathbf{A}\cdot\mathbf{v} = 0. \tag{12}$$

Addition and subtraction of

$$\frac{e}{c}\iint d^3x\, d^3v\, \mathbf{v}\cdot\frac{\partial\mathbf{A}}{\partial t}$$

and utilization of (3a) and (3b) yields

$$\frac{\partial K}{\partial t} + \int d^3x\, \mathbf{E}\cdot\mathbf{j} + \frac{e}{c}\frac{\partial}{\partial t}\int d^3x\, \mathbf{j}\cdot\mathbf{A} + \iint d^3x\, d^3v\left[\frac{e^2}{mc}\mathbf{A}\cdot\frac{\partial g}{\partial\mathbf{v}}\mathbf{v}\cdot\frac{\partial\phi}{\partial\mathbf{x}} - \frac{e^2}{mc}\frac{\partial g}{\partial\mathbf{v}}\cdot\frac{\partial\phi}{\partial\mathbf{x}}\mathbf{A}\cdot\mathbf{v} - \frac{e^2}{mc^2}\frac{\partial\mathbf{A}}{\partial t}\cdot\frac{\partial g}{\partial\mathbf{v}}\mathbf{A}\cdot\mathbf{v} + \frac{e^2}{mc^2}\frac{\partial g}{\partial v}\cdot\frac{\partial}{\partial\mathbf{x}}\mathbf{A}\cdot\mathbf{v}\mathbf{A}\cdot\mathbf{v}\right] = 0. \tag{13}$$

Integration by parts with respect to $\mathbf{v}$ shows that the first two terms in brackets cancel, while the last is a perfect $\mathbf{x}$ derivative and hence vanishes upon integration. Finally integration by parts with respect to $\mathbf{v}$ on the remaining term in the brackets and the use of (2c) and (2d) on the second integral gives

$$\frac{\partial}{\partial t}\left\{K - \int d^3x\left[\frac{1}{8\pi}\left(\mathbf{E}^2 + \mathbf{B}^2 - \frac{\omega_p^2}{c^2}\mathbf{A}^2\right) - \frac{1}{c}\mathbf{j}\cdot\mathbf{A}\right]\right\} = 0. \tag{14}$$

We have thus exhibited our first constant. Before proceeding further we rewrite K in a suggestive alternative form by noting that

$$F = \int_{-\infty}^{x_\parallel} \bar{f}(\mathbf{x}_\perp, x'_\parallel, \mathbf{v}, t)\, dx'_\parallel \tag{15}$$

or, with $u \equiv x'_\parallel - x_\parallel$,

$$F = \int_{-\infty}^{0} \bar{f}(\mathbf{x} + u\mathbf{e}_\parallel, \mathbf{v}, t)\, du, \tag{16}$$

where

$$e_\parallel \equiv \frac{\partial g}{\partial \mathbf{v}} \Big/ \left|\frac{\partial g}{\partial \mathbf{v}}\right|.$$

Therefore

$$\frac{F}{|\partial g/\partial \mathbf{v}|} = \int_0^\infty ds\, \bar{f}\left(\mathbf{x} - s\frac{\partial g}{\partial \mathbf{v}}, \mathbf{v}, t\right). \tag{17}$$

Hence the constant can be written as

$$c_2 = \frac{m}{2}\iint d^3x\, d^3v \times \int_0^\infty ds\, \bar{f}(\mathbf{x}, \mathbf{v}, t)\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\bar{f}\left(\mathbf{x} - s\frac{\partial g}{\partial \mathbf{v}}, \mathbf{v}, t\right) - \int d^3x\left[\frac{1}{8\pi}\left(\mathbf{E}^2 + \mathbf{B}^2 - \frac{\omega_p^2}{c^2}\mathbf{A}^2\right) - \frac{1}{c}\mathbf{j}\cdot\mathbf{A}\right]. \tag{18}$$

A second (vector) constant is obtained by multiplying (8) by $\frac{1}{2}\partial F/\partial \mathbf{x}$, operating on (10) with $\bar{f}\partial/\partial \mathbf{x}$, then adding the two equations and integrating over the phase space. There results

$$\frac{m}{2}\frac{\partial}{\partial t}\iint d^3x\, d^3v\, \bar{f}\frac{\partial F/\partial \mathbf{x}}{|\partial g/\partial \mathbf{v}|} + e\iint d^3x\, d^3v\, \bar{f}\frac{\partial}{\partial \mathbf{x}}\left(-\phi + \frac{1}{c}\mathbf{A}\cdot\mathbf{v}\right) = 0. \tag{19}$$

If we denote $m/2$ times the first integral by $\mathbf{P}$ and employ (6), we have

$$\frac{\partial \mathbf{P}}{\partial t} - e\iint d^3x\, d^3v\left(f - \frac{e}{mc}\mathbf{A}\cdot\frac{\partial g}{\partial \mathbf{v}}\right)\frac{\partial \phi}{\partial \mathbf{x}} + \frac{e}{c}\iint d^3x\, d^3v\left(f - \frac{e}{mc}\mathbf{A}\cdot\frac{\partial g}{\partial \mathbf{v}}\right)\left(\frac{\partial}{\partial \mathbf{x}}\mathbf{A}\right)\cdot\mathbf{v} = 0. \tag{20}$$

Both terms in (20) involving $\partial g/\partial \mathbf{v}$ vanish upon integration. Thus

$$\frac{\partial \mathbf{P}}{\partial t} - \int d^3x\, \sigma\frac{\partial \phi}{\partial \mathbf{x}} + \frac{e}{c}\int d^3x\, f\frac{\partial}{\partial \mathbf{x}}\mathbf{A}\cdot\mathbf{v} = 0, \tag{21}$$

which may quickly be rewritten as

$$\frac{\partial \mathbf{P}}{\partial t} - \int d^3x\, \sigma\frac{\partial \phi}{\partial \mathbf{x}} + \frac{1}{c}\int d^3x\, \mathbf{j}\times\mathbf{B} + \frac{e}{c}\iint d^3x\, d^3v\, f\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\mathbf{A} = 0. \tag{22}$$

We now transfer the $\mathbf{x}$ derivative in the last term onto f and employ (1) to obtain

$$\frac{\partial \mathbf{P}}{\partial t} - \int d^3x\, \sigma\frac{\partial \phi}{\partial \mathbf{x}} + \frac{1}{c}\int d^3x\, \mathbf{j}\times\mathbf{B} + \frac{e}{c}\iint d^3x\, d^3v\left[\frac{\partial f}{\partial t} + e\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)\cdot\frac{\partial g}{\partial \mathbf{v}}\right]\mathbf{A} = 0. \tag{23}$$

The term involving $\partial g/\partial \mathbf{v}$ goes out upon velocity integration, so that, employing (4a), we have

$$\frac{\partial \mathbf{P}}{\partial t} + \frac{1}{c}\frac{\partial}{\partial t}\int d^3x\sigma\mathbf{A} + \int d^3x\left[\sigma\mathbf{E} + \frac{1}{c}\mathbf{j}\times\mathbf{B}\right] = 0. \tag{24}$$

If we now employ all the Maxwell equations (2a), (2b), (2c), and (2d) in the last integral, we have

$$\frac{\partial}{\partial t}\left[\mathbf{P} + \frac{1}{c}\int d^3x\, \sigma\mathbf{A} - \frac{1}{4\pi c}\int d^3x\, \mathbf{E}\times\mathbf{B}\right] = 0, \tag{25}$$

or finally

$$\mathbf{c}_1 = \frac{m}{2}\iint d^3x\, d^3v \times \int_0^\infty ds\, \bar{f}(\mathbf{x}, \mathbf{v}, t)\frac{\partial}{\partial \mathbf{x}}\bar{f}\left(\mathbf{x} - s\frac{\partial g}{\partial \mathbf{v}}, \mathbf{v}, t\right) - \frac{1}{c}\int d^3x\left[\frac{1}{4\pi}\mathbf{E}\times\mathbf{B} - \sigma\mathbf{A}\right]. \tag{26}$$

III. INVARIANCE PROPERTIES

We now demonstrate two invariance properties, gauge invariance and invariance under the displacement of F, the primitive from which $\bar{f}$ is derived. It is sufficient to prove these invariances under infinitesimal transformations, with the group property completing the proof to finite transformations. First the gauge invariance.

Let

$$\mathbf{A} \to \mathbf{A} + \delta\mathbf{A}, \tag{27a}$$

$$\phi \to \phi + \delta\phi. \tag{27b}$$

That $\mathbf{B}$ and $\mathbf{E}$ (and f) remain unchanged requires

$$(\partial/\partial \mathbf{x}) \times \delta\mathbf{A} = 0, \tag{28a}$$

$$\frac{\partial \delta\phi}{\partial \mathbf{x}} + \frac{1}{c}\frac{\partial \delta\mathbf{A}}{\partial t} = 0. \tag{28b}$$

Therefore there exists a $\delta\psi$ such that

$$\delta A \equiv \partial\delta\psi/\partial \mathbf{x}. \tag{29}$$

Note that

$$\frac{\partial \mathbf{A}\cdot\partial g/\partial \mathbf{v}}{|\partial g/\partial \mathbf{v}|} = \frac{\partial \delta\psi}{\partial x_\parallel}. \tag{30}$$

If we employ (29) and (30) in (14) we find

$$c_2 = -\frac{e}{2c}\iint d^3x\, d^3v\, \frac{\partial \delta\psi}{\partial x_\parallel}\, \mathbf{v}\cdot\frac{\partial F}{\partial \mathbf{x}} - \frac{e}{2c}\iint d^3x\, d^3v \left(f - \frac{e}{mc}\mathbf{A}\cdot\frac{\partial g}{\partial \mathbf{v}}\right)\mathbf{v}\cdot\frac{\partial \delta\psi}{\partial \mathbf{x}} + \int d^3x\left[\frac{1}{4\pi}\frac{\omega_p^2}{c^2}\mathbf{A} + \frac{1}{c}\mathbf{j}\right]\cdot\delta\mathbf{A}. \tag{31}$$

Two integrations by parts, first with respect to $\mathbf{x}$ and then with respect to $x_\parallel$ show that the second integral is equal to the first, hence

$$\delta c_2 = -\frac{e}{c}\iint d^3x\, d^3v\, f\mathbf{v}\cdot\delta\mathbf{A} + \frac{e^2}{mc^2}\iint d^3x\, d^3v\, \mathbf{A}\cdot\frac{\partial g}{\partial \mathbf{v}}\,\mathbf{v}\cdot\delta\mathbf{A} + \int d^3x\left[\frac{1}{4\pi}\frac{\omega_p^2}{c^2}\mathbf{A} + \mathbf{j}\right]\cdot\delta\mathbf{A}. \tag{32}$$

Finally an integration by parts with respect to $\mathbf{v}$ in the second integral shows that $\delta c_2 = 0$. Analogously $\delta \mathbf{c}_1 = 0$.

The invariance under change of primitive

$$F \to F + \delta F(\mathbf{x}_\perp, \mathbf{v}, t)$$

is quite trivial.

$$\delta c_2 = \frac{m}{2}\iint d^3x\, d^3v\, \frac{\bar{f}}{|\partial g/\partial \mathbf{v}|}\,\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\,\delta F(\mathbf{x}_\perp, \mathbf{v}, t). \tag{33}$$

But $\bar{f} = \partial F/\partial x_\parallel$ so that

$$\delta c_2 = \frac{m}{2}\iint d^3x\, d^3v\, \frac{1}{|\partial g/\partial \mathbf{v}|}\,\frac{\partial F}{\partial x_\parallel}\,\mathbf{v}\cdot\frac{\partial \delta F}{\partial \mathbf{x}}. \tag{34}$$

Transfering the $x_\parallel$ derivative nullifies the integral. Likewise, $\delta \mathbf{c}_1 = 0$.

IV. REMARKS AND SAMPLE STABILITY PROBLEM

These constants, at least in their present ungeneralized form, are intimately related to the second-order momentum and energy constants of the system

$$\mathrm{II}_2 = m\iint d^3x\, d^3v\, \mathbf{v} f_2(x, v, t) + \frac{1}{4\pi c}\int d^3x\, \mathbf{E}\times\mathbf{B}, \tag{35}$$

and

$$\mathcal{E}_2 = \frac{m}{2}\iint d^3x\, d^3v\, v^2 f_2 + \frac{1}{8\pi}\int d^3x(\mathbf{E}^2 + \mathbf{B}^2), \tag{36}$$

since one sees the electromagnetic momentum and energy as ingredients of (26) and (18). The existence of other constants as in Ref. 2 between which and the second-order momentum and energy the explicitly second-order particle momentum and kinetic energy may be eliminated, has not been demonstrated. Since they are not revealed by the rather more systematic derivation given in the Appendix, their existence is, in general, doubted.

To give some insight into the physical significance of these constants as well as an inkling of their power in stability considerations let us consider the situation when $g(\mathbf{v}) = h[\frac{1}{2}(\mathbf{v} - \mathbf{V}_0)^2]$, i.e., when the equilibrium distribution function is isotropic around some center $\mathbf{V}_0$. Let us consider the combination of constants

$$c_2 - \mathbf{V}_0\cdot\mathbf{c}_1 = \frac{m}{2}\iint d^3x\, d^3v\, \frac{\bar{f}(\mathbf{v} - \mathbf{V}_0)\cdot\partial F/\partial \mathbf{x}}{|\partial g/\partial \mathbf{v}|} + \frac{1}{c}\int d^3x\,(\mathbf{j} - \sigma\mathbf{V}_0)\cdot\mathbf{A} - \frac{1}{8\pi}\int d^3x\left[\mathbf{E}^2 + \mathbf{B}^2 - \frac{\omega_p^2}{c^2}\mathbf{A} + 2\mathbf{E}\cdot\frac{\mathbf{V}_0}{c}\times\mathbf{B}\right]. \tag{37}$$

If we note that

$$\frac{(\mathbf{v} - \mathbf{V}_0)}{|\partial g/\partial \mathbf{v}|}\cdot\frac{\partial}{\partial x} = \frac{1}{h'}\,e_\parallel\cdot\frac{\partial}{\partial \mathbf{x}} = \frac{1}{h'}\,\frac{\partial}{\partial x_\parallel} \tag{38}$$

and employ (6) and (9), then (37) becomes

$$c_2 - \mathbf{V}_0\cdot\mathbf{c}_1 = \frac{m}{2}\iint d^3x\, d^3v\, \frac{f^2}{h'} - \frac{e}{c}\iint d^3x\, d^3v\, \mathbf{A}\cdot(\mathbf{v} - \mathbf{V}_0)f + \frac{e^2}{2mc^2}\iint d^3x\, d^3v\, \mathbf{A}\cdot\frac{\partial g}{\partial \mathbf{v}}\,\mathbf{A}\cdot(\mathbf{v} - \mathbf{V}_0) + \frac{1}{c}\int d^3x\,(\mathbf{j} - \sigma\mathbf{V}_0)\cdot\mathbf{A} - \frac{1}{8\pi}\int d^3x\left[\mathbf{E}^2 + \mathbf{B}^2 - \frac{\omega_p^2}{c^2}\mathbf{A} + 2\mathbf{E}\cdot\frac{\mathbf{V}_0}{c}\times\mathbf{B}\right]. \tag{39}$$

Now all terms involving $\mathbf{A}$ cancel and we are left with

$$c_2 - \mathbf{V}_0\cdot\mathbf{c}_1 = \frac{m}{2}\iint d^3x\, d^3v\, \frac{f^2}{h'} - \frac{1}{8\pi}\int d^3x \times\left[\left(\mathbf{E} + \frac{\mathbf{V}_0}{c}\times\mathbf{B}\right)^2 + \mathbf{B}^2 - \frac{1}{c^2}(\mathbf{V}_0\times\mathbf{B})^2\right]. \tag{40}$$

This expression is just a slight generalization of the "free energy" used by Newcomb (see Appendix I, Ref. 1) to show stability of the Maxwell distribution. It shows at once that any distribution which is a decreasing monotone (about any shifted velocity $\mathbf{V}_0$) function of the particle kinetic energy ($h' < 0$), is

stable since the quadratic form (40) is (negative) definite. Note that in this elementary situation the integrand of the first integral appearing in (42) has become local.

V. GENERALIZATIONS

(A) Actually each of these constants is just one member of a continuous family of constants the existence of which reflects the invariance of the equilibrium under spatial translations. An alternate aspect of this invariance is that in any quadratic global constant, there is no coupling of the different $\mathbf{k}$ modes resulting from Fourier transformation on $\mathbf{x}$ (see Appendix). Namely, if preceding (11) and (19) we displace the $\mathbf{x}$ variable in the equation for F by a constant ξ we find the derivations still go through, so that we have the generalized constants

$$C_1 = \int_{-\infty}^{\infty} d^3\xi\, \mathbf{V}(\xi)\cdot\left\{\frac{m}{2}\iint d^3x\, d^3v \int_0^{\infty} ds \times \frac{\partial f}{\partial \mathbf{x}}\left(\mathbf{x} + \xi - s\frac{\partial g}{\partial \mathbf{v}}, v, t\right) f(\mathbf{x}, \mathbf{v}, t) - \frac{1}{c}\int d^3x \left[\frac{1}{4\pi}\mathbf{E}(\mathbf{x}, t)\times\mathbf{B}(\mathbf{x}+\xi, t) - \sigma(\mathbf{x}, t)\mathbf{A}(\mathbf{x}+\xi, t)\right]\right\}, \tag{41}$$

and

$$C_2 = \int_{-\infty}^{\infty} d^3\xi\, S(\xi)\cdot\left\{\frac{m}{2}\iint d^3x\, d^3v \int_0^{\infty} ds\, \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}} \times \left(\mathbf{x} + \xi - s\frac{\partial g}{\partial \mathbf{v}}, \mathbf{v}, t\right) f(\mathbf{x}, \mathbf{v}, t) - \int d^3x \frac{1}{8\pi}(\mathbf{E}(\mathbf{x}, t)\cdot E(\mathbf{x}+\xi, t) + B(\mathbf{x}, t)\cdot B(\mathbf{x}+\xi, t) - (\omega_p^2/c^2)\mathbf{A}(\mathbf{x}, t)\cdot A(\mathbf{x}+\xi, t)) - (1/c)j(\mathbf{x}, t)\cdot A(\mathbf{x}+\xi, t)\right]\right\}, \tag{42}$$

where $\mathbf{V}$ and S are arbitrary vector and scalar functions of ξ, respectively. This generalization applies, of course, only for the spatially homogeneous equilibrium. [In (41) there are actually three such constants corresponding to the three independent components of $\mathbf{V}$.]

(B) The constants (18) and (26) persist, with slight modification, in a completely relativistic theory, for if we write down the relativistic generalization of (1),

$$\frac{\partial f(\mathbf{x}, \mathbf{p}, t)}{\partial t} + \mathbf{v}(\mathbf{p})\cdot\frac{\partial f}{\partial \mathbf{x}} + e\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)\cdot\frac{\partial g(\mathbf{p})}{\partial \mathbf{p}} = 0, \tag{43}$$

with

$$\mathbf{p} \equiv (1 - v^2/c^2)^{-\frac{1}{2}} m\mathbf{v}, \tag{44}$$

we find corresponding to (26) and (18)

$$\mathbf{c}_{1r} = \frac{1}{2}\iint d^3x\, d^3p \frac{\bar{f}_r \nabla F_r}{|\partial g/\partial p|} + \frac{1}{c}\int d^3x \left[\sigma\mathbf{A} - \frac{1}{4\pi}\mathbf{E}\times\mathbf{B}\right], \tag{45}$$

$$c_{2r} = \frac{1}{2}\iint d^3x\, d^3p \frac{\bar{f}_r \mathbf{v}(\mathbf{p})\cdot\nabla F_r}{|\partial g/\partial \mathbf{p}|} + \frac{1}{c}\int d^3x \left[\mathbf{j}\cdot\mathbf{A} - \frac{(E^2 + B^2)}{8\pi}\right] + \frac{e^2}{2c^2}\iint d^3x\, d^3p\, g(\mathbf{p})\mathbf{A}\cdot\frac{\partial \mathbf{v}}{\partial \mathbf{p}}\cdot\mathbf{A}. \tag{46}$$

Here, from (44)

$$\partial \mathbf{v}/\partial p = c(p^2 + m^2c^2)^{-\frac{1}{2}}[(p^2 + m^2c^2)\mathbf{I} - \mathbf{pp}], \tag{47}$$

while

$$\bar{f}_r = f - (e/c)\mathbf{A}\cdot\partial g/\partial \mathbf{p}, \tag{48}$$

and F_r is defined by

$$\bar{f}_r \equiv \partial F_r/\partial x_1. \tag{49}$$

$\mathbf{I}$ is the unit dyadic.

(C) It is readily verified that if one considers perturbations about the unidimensional nonlinear electrostatic solutions of Ref. 4, i.e. about the solutions of

$$v\frac{\partial g(x, v)}{\partial x} - \frac{e}{m}\frac{\partial \Phi}{\partial x}\frac{\partial g(x, v)}{\partial v} = 0, \tag{50}$$

and

$$\frac{\partial^2 \Phi}{\partial x^2} = -4\pi e\left[\int dv\, g - n_0\right], \tag{51}$$

one finds a constant corresponding to (18),

$$c_2 = \frac{m}{2}\iint d^3x\, d^3v \frac{vf^2}{\partial g/\partial v} - \frac{1}{8\pi}\int d^3x\left(\frac{\partial \phi}{\partial x}\right)^2, \tag{52}$$

where f and ϕ are the perturbed distribution function and electrostatic potential respectively. No analog of c_1 is found. This constant c_2 is of particular value in studying the stability of plasma sheaths.[5]

[5] See e.g., M. N. Rosenbluth, L. M. Pearlstein, and G. Stuart, Phys. Fluids 6, 1289 (1963).

(D) So far we have dealt with constants which are local in the velocity space. There is an important generalization away from this. To illustrate this particular generalization we shall deal for simplicity in this subsection with perturbations of a spatially uniform plasma and consider only the electrostatic interaction. In $\mathbf{k}$ space we then have

$$\frac{\partial f_k}{\partial t} + i\mathbf{k}\cdot\mathbf{v}f_k + \frac{e}{mk^2}\mathbf{E}\cdot\mathbf{k}\mathbf{k}\cdot\frac{\partial g}{\partial v} = 0, \tag{53}$$

$$i\mathbf{k}\cdot\mathbf{E}_k = 4\pi e\int d^3v\, f_k, \tag{54}$$

$$\mathbf{k}\times\mathbf{E}_k = 0. \tag{55}$$

If we proceed as in the appendix we find not only the aforementioned constants with $\mathbf{B} = \mathbf{A} = 0$, but also a *third* constant

$$c_3 = \int d^3k\, B_*(\mathbf{k})\cdot\mathbf{k}\int d^3v\Big[m\frac{(\mathbf{k}\cdot\mathbf{v})^2}{\mathbf{k}\cdot\partial g/\partial\mathbf{v}} f_k f_{-k} - ie(\mathbf{E}_k\cdot\mathbf{v}f_{-k} - \mathbf{E}_{-k}\cdot\mathbf{v}f_k)\Big]. \tag{56}$$

Are there even more constants if we appropriately generalize the form (A1)? Before going into detail we point out there must be more by noting that we may first multiply (53) by $\delta(u - \hat{\mathbf{k}}\cdot\mathbf{v})$, where $\hat{k} = \mathbf{k}/k$, and then integrate over the velocity space to obtain

$$\frac{\partial\tilde{f}_k(u,\,t)}{\partial t} + iku\tilde{f}_k + \frac{e}{m}\mathbf{E}_k\cdot\hat{\mathbf{k}}\frac{\partial\tilde{g}}{\partial u} = 0, \tag{57}$$

$$i\mathbf{k}\cdot\mathbf{E}_k = 4\pi e\int du\,\tilde{f}_k, \tag{58}$$

where the operation indicated with a tilde is given by

$$\tilde{f}_k(u,\,t) = \int d^3v\, f_k(\mathbf{v},\,t)\,\delta(u - \hat{\mathbf{k}}\cdot\mathbf{v}), \quad \text{etc.} \tag{59}$$

Here δ is the Dirac delta function. We may now construct constants by the previous method on this set of equations, e.g.,

$$c_2 = \int d^3k\, B_2(\mathbf{k})\Big[\int du\,\frac{mu\tilde{f}_k\tilde{f}_{-k}}{2\tilde{g}'(u)} - \frac{|E_k|^2}{8\pi}\Big]. \tag{60}$$

This set of constants is in a sense more powerful in that one can show at once that any isotropic (not necessarily monotone!) equilibrium $g(\mathbf{v})$ is stable. [For $g(u)$ is monotone decreasing in u, since it is readily shown that every uniformly populated spherical shell in $\mathbf{v}$ space projects into a symmetric positive block in u space.]

All types of these constants so far considered (for the spatially homogeneous equilibria) are embraced by

$$C = \iiint d^3k\, d^3v\, d^3\bar{v}\, A_k(\mathbf{v},\,\bar{\mathbf{v}})f_k(\mathbf{v})f_{-k}(\bar{\mathbf{v}}), \tag{61}$$

where without loss of generality we may take

$$A_{-k}(\bar{\mathbf{v}},\,\mathbf{v}) = A_k(\mathbf{v},\,\bar{\mathbf{v}}). \tag{62}$$

For this problem we regard $\mathbf{E}_k$ as having been eliminated, so that f_k satisfies

$$\frac{\partial f_k}{\partial t} = i\mathbf{k}\cdot\mathbf{v}f_k + \frac{i4\pi e^2}{mk^2}\mathbf{k}\cdot\frac{\partial g}{\partial\mathbf{v}}\int d^3v\, f_k. \tag{63}$$

If, as in the Appendix, we now take the time derivative of (61), use (62) to eliminate time derivatives, demand that the resultant quadratic form in f vanish for arbitrary f, and hence set equal to zero the second functional derivative of this resultant form with respect to f_k and f_{-k}, we obtain the following equation for the determination of A_k:

$$(\hat{\mathbf{k}}\cdot\mathbf{v} - \hat{\mathbf{k}}\cdot\bar{\mathbf{v}})A_k(\mathbf{v},\,\bar{\mathbf{v}}) = R_k(\bar{\mathbf{v}}) - R_k(\mathbf{v}), \tag{64}$$

where

$$R_k(\mathbf{v}) = \frac{4\pi e^2}{mk^2}\int d^3\bar{v}\,\hat{\mathbf{k}}\cdot\frac{\partial g(\bar{\mathbf{v}})}{\partial\bar{\mathbf{v}}}\,A_k(\mathbf{v},\,\bar{\mathbf{v}}). \tag{65}$$

(A_k is not to be confused with the vector potential $\mathbf{A}$ introduced earlier.) [From here on we absorb the factor in front of the integral (65) into g and we drop the subscript k.] The equation for A may be solved. From (64)

$$A(\mathbf{v},\,\bar{\mathbf{v}}) = [R(\mathbf{v}) - R(\bar{\mathbf{v}})]/[\hat{\mathbf{k}}\cdot\bar{\mathbf{v}} - \hat{\mathbf{k}}\cdot\mathbf{v}] + Q(\mathbf{v},\,\bar{\mathbf{v}})\,\delta(\hat{\mathbf{k}}\cdot\bar{\mathbf{v}} - \hat{\mathbf{k}}\cdot\mathbf{v}), \tag{66}$$

and thus from (65)

$$R(\mathbf{v})\Big[1 - P\int d^3\bar{v}\,\frac{\hat{\mathbf{k}}\cdot(\partial g/\partial\bar{\mathbf{v}})}{\hat{\mathbf{k}}\cdot\bar{\mathbf{v}} - \hat{\mathbf{k}}\cdot\mathbf{v}}\Big] + P\int d^3\bar{v}\,\frac{\hat{\mathbf{k}}\cdot(\partial g/\partial\bar{\mathbf{v}})R(\mathbf{v})}{\hat{\mathbf{k}}\cdot\bar{\mathbf{v}} - \hat{\mathbf{k}}\cdot\mathbf{v}} = Y(\mathbf{v}), \tag{67}$$

where

$$Y(\mathbf{v}) = \int d^3\bar{v}\,\mathbf{k}\cdot\frac{\partial g}{\partial\bar{\mathbf{v}}}\,Q(\mathbf{v},\,\bar{\mathbf{v}})\,\delta(\hat{\mathbf{k}}\cdot\bar{\mathbf{v}} - \hat{\mathbf{k}}\cdot\mathbf{v}), \tag{68}$$

and the symbol P denotes principal value of the integrals. If we now define $S(\mathbf{v}) \equiv R(\mathbf{v})\hat{\mathbf{k}}\cdot\partial g/\partial\mathbf{v}$, $Z(\mathbf{v}) \equiv Y(\mathbf{v})\hat{\mathbf{k}}\cdot\partial g/\partial\mathbf{v}$, and the tilde operation

$$\tilde{S}(u) = \int d^3v\, S(\mathbf{v})\,\delta(u - \hat{\mathbf{k}}\cdot\mathbf{v}), \quad \text{etc.}, \tag{69}$$

then multiplying (67) by $\hat{\mathbf{k}}\cdot\partial g/\partial\mathbf{v}$ and performing

the tilde operation yields

$$\tilde{S}(u)\left[1 - P\int du' \frac{\partial\tilde{g}/\partial u'}{u' - u}\right] + \frac{\partial\tilde{g}}{\partial u} P\int du' \frac{\tilde{S}(u')}{u' - u} = \tilde{Z}(u). \quad (70)$$

The problem is now reduced to the standard inhomogeneous Hilbert problem.[6] Define

$$S(z) = \int du \frac{\tilde{S}(u)}{u - z} \quad (71)$$

and

$$\rho(z) = 1 - \int du \frac{\partial\tilde{g}/\partial u}{u - z}. \quad (72)$$

Then (70) reads

$$S_+(u)\rho_-(u) - S_-(u)\rho_+(u) = 2\pi i\tilde{Z}(u), \quad (73)$$

where

$$S_\pm = \lim_{\epsilon\to 0^+} \int du' \frac{\tilde{S}(u')}{u' - u \mp i\epsilon}, \quad \text{etc.} \quad (74)$$

We may proceed to the solution at once if the analytic properties of $\rho(z)$ are known! This, on the surface, would seem a painful step for us to take, because the initial motivation for this whole investigation was to ultimately obtain stability criteria (not specifically in this paper) without ultilizing a detailed *a priori* knowledge of the dispersion function, i.e., of the stability of g. Indeed, we have obtained all the constants previously discussed without this knowledge.

For the moment we proceed as if the system were stable, i.e., $\rho(z)$ is sectionally regular and nonvanishing, and $\rho(z) \to 1$ as $z \to \infty$. In this case the index of the integral equation (73) is zero and the equation has a unique solution vanishing at infinity,

$$S(z) = \rho(z)\int du \frac{\tilde{Z}(u)}{\rho_+(u)\rho_-(u)(u - z)}. \quad (75)$$

This gives at once, from (67), (71), and (72),

$$R(\mathbf{v}) = \frac{2Y(\mathbf{v})}{\rho_+(\hat{\mathbf{k}}\cdot\mathbf{v}) + \rho_-(\hat{\mathbf{k}}\cdot\mathbf{v})} - \frac{S_+(\hat{\mathbf{k}}\cdot\mathbf{v}) + S_-(\hat{\mathbf{k}}\cdot\mathbf{v})}{\rho_+(\hat{\mathbf{k}}\cdot\mathbf{v}) + \rho_-(\hat{\mathbf{k}}\cdot\mathbf{v})}. \quad (76)$$

We now demonstrate a multitude of constants. Let us assume $Y_1(\mathbf{v}) = \hat{\mathbf{k}}$, then $\tilde{Z}(u) = \hat{\mathbf{k}}\partial\tilde{g}/\partial u$.

[6] N. T. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff, Ltd., Groningen, The Netherlands, 1953), p. 86, *et seq.*

Then

$$R(\mathbf{v}) = \hat{\mathbf{k}}\left[\frac{2}{\rho_+(\hat{\mathbf{k}}\cdot\mathbf{v}) + \rho_-(\hat{\mathbf{k}}\cdot\mathbf{v})} - \frac{\rho_+(\hat{\mathbf{k}}\cdot\mathbf{v})}{\rho_+(\hat{\mathbf{k}}\cdot\mathbf{v}) + \rho_-(\hat{\mathbf{k}}\cdot\mathbf{v})} \times \int du \frac{\partial\tilde{g}/\partial u}{\rho_+(u)\rho_-(u)(u - \hat{\mathbf{k}}\cdot\mathbf{v} - i\epsilon)} - \frac{\rho_-(\hat{\mathbf{k}}\cdot\mathbf{v})}{\rho_+ + \rho_-}\int du \frac{\partial\tilde{g}/\partial u}{\rho_+(u)\rho_-(u)(u - \hat{\mathbf{k}}\cdot\mathbf{v} + i\epsilon)}\right]. \quad (77)$$

We now examine the integrals occurring in (77), for instance,

$$I_+(\hat{\mathbf{k}}\cdot\mathbf{v}) \equiv \int \frac{\partial\tilde{g}/\partial u}{\rho_+(u)\rho_-(u)(u - \hat{\mathbf{k}}\cdot\mathbf{v} - i\epsilon)} \quad (78)$$

or

$$I_+ = -\frac{1}{2\pi i}\int \frac{du}{u - \hat{\mathbf{k}}\cdot\mathbf{v} - i\epsilon} \times \left[\left(\frac{1}{\rho_-(u)} - 1\right) - \left(\frac{1}{\rho_+(u)} - 1\right)\right]. \quad (79)$$

The addition and subtraction of unity has made each of the terms in the bracket of (70) vanishing (like $1/z^2$) as $z \to \infty$. For the first parentheses we now close the contour in the lower half-plane to give zero, while for the second parentheses we close in the upper half-plane to obtain

$$I_\pm = 1/\rho_\pm(\hat{\mathbf{k}}\cdot\mathbf{v}) - 1, \quad (80)$$

and thus

$$R_1(\mathbf{v}) = \hat{\mathbf{k}}. \quad (81)$$

Likewise, if $Y_2(\mathbf{v}) = \hat{\mathbf{k}}\cdot\mathbf{v}$ then $R_2(\mathbf{v}) = \hat{\mathbf{k}}\cdot\mathbf{v}$. [These solutions are trivially verified by inspection of (67).] These two expressions for $Y(\mathbf{v})$ could emanate, for example, *either* from

$$Q_1(\mathbf{v}, \bar{\mathbf{v}}) = \frac{\hat{\mathbf{k}}}{\hat{\mathbf{k}}\cdot\partial g/\partial v}\,\delta(\mathbf{v}_\perp - \bar{\mathbf{v}}_\perp), \quad (82)$$

and

$$Q_2(\mathbf{v}. \bar{\mathbf{v}}) = \frac{\hat{\mathbf{k}}\cdot\mathbf{v}}{\hat{\mathbf{k}}\cdot\partial g/\partial\mathbf{v}}\,\delta(\mathbf{v}_\perp - \bar{\mathbf{v}}_\perp), \quad (83)$$

or from

$$Q_1'(\mathbf{v}, \bar{\mathbf{v}}) = \hat{\mathbf{k}}\Big/\int d^3v'\,\hat{\mathbf{k}}\cdot\frac{\partial g}{\partial\mathbf{v}'}\,\delta(\hat{\mathbf{k}}\cdot\mathbf{v} - \hat{\mathbf{k}}\cdot\mathbf{v}'), \quad (84)$$

and

$$Q_2'(\mathbf{v}, \bar{\mathbf{v}}) = \hat{\mathbf{k}}\cdot\mathbf{v}\Big/\int d^3v'\,\hat{\mathbf{k}}\cdot\frac{\partial g}{\partial\mathbf{v}'}\,\delta(\hat{\mathbf{k}}\cdot\mathbf{v} - \hat{\mathbf{k}}\cdot\mathbf{v}'). \quad (85)$$

These Q's and Q''s with their corresponding R's (the same R's for both Q and Q'!) give rise to the constants c_1 and c_2 emanating from (53) and (57).

More generally, it is readily seen that a Q (and similarly for Q') of the form

$$Q_n = \frac{(\hat{\mathbf{k}}\cdot\mathbf{v})^n}{\hat{\mathbf{k}}\cdot\partial g/\partial \mathbf{v}}\,\delta(\mathbf{v}_\perp - \bar{\mathbf{v}}_\perp) \tag{86}$$

gives rise to a $R_n(\mathbf{v})$ which is a polynomial of the nth degree in $(\hat{\mathbf{k}}\cdot\mathbf{v})$ with coefficients made up of moments of g. [Here one must add and subtract more and more terms in the large z expansion of $1/\rho(z)$ as in (79).]

This homomorphism between Q and Y has not been fully explored, i.e., we have not given the general solution of Q in terms of Y from (68), but this should not be too difficult.

We choose this paper by asserting that if the distribution is unstable [$\rho(z)$ has zeros, as a matter of fact in pairs since from (72) both z and z^* are roots] then the integral equation is of positive even index. Now it turns out that the constants (86) persist, but in addition there are new constants associated with the now nontrivial solutions of the homogeneous equation corresponding to (73). This is not surprising because we now have some discrete unstable Van Kampen–Case[7] modes in addition to the continuum modes. We do not elaborate further here.

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APPENDIX

We give here an alternative derivation of these constants, in one sense more straightforward, but in another sense more limited in that it is only appropriate, without severe generalization, to the case where the equilibrium is independent of position. That is, we shall take advantage of the knowledge that if the $\mathbf{x}$ variable is Fourier-transformed then different $\mathbf{k}$ modes do not couple. We begin by demanding that the rather general quadratic form

$$\begin{aligned} Q = \int d^3k \Big\{ \int d^3v [&\tfrac{1}{2}\alpha_k(\mathbf{v}) f_k(\mathbf{v}, t) f_{-k}(\mathbf{v}, t) \\ &+ \beta_k(\mathbf{v})\cdot\mathbf{B}_k(t) f_{-k} + \varepsilon_k(\mathbf{v})\cdot\mathbf{E}_k(t) f_{-k}] \\ &+ \tfrac{1}{2}\mathbf{E}_k\cdot\lambda_k\cdot\mathbf{E}_{-k} + \mathbf{E}_k\cdot\mu_k\cdot\mathbf{B}_{-k} + \tfrac{1}{2}\mathbf{B}_k\cdot\nu_k\cdot\mathbf{B}_{-k} \Big\} \end{aligned} \tag{A1}$$

be a constant of the motion, with the scalar α, the vectors β and ε, and the dyadics λ, μ, ν to be determined. Without loss of generality we may assume

$$\alpha_k(\mathbf{v}) = \alpha_{-k}(\mathbf{v}), \quad \tilde{\lambda}_{-k} = \lambda_k, \quad \tilde{\nu}_{-k} = \nu_k, \tag{A2}$$

and

$$\hat{\mathbf{k}}\cdot\beta_k = 0, \quad \mu_k\cdot\mathbf{k} = 0, \quad \nu_k\cdot\mathbf{k} = \mathbf{k}\cdot\nu_k = 0. \tag{A3}$$

The symbol $\sim$ here means transpose.

Now upon taking the time derivative of (A1), demanding that it vanish, and utilizing the equations of motion, there results

$$\begin{aligned} 0 = \int d^3k \Big\{ \int d^3v \Big[&-(\alpha_k f_k + \beta_k\cdot\mathbf{B}_k + \varepsilon_k\cdot\mathbf{E}_k) \\ &\times [-i\mathbf{k}\cdot\mathbf{v} f_k + (\mathbf{E}_{-k} + \mathbf{v}\times\mathbf{B}_{-k})\cdot\partial g/\partial\mathbf{v}] \\ &+ \Big(-i\mathbf{k}\times\mathbf{E}_k\cdot\beta_k + i\mathbf{k}\times\mathbf{B}_k\cdot\epsilon_k \\ &- \varepsilon_k\cdot\int d^3v'\, \mathbf{v}' f_k(\mathbf{v}')\Big) f_{-k}\Big] \\ &+ i\mathbf{k}\times\mathbf{B}_k\cdot\lambda_k\cdot\mathbf{E}_{-k} - \int d^3v'\, \mathbf{v}' f_k(\mathbf{v}')\cdot\lambda_k\cdot E_{-k} \\ &- i\mathbf{k}\times\mathbf{E}_k\cdot\nu_k\cdot\mathbf{B}_{-k} + i\mathbf{k}\times\mathbf{B}\cdot\mu_k\cdot\mathbf{B}_{-k} \\ &- \int d^3v'\, \mathbf{v}' f(\mathbf{v}')\cdot\mu_k\cdot\mathbf{B}_{-k} + i\mathbf{E}_k\cdot\mu_k\cdot\mathbf{k}\times\mathbf{E}_k \Big\}. \end{aligned} \tag{A4}$$

Since this must be true for all f_k, $\mathbf{E}_k$, $\mathbf{B}_k$, after eliminating $\mathbf{k}\cdot\mathbf{E}_k$ and $\mathbf{k}\cdot\mathbf{B}_k$ by

$$i\mathbf{k}\cdot\mathbf{E}_k = \int d^3v\, f_k \tag{A5}$$

and

$$\mathbf{k}\cdot\mathbf{B}_k = 0, \tag{A6}$$

we set all the second functional derivatives with respect to f_k, $\mathbf{k}\times\mathbf{E}_k$, and $\mathbf{k}\times\mathbf{B}_k$ equal to zero to obtain the following set of equations for the undetermined coefficients:

$$\begin{aligned} &i\alpha_k\mathbf{k}\cdot\frac{\partial g}{\partial\mathbf{v}} - i\bar{\alpha}_k\mathbf{k}\cdot\frac{\partial\bar{g}}{\partial\bar{\mathbf{v}}} + \mathbf{k}\cdot\mathbf{v}\epsilon_k\cdot\frac{\mathbf{k}}{k^2} + \mathbf{k}\cdot\bar{\mathbf{v}}\,\frac{\mathbf{k}}{k^2}\,\bar{\varepsilon}_{-k} \\ &\quad - \mathbf{v}\cdot\bar{\varepsilon}_{-k} - \bar{\mathbf{v}}\cdot\varepsilon_k + i\mathbf{v}\cdot\lambda_{-k}\cdot\frac{\mathbf{k}}{k^2} - i\bar{\mathbf{v}}\cdot\lambda_k\cdot\frac{\mathbf{k}}{k^2} \\ &\quad - \frac{1}{k^4}\int d^3v\, \mathbf{k}\cdot(\varepsilon_k + \varepsilon_{-k})\mathbf{k}\cdot\frac{\partial g}{\partial\mathbf{v}} = 0, \end{aligned} \tag{A7}$$

$$\begin{aligned} &\frac{1}{k^2}\alpha_k\mathbf{k}\times\Big(\mathbf{v}\times\frac{\partial g}{\partial\mathbf{v}}\Big) + i\varepsilon_k - \lambda_k\cdot\frac{\mathbf{k}}{k^2} \\ &\quad + \mathbf{v}\cdot\mu_{-k}\times\frac{\mathbf{k}}{k^2} + \frac{i}{k^2}\,\mathbf{k}\cdot\mathbf{v}\mathbf{k}\times\beta_k \\ &\quad - \frac{i}{k^4}\int d^3v\, \mathbf{k}\cdot\frac{\partial g}{\partial\mathbf{v}}\,\mathbf{k}\times\beta_k \\ &\quad + \frac{i}{k^4}\int d^3v\, \mathbf{k}\times\Big(\mathbf{v}\times\frac{\partial g}{\partial\mathbf{v}}\Big)\mathbf{k}\cdot\varepsilon_{-k} = 0, \end{aligned} \tag{A8}$$

[7] See K. M. Case, Ann. Phys. 7, 349 (1959).

$$-\frac{1}{k^2}\alpha_k\mathbf{k}\times\frac{\partial g}{\partial \mathbf{v}} - i\beta_k + \frac{\mathbf{k}}{k^2}\cdot\mathfrak{y}_{-k} + \mathbf{v}\cdot\lambda_{-k}\times\frac{k}{k^2} + i\mathbf{k}\cdot\mathbf{v}\frac{k}{k^2}\times\varepsilon_k - \frac{i}{k^4}\int d^3v\,\mathbf{k}\cdot\frac{\partial g}{\partial \mathbf{v}}\mathbf{k}\times\varepsilon_k - \frac{i}{k^4}\int d^3v\,\mathbf{k}\times\frac{\partial g}{\partial \mathbf{v}}\epsilon_{-k}\cdot k = 0, \tag{A9}$$

$$\frac{i}{k^2}\mathbf{k}\times\tilde{\mathfrak{y}}_k + \frac{i}{k^2}\mathfrak{y}_{-k}\times\mathbf{k} + \frac{1}{k^4}\int d^3v\,\mathbf{k}\times\left(\mathbf{v}\times\frac{\partial g}{\partial \mathbf{v}}\right)\times\mathbf{k}\times(\beta_k + \beta_{-k}) = 0, \tag{A10}$$

$$\frac{i}{k^2}\tilde{\mathfrak{y}}_k\times\mathbf{k} + \frac{i}{k^2}\mathbf{k}\times\mathfrak{y}_{-k} + \frac{1}{k^4}\int d^3v\,\mathbf{k}\times\frac{\partial g}{\partial \mathbf{v}}\times\mathbf{k}\times(\varepsilon_k + \varepsilon_{-k}) = 0, \tag{A11}$$

$$\frac{i}{k^2}\mathbf{k}\times\lambda_{-k} - \frac{i}{k^2}\mathbf{v}_{-k}\times\mathbf{k} - \frac{1}{k^4}\int d^3v\,\mathbf{k}\times\frac{\partial g}{\partial \mathbf{v}}\mathbf{k}\times\beta_k + \frac{1}{k^4}\int d^3v\,\mathbf{k}\times\varepsilon_{-k}\mathbf{k}\times\left(\mathbf{v}\times\frac{\partial g}{\partial \mathbf{v}}\right) = 0. \tag{A12}$$

Here $\bar{\alpha}_k \equiv \alpha_k(\bar{\mathbf{v}})$, etc. Actually this rather formidable looking set of equations is not difficult to solve. Upon dotting (A8)–(A12) with $\mathbf{k}$ and using (A2) and (A3), we obtain

$$\mathbf{k}\cdot\varepsilon_k = -i(\mathbf{kk}/k^2) : \lambda_k, \tag{A13a}$$

hence

$$\mathbf{k}\cdot(\varepsilon_k + \varepsilon_{-k}) = 0, \tag{A13b}$$

$$\mathbf{k}\cdot\mathfrak{y}_k\cdot\mathbf{k} = \mathbf{k}\cdot\mathfrak{y}_k\times\mathbf{k} = \mathbf{k}\times\mathfrak{y}_k\cdot\mathbf{k} = \mathbf{k}\cdot\lambda_k\times\mathbf{k} = \mathbf{k}\times\lambda_k\cdot\mathbf{k} = \mathbf{k}\cdot\mathbf{v}_k\times\mathbf{k} = \mathbf{k}\times\mathbf{v}_k\cdot\mathbf{k} = 0. \tag{A13c}$$

If we set $\bar{v} = 0$ in (A7) we find, with $C_k \equiv \alpha_k\mathbf{k}\cdot\partial g/\partial\mathbf{v}$, that C_k is a linear form in $\mathbf{v}$,

$$C_k = C_k^0 + \mathbf{C}_k\cdot\mathbf{v}. \tag{A14}$$

If now (A9) is inserted into (A8) there results

$$C_k[\mathbf{v} - (\mathbf{kk}/k^2)\cdot\mathbf{v}] + i\varepsilon_{k\perp}[k^2 - (\mathbf{k}\cdot\mathbf{v})^2] + \mathbf{v}\cdot\mathfrak{y}_{-k}\times\mathbf{k} + \mathbf{k}\cdot\mathbf{v}\cdot\lambda_{-k}\cdot\left[\mathbf{I} - \frac{\mathbf{kk}}{k^2}\right] + \frac{i}{k^2}\mathbf{k}\cdot\mathbf{v}\int d^3v\,\mathbf{k}\cdot\frac{\partial g}{\partial \mathbf{v}}\varepsilon_{k\perp} = \frac{1}{k^2}\int d^3v\,\mathbf{k}\cdot\frac{\partial g}{\partial \mathbf{v}}\left[\frac{\alpha_k}{k^2}\mathbf{k}\times\left(\frac{\partial g}{\partial \mathbf{v}}\times\mathbf{k}\right) - i\mathbf{k}\cdot\mathbf{v}\varepsilon_{k\perp}\right]. \tag{A15}$$

Here $\varepsilon_{k\perp} = \varepsilon_k\cdot[\mathbf{I} - \mathbf{kk}/k^2]$. The integral on the rhs of (A15) is zero, which is seen by taking $\mathbf{v}$ first in the direction of $\mathbf{k}$ and then oppositely oriented. Next, if $\mathbf{v}$ is taken zero we conclude

$$\varepsilon_{k\perp}^0 = 0. \tag{A16}$$

Thus, taking $\bar{\mathbf{v}} = 0$ in (A7) and using (A13a) results in

$$C_k = C_k^0 - {}_*i\mathbf{v}\cdot\varepsilon_{-k}^0 = A_k^0 + \frac{1}{k^4}\mathbf{kk} : \lambda_k(\mathbf{k}\cdot\mathbf{v}). \tag{A17}$$

If (A17) is now reinserted into (A7) there results

$$-\mathbf{v}\cdot\bar{\varepsilon}_{-k\perp} - \bar{\mathbf{v}}\cdot\varepsilon_{k\perp} = 0. \tag{A18}$$

If (A18) is multiplied $\bar{\mathbf{v}}\gamma(|\bar{\mathbf{v}}|)$, where γ is an arbitrary function, and integrated over $\bar{\mathbf{v}}$ we find

$$\varepsilon_{k\perp} = \mathbf{D}_k\cdot(\mathbf{k}\times\mathbf{v}), \tag{A19}$$

a linear function of $\bar{\mathbf{v}}_\perp$. But $\mathbf{D}_k$ must be zero as seen by inserting (A19) into (A15) because there is no term to cancel the cubic term, since (A15) is now a polynomial in $\mathbf{v}$. Setting the linear and quadratic terms in the resultant (A15) separately to zero gives

$$\frac{1}{k^4}\mathbf{kk} : \lambda_k\left(\mathbf{v} - \frac{\mathbf{kk}\cdot\mathbf{v}}{k^2}\right) + \mathbf{v}\cdot\lambda_{-k}\cdot\left[\mathbf{I} - \frac{\mathbf{kk}}{k^2}\right] = 0,$$

or

$$\lambda_{k\perp} = -(\mathbf{kk}/k^4) : \lambda_k[\mathbf{I} - \mathbf{kk}/k^2] \tag{A20}$$

and

$$\mathfrak{y}_k = -(C_k^0/k^2)\mathbf{I}\times\mathbf{k}.$$

The remainder of the coefficients are now trivially found in terms of C_k^0 and $\mathbf{kk} : \lambda_k/k^2$ and we have (now in Gaussian units)

$$Q_1 = \int d^3k\,\mathbf{B}_1(k)\cdot\mathbf{k}\left\{\int d^3v\left[\frac{1}{2\mathbf{k}\cdot\partial g/\partial\mathbf{v}}\left(mf_kf_{-k} + \frac{ie}{ck^2}(f_k\mathbf{k}\times\mathbf{B}_{-k} - f_{-k}\mathbf{k}\times\mathbf{B}_k)\cdot\frac{\partial g}{\partial\mathbf{v}} + \frac{e^2}{mc^2k^4}\frac{\partial g}{\partial\mathbf{v}}\cdot(\mathbf{k}\times\mathbf{B}_k\mathbf{k}\times\mathbf{B}_{-k})\cdot\frac{\partial g}{\partial\mathbf{v}}\right)\right] + \frac{1}{4\pi ck^2}[\mathbf{B}_{-k}\cdot(\mathbf{E}_k\times\mathbf{k}) + \mathbf{B}_k\cdot(\mathbf{E}_{-k}\times\mathbf{k})]\right\} \tag{A21}$$

and

$$Q_2 = \int d^3k\,B_2(\mathbf{k})\left\{\int d^3v\left[\frac{\mathbf{k}\cdot\mathbf{v}}{2\mathbf{k}\cdot\partial g/\partial\mathbf{v}}\left(mf_kf_{-k} + \frac{ie}{ck^2}(f_k\mathbf{k}\times\mathbf{B}_{-k} - f_{-k}\mathbf{k}\times\mathbf{B}_k)\cdot\frac{\partial g}{\partial\mathbf{v}} + \frac{e^2}{mc^2k^4}\frac{\partial g}{\partial\mathbf{v}}\cdot(\mathbf{k}\times\mathbf{B}_k\mathbf{k}\times\mathbf{B}_{-k})\cdot\frac{\partial g}{\partial\mathbf{v}}\right) + \frac{ie}{2ck^2}\mathbf{v}\cdot(\mathbf{k}\times\mathbf{B}_kf_{-k} - \mathbf{k}\times\mathbf{B}_{-k}f_k)\right] - (1/8\pi)\left(|\mathbf{E}_k|^2 + \left(1 - \frac{\kappa^2}{k^2}\right)|\mathbf{B}_k|^2\right)\right\}. \tag{A22}$$

Here $\kappa^2 = \omega_p^2/c^2$ and $\mathbf{B}_1$ and B_2 are arbitrary functions of $\mathbf{k}$. Notice that only two constants are found, and these are just those previously stated in (35) and (36), as found upon inversion.

Mathematical Methods for Evaluating Three-Body Interactions Between Closed-Shell Atoms or Ions*

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The mathematical methods involved in the evaluation of three-body interactions between rare-gas atoms or alkali-halide ions with Gaussian type electron wavefunctions are outlined in first and second orders of perturbation theory. These methods are of general applicability for the analysis of many-center coulombic and exchange integrals occurring in problems of atomic and solid-state physics in which Gaussian functions can be used as a basis.

1. INTRODUCTION

FUNCTIONS of the Gaussian-type exp $(-\alpha r^2)$ have recently found increased interest as a basis for the evaluation of two-center and many-center integrals in atomic physics and solid-state theory. This interest arises from the fact that coulombic and exchange integrals with electron wavefunctions of Gaussian type are much less difficult to calculate than those using Slater-type orbitals, for example, as was first noted by Boys[1] and McWeeny.[2] For a detailed account of this type of applications we refer to a recent treatise by Shavitt[3] and an analysis by Krauss,[4] where many additional references can be found.

In this paper we will outline the mathematical methods used in a somewhat different application of Gaussian functions, namely in the analysis of stability of rare-gas crystals and alkali-halide solids as given recently by Jansen and collaborators.[5-8] It can be shown that in the stability analysis the electron wavefunctions of the rare-gas atoms and those of the alkali-halide ions may be replaced by those characterizing the charge distribution of *effective* electrons, one such electron per atom or ion. This charge distribution is chosen to be of Gaussian form

$$\rho(r) = (\beta/\Pi^{\frac{1}{2}})^3 \exp(-\beta^2 r^2),$$

where r is the distance from the effective electron to its nucleus, and where β is a characteristic parameter, different for different atoms or ions.

Crystal stability is then analyzed in terms of *three-body interactions* between atoms or ions, which are of exchange type; these interactions are evaluated in first and second orders of perturbation theory, where the unperturbed ground-state wavefunction, $\varphi(r)$, of an atom or ion is taken as the positive square root of the charge distribution $\rho(r)$. The problem thus reduces to the evaluation of three-body exchange interactions for different triplets of atoms or ions in the crystals with unperturbed wavefunctions which are of the Gaussian form.

In the following sections we analyze the first- and second-order perturbation calculations for three-body interactions between the atoms or the ions, first for a general triplet (abc) of atoms or ions. Detailed results will be given for specific triangles of rare-gas atoms occurring in the face-centered cubic and hexagonal close-packed configurations in their solid states. In this sense the present paper is complementary to Refs. 5–8. The methods outlined are, however, of general applicability for the evaluation of many-center integrals with Gaussian functions in atomic physics and solid-state theory.

2. DEVELOPMENT OF RELATIVE FIRST- AND SECOND-ORDER THREE-BODY INTERACTION ENERGIES AS A LINEAR COMBINATION OF A PRODUCT OF OVERLAP INTEGRALS AND SOME BASIC FUNCTIONS

A. Notation

We will denote by E_1 and E_2, respectively, the total first- and second-order interaction energies for a triplet of atoms (abc); by $E_1^{(0)}$ and $E_2^{(0)}$ the respective sums of the first- and second-order interactions between the isolated pairs (ab), (ac), and (bc).

We will evaluate the relative first- and second-order three-body interaction energies, defined, re-

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spectively, as

$$\Delta E_1/E_1^{(0)} \equiv (E_1 - E_1^{(0)})/E_1^{(0)}, \quad (1)$$

and

$$\Delta E_2/E_2^{(0)} \equiv (E_2 - E_2^{(0)})/E_2^{(0)}. \quad (2)$$

B. First-Order Three-Body Energy for Triplets of Identical Atoms

We introduce the following notations:

φ_a, φ_b and φ_c are the ground-state wavefunctions for atoms a, b and c, respectively (we have $\varphi_a(1) = (\beta/\Pi^{\frac{1}{2}})^{\frac{3}{2}} e^{-\beta^2 r_{a1}^2/2}$, etc.);

H'_{ab} is the electrostatic interaction (perturbation Hamiltonian) between atoms a and b;

$\Delta_{ab} = \int \varphi_a \varphi_b \, d\tau$ is the overlap integral between a and b;

$$\Delta^2_{abc} = \Delta^2_{ab} + \Delta^2_{ac} + \Delta^2_{bc} - 2\Delta_{ab}\Delta_{ac}\Delta_{bc}, \quad (3)$$

Ψ is the zero-order total wavefunction (Slater determinant),

$$\Psi = [3!(1 - \Delta^2_{abc})]^{-\frac{1}{2}} \det \{\varphi_a(1)\varphi_b(2)\varphi_c(3)\}, \quad (4)$$

and

$$\Psi_{0(ab)} = [2!(1 - \Delta^2_{ab})]^{-\frac{1}{2}} \det \{\varphi_a(1)\varphi_b(2)\}, \quad (5)$$

the zero wavefunction for the pair (ab). We have

$$E_1 = \langle H'_{abc} \rangle = \langle H'_{ab} \rangle + \langle H'_{ac} \rangle + \langle H'_{bc} \rangle, \quad (6)$$

where

$$\langle H'_{ab} \rangle = \iiint \Psi^* H'_{ab} \Psi \, d\tau_1 \, d\tau_2 \, d\tau_3, \quad (7)$$

and

$$E_1^{(0)} = \langle H'_{abc} \rangle_0 = \langle H'_{ab} \rangle_0 + \langle H'_{ac} \rangle_0 + \langle H'_{bc} \rangle_0, \quad (8)$$

$$\langle H'_{ab} \rangle_0 = \iint \Psi^*_{0(ab)} H'_{ab} \Psi_{0(ab)} \, d\tau_1 \, d\tau_2. \quad (9)$$

Similar expressions hold for the pairs (ac) and (bc).

$\langle H'_{ab} \rangle$ and $\langle H'_{ab} \rangle_0$ in Terms of Auxiliary Functions A_1, A_2, A_3, and A_4

By substituting (4) in (7), we obtain 36 volume integrals, which can be expressed in terms of the four auxiliary functions A_1, A_2, A_3 and A_4, defined as follows:

$$\beta A_1(\beta R_{ab}) \equiv \iint \varphi_a^2(1)\varphi_b^2(2) H'_{ab} \, d\tau_1 \, d\tau_2, \quad (10)$$

$$\beta \Delta^2_{ab} A_2(\beta R_{ab}) \equiv \iint \varphi_a(1)\varphi_a(2)\varphi_b(1)\varphi_b(2) H'_{ab} \, d\tau_1 \, d\tau_2, \quad (11)$$

$$\beta \Delta^2_{bc} A_3(\beta R_{ab}, \beta R_{a(bc)}) \equiv \iiint \varphi_a^2(1)\varphi_b(2)\varphi_b(3)\varphi_c(2)\varphi_c(3) H'_{ab} \, d\tau_1 \, d\tau_2 \, d\tau_3, \quad (12)$$

and

$$\beta \Delta_{ab}\Delta_{ac}\Delta_{bc} A_4(\beta R_{ab}, \beta R_{a(bc)}, \beta R_{(ab)(bc)}) \equiv \iiint \varphi_a(1)\varphi_a(2)\varphi_b(2)\varphi_b(3)\varphi_c(1)\varphi_c(3) H'_{ab} \, d\tau_1 \, d\tau_2 \, d\tau_3. \quad (13)$$

In the above notation, $R_{a(bc)}$ denotes the distance between atom a and the middle of R_{bc}, whereas $R_{(ab)(bc)}$ stands for the distance between the middle of R_{ab} and the middle of R_{bc}.

The final first-order expression then becomes

$$\begin{aligned} \frac{\langle H'_{ab} \rangle}{\beta e^2}(1 - \Delta^2_{abc}) &= A_1(\beta R_{ab}) - \Delta^2_{ab} A_2(\beta R_{ab}) \\ &- \Delta^2_{ac} A_3(\beta R_{ab}, \beta R_{b(ac)}) - \Delta^2_{bc} A_3(\beta R_{ab}, \beta R_{a(bc)}) \\ &+ \Delta_{ab}\Delta_{ac}\Delta_{bc}[A_4(\beta R_{ab}, \beta R_{a(bc)}, \beta R_{(ab)(bc)}) \\ &+ A_4(\beta R_{ab}, \beta R_{b(ac)}, \beta R_{(ab)(bc)})]. \end{aligned} \quad (14)$$

As a special case, we obtain for the pair-energy $\langle H'_{ab} \rangle_0$

$$\begin{aligned} \frac{\langle H'_{ab} \rangle_0}{\beta e^2}(1 - \Delta^2_{ab}) &= \lim_{\substack{R_{ac}\to\infty \\ R_{bc}\to\infty}} \left\{ \frac{\langle H'_{ab} \rangle}{\beta e^2}(1 - \Delta^2_{abc}) \right\} \\ &= A_1(\beta R_{ab}) - \Delta^2_{ab} A_2(\beta R_{ab}). \end{aligned} \quad (15)$$

Similar expressions hold for $\langle H'_{ac} \rangle$, $\langle H'_{ac} \rangle_0$ and $\langle H'_{bc} \rangle$, $\langle H'_{bc} \rangle_0$.

Auxiliary functions A_1, A_2, A_3, and A_4 in Terms of the Basic Function $L(x) = \operatorname{erf} x/x$

By substituting the explicit expression of H'_{ab} into (10)–(13) [for example $H'_{ab} = 1/R_{ab} - 1/r_{b2} - 1/r_{a1} + 1/r_{12}$ in (11)], it is easily found that the auxiliary functions A_1 to A_4 can be expressed in terms of the basic integral

$$L(x) \equiv \operatorname{erf} x/x$$

as follows:

$$\begin{aligned} A_1(x) &= 1/x - 2L(x) + 2^{-\frac{1}{2}} L(2^{-\frac{1}{2}}x), \\ A_2(x) &= 1/x - 2L(x/2) + (2/\Pi)^{\frac{1}{2}}, \\ A_3(x_1, x_2) &= 1/x_1 - L(x_1) - L(x_2) + 2^{\frac{1}{2}} L(2^{\frac{1}{2}}x_2), \end{aligned} \quad (16)$$

and

$$A_4(x_1, x_2, x_3) = 1/x_1 - L(x_1/2) - L(x_2) + 2^{\frac{1}{2}} L(2^{\frac{1}{2}}x_3).$$

The final equation for $\langle H'_{ab}\rangle$ can then be written as

$$\frac{\langle H'_{ab}\rangle}{\beta e^2}(1-\Delta^2_{abc}) = (1-\Delta^2_{abc})/\beta R_{ab} - 2\{1-(\tfrac{1}{2})(\Delta^2_{ac}+\Delta^2_{bc})\}L(\beta R_{ab}) + 2\Delta_{ab}\{\Delta_{ab}-\Delta_{ac}\Delta_{bc}\}L(\beta R_{ab}/2) + \Delta_{ac}\{\Delta_{ac}-\Delta_{ab}\Delta_{bc}\}L(\beta R_{b(ac)}) + \Delta_{bc}\{\Delta_{bc}-\Delta_{ab}\Delta_{ac}\}L(\beta R_{a(bc)}) + 2^{-\frac{1}{2}}\{L(2^{-\frac{1}{2}}\beta R_{ab}) - \Pi^{-\frac{1}{2}}\Delta^2_{ab}\}, \quad (17)$$

and

$$\frac{\langle H'_{ab}\rangle_0}{\beta e^2}(1-\Delta^2_{ab}) = (1-\Delta^2_{ab})/\beta R_{ab} - 2L(\beta R_{ab}) + 2\Delta^2_{ab}L(\beta R_{ab}/2) + 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}\beta R_{ab}) - (2/\Pi)^{\frac{1}{2}}\Delta^2_{ab}. \quad (18)$$

C. First-Order Calculation for Different Atoms

We note that the expressions for the first-order three-body interactions given above can readily be extended to the case of atoms (or ions) of *different* size, such as occur for mixed molecular crystals and for ionic solids. Let a and b denote two different atoms, characterized by the Gaussian parameters β' and β, respectively. The Gaussian wavefunctions for the two atoms are

$$\varphi_a(1) = (\beta'/\Pi^{\frac{1}{2}})^{\frac{3}{4}}\exp(-\beta' r^2_{a1}/2),$$

and

$$\varphi_b(2) = (\beta/\Pi^{\frac{1}{2}})^{\frac{3}{4}}\exp(-\beta r^2_{b2}/2).$$

Consequently, the integrals occurring in the evaluation of $\langle H'_{ab}\rangle$ are slightly modified.

We introduce a new parameter γ, defined by

$$\gamma = (\beta'/\beta)^2$$

and use the identity

$$\gamma r^2_{a1} + r^2_{b1} = [\gamma/(\gamma+1)]R^2_{ab} + (\gamma+1)r^2_{(d)1}, \quad (19)$$

where the point (d) is defined by

$$\gamma = R_{(d)b}/R_{(d)a}.$$

Using (19), all the integrals become of the following four types:

$$(\alpha/\Pi^{\frac{1}{2}})^3\int \exp(-\alpha^2 r^2_{a1})/r_{b1}\,d\tau_1 = \operatorname{erf}(\alpha R_{ab})/R_{ab} = \alpha L(\alpha R_{ab}), \quad (20)$$

$$(\alpha/\Pi^{\frac{1}{2}})^6\iint \exp[-\alpha^2(r^2_{a1}+r^2_{b2})]/r_{12}\,d\tau_1\,d\tau_2 = \operatorname{erf}(2^{-\frac{1}{2}}\alpha R_{ab})/R_{ab} = 2^{-\frac{1}{2}}\alpha L(2^{-\frac{1}{2}}\alpha R_{ab}), \quad (21)$$

$$(\alpha/\Pi^{\frac{1}{2}})^6\iint \exp[-\alpha^2(r^2_{a1}+r^2_{a2})]/r_{12}\,d\tau_1\,d\tau_2 = 2^{-\frac{1}{2}}\alpha L(0) = (2/\Pi)^{\frac{1}{2}}\alpha, \quad (22)$$

and

$$k^{\frac{1}{2}}(\alpha/\Pi^{\frac{1}{2}})^6\iint \exp[-\alpha^2(kr^2_{a1}+r^2_{b2})]/r_{12}\,d\tau_1\,d\tau_2 = \operatorname{erf}[(k/k+1)^{\frac{1}{2}}\alpha R_{ab}]/R_{ab} = \alpha(k/k+1)^{\frac{1}{2}}L[(k/k+1)^{\frac{1}{2}}\alpha R_{ab}], \quad (23)$$

where the parameters α and k are given functions of β and γ.

The first three types of integrals occurred already in the first-order calculations for identical atoms ($\gamma = 1$); consequently, only (23) is a new type of integral. The formula (23) is obtained by using the three following identities:

$$\int_{-1}^{1}\exp[-\alpha^2(a^2+b^2-2ab\zeta)]\;\zeta = \{\exp[-\alpha^2(a-b)^2] - \exp[-\alpha^2(a+b)^2]\}/2\alpha^2 ab, \quad (24)$$

$$\int_0^\infty\int_{-1}^{1}(a^2+u^2-2au\zeta)^{-\frac{1}{2}}u^2\operatorname{erf}(-u^2)\,d\zeta\,du = \Pi^{\frac{1}{2}}\operatorname{erf} a/2a = \Pi^{\frac{1}{2}}L(a)/2, \quad (25)$$

$$\int_0^\infty\{\exp[-(au-b)^2] - \exp[-(au+b)^2]\}\operatorname{erf} u\,du = \Pi^{\frac{1}{2}}\operatorname{erf}[b/(a^2+1)^{\frac{1}{2}}]/a. \quad (26)$$

As is seen from Eqs. (20)–(23), in the case of $\gamma \neq 1$, also, all first-order integrals can be expressed in terms of erf x functions.

D. Second-Order Interaction Energy

For the second-order energy we have to evaluate

$$E_2 = \sum_{\kappa\neq 0}(H'_{abc})_{0\kappa}(H'_{abc})_{\kappa 0}/(E_0 - E_\kappa) \equiv -\{\langle H'^2_{abc}\rangle - \langle H'_{abc}\rangle^2\}/E_{av}, \quad (27)$$

where E_{av} is defined by the averaging procedure, and where κ numbers the excited states of the system (energy E_κ). On the other hand,

$$E_2^{(0)} = -\frac{1}{E_{av}}\{\langle H'^2_{ab}\rangle_0 - \langle H'_{ab}\rangle^2_0 + [(ac),(bc)]\}; \quad (28)$$

$[(ac),(bc)]$ signify that the corresponding expressions for the pairs (ac) and (bc) must be added. It should be noted that the quantities E_{av} in (27) and (28) are not precisely the same. Their difference can, however, be ignored for our purpose.

Since $\langle H'_{abc}\rangle$ and $\langle H'_{abc}\rangle_0$ are already known from the first-order interactions, the only unknown quantity is $\langle H'^2_{abc}\rangle$, defined by

$$\langle H'^2_{abc}\rangle \equiv \iiint \Psi^* H'^2_{abc}\Psi \, d\tau_1 \, d\tau_2 \, d\tau_3. \tag{29}$$

Development of $\langle H'^2_{abc}\rangle$ as a Linear Combination of a Product of Overlap Integrals and the Auxiliary Functions $\mathfrak{A}$ to $\mathfrak{K}$

For the evaluation of $\langle H'^2_{abc}\rangle$ we substitute the value of $\Psi = \Psi^*$ given by (4) into (29) and decompose in each term H'^2_{abc} into squares and double products,

$$H'^2_{abc} = H'^2_{ab} + H'^2_{ac} + H'^2_{bc} + 2H'_{ab}H'_{ac} + 2H'_{ab}H'_{bc} + 2H'_{ac}H'_{bc}.$$

Thus we obtain 126 volume integrals, all of them of the eight following types (except for permutations):

$$\beta^2\mathfrak{A}(\beta R_{ab}) \equiv \iint \varphi_a(1)\varphi_b(2)H'^2_{ab}\varphi_a(1)\varphi_b(2) \, d\tau_1 \, d\tau_2, \tag{30}$$

$$\beta^2\Delta^2_{ab}\mathfrak{B}(\beta R_{ab}) \equiv \iint \varphi_a(1)\varphi_b(2)H'^2_{ab}\varphi_a(2)\varphi_b(1) \, d\tau_1 \, d\tau_2, \tag{31}$$

$$\beta^2\mathfrak{C}(\beta R_{ab}, \beta R_{ac}, \sphericalangle bac) \equiv \iiint \varphi_a(1)\varphi_b(2)\varphi_c(3)H'_{ab}H'_{ac}\varphi_a(1)\varphi_b(2)\varphi_c(3) \, d\tau_1 \, d\tau_2 \, d\tau_3, \tag{32}$$

$$\beta^2\Delta^2_{ab}\mathfrak{D}(\beta R_{ac}, \beta R_{c(ab)}, \sphericalangle ac(ab)) \equiv \iiint \varphi_a(1)\varphi_b(2)\varphi_c(3)H'^2_{ac}\varphi_a(2)\varphi_b(1)\varphi_c(3) \, d\tau_1 \, d\tau_2 \, d\tau_3, \tag{33}$$

$$\beta^2\Delta^2_{ab}\mathfrak{E}(\beta R_{ac}, \beta R_{bc}, \beta R_{c(ab)}) \equiv \iiint \varphi_a(1)\varphi_b(2)\varphi_c(3)H'_{ac}H'_{bc}\varphi_a(2)\varphi_b(1)\varphi_c(3) \, d\tau_1 \, d\tau_2 \, d\tau_3, \tag{34}$$

$$\beta^2\Delta^2_{ab}\mathfrak{F}(\beta R_{ab}, \beta R_{ac}, \beta R_{c(ab)}) \equiv \iiint \varphi_a(1)\varphi_b(2)\varphi_c(3)H'_{ab}H'_{ac}\varphi_a(2)\varphi_b(1)\varphi_c(3) \, d\tau_1 \, d\tau_2 \, d\tau_3, \tag{35}$$

$$\beta^2\Delta_{ab}\Delta_{ac}\Delta_{bc}\mathfrak{G}(\beta R_{ab}, \beta R_{a(bc)}, \beta R_{(ab)(bc)}) \equiv \iiint \varphi_a(1)\varphi_b(2)\varphi_c(3)H'^2_{ab}\varphi_a(2)\varphi_b(3)\varphi_c(1) \, d\tau_1 \, d\tau_2 \, d\tau_3, \tag{36}$$

and

$$\beta^2\Delta_{ab}\Delta_{ac}\Delta_{bc}\mathfrak{K}(\beta R_{ac}, \beta R_{bc}, \beta R_{b(ac)}) \equiv \iiint \varphi_a(1)\varphi_b(2)\varphi_c(3)H'_{ac}H'_{bc}\varphi_a(2)\varphi_b(3)\varphi_c(1) \, d\tau_1 \, d\tau_2 \, d\tau_3. \tag{37}$$

In (30)–(37) we use the same notation as in (10)–(13). We then obtain for $\langle H'^2_{abc}\rangle$ the following expression:

$$\begin{aligned}\frac{(1-\Delta^2_{abc})\langle H'^2_{abc}\rangle}{\beta^2 e^4} = {} & \{\mathfrak{A}(\beta R_{ab}) - \Delta^2_{ab}\mathfrak{B}(\beta R_{ab}) \\ & + 2\mathfrak{C}(\beta R_{ab}, \beta R_{ac}, \sphericalangle bac) \\ & - 2\Delta^2_{ab}\mathfrak{E}(\beta R_{ac}, \beta R_{bc}, \beta R_{c(ab)}) + [(ac),(bc)]\} \\ & + \{-\Delta^2_{ab}\mathfrak{D}(\beta R_{ac}, \beta R_{c(ab)}, \sphericalangle ac(bc)) \\ & - 2\Delta^2_{ab}\mathfrak{F}(\beta R_{ab}, \beta R_{ac}, \beta R_{c(ab)}) \\ & + 2\Delta_{ab}\Delta_{ac}\Delta_{bc}\mathfrak{G}(\beta R_{ab}, \beta R_{a(bc)}, \beta R_{(ab)(bc)}) \\ & + 2\Delta_{ab}\Delta_{ac}\Delta_{bc}\mathfrak{K}(\beta R_{ab}, \beta R_{ac}, \beta R_{c(ab)}) \\ & + [(ba),(ac),(ca),(bc),(cb)]\},\end{aligned} \tag{38}$$

and for $\langle H'^2_{ab}\rangle_0$,

$$\langle H'^2_{ab}\rangle_0/\beta^2 e^4 = \{\mathfrak{A}(\beta R_{ab}) - \Delta^2_{ab}\mathfrak{B}(\beta R_{ab})\}/(1-\Delta^2_{ab}). \tag{39}$$

In (38) the notation $[(ac),(bc)]$ has the same meaning as in (28). It is to be noted that the total number of permutations for the last four terms in (38) is six, compared with three for the first four terms of this equation, since for the last terms permuting a and b, or a and c, or b and c is geometrically different for the arguments of the functions $\mathfrak{D}$, $\mathfrak{F}$, $\mathfrak{G}$, and $\mathfrak{K}$.

From (27), (28), (38), and (39) we note that, to obtain the final result for $\Delta E_2/E_2^{(0)}$, it is sufficient to evaluate the eight auxiliary functions $\mathfrak{A}$ to $\mathfrak{K}$ for the corresponding values of the distances βR_{ab}, βR_{ac}, etc.

The Auxiliary Functions $\mathfrak{A}$–$\mathfrak{K}$ as Linear Combinations of the Basic Integrals K–S

We will now express the auxiliary functions $\mathfrak{A}$ to $\mathfrak{K}$ in terms of nine basic integrals K to S. To do so, we observe that all auxiliary functions contain volume integrals of the following forms:

$$I_1 = \beta^3\Pi^{-\frac{1}{2}}\int \exp\left[-(\beta^2/2)(r^2_{a1}+r^2_{b1})\right] d\tau_1 = \exp(-\beta^2R^2_{ab}/4) = \Delta_{ab}, \tag{40}$$

$$I_2 = \beta^3\Pi^{-\frac{1}{2}}\int \exp(-\beta^2 r_{a1})/r_{b1} \, d\tau_1, \tag{41}$$

$$I_3 = \beta^6\Pi^{-3}\iint \exp\left[-\beta^2(r^2_{a1}+r^2_{b2})\right]/r_{12} \, d\tau_1 \, d\tau_2, \tag{42}$$

$$I_4 = \beta^6\Pi^{-3}\iint \exp\left[-\beta^2(r^2_{a1}+r^2_{b2})\right]/r^2_{12} \, d\tau_1 \, d\tau_2, \tag{43}$$

$$I_5 = \beta^3\Pi^{-\frac{1}{2}}\int \exp(-\beta^2 r^2_{a1})/r^2_{b1} \, d\tau_1, \tag{44}$$

$$I_6 = \beta^6\Pi^{-3}\iint \exp\,[-\beta^2(r_{a1}^2 + r_{b2}^2)]/r_{a2}r_{12}\,d\tau_1\,d\tau_2, \tag{45}$$

$$I_7 = \beta^3\Pi^{-\frac{3}{2}}\int \exp\,(-\beta^2 r_{a1}^2)/r_{b1}r_{c1}\,d\tau_1, \tag{46}$$

$$I_8 = \beta^6\Pi^{-3}\iint \exp\,[-\beta^2(r_{a1}^2 + r_{b2}^2)]/r_{c1}r_{12}\,d\tau_1\,d\tau_2, \tag{47}$$

$$I_9 = \beta^9\Pi^{-9/2}\iiint \exp\,[-\beta^2(r_{a1}^2 + r_{b2}^2 + r_{c3}^2)]/r_{12}r_{13} \times d\tau_1\,d\tau_2\,d\tau_3, \tag{48}$$

$$I_{10} = \beta^6\Pi^{-3}\iint \exp\,[-\beta^2(r_{a1}^2 + r_{a2}^2)]/r_{c1}r_{12}\,d\tau_1\,d\tau_2, \tag{49}$$

and

$$I_{11} = \beta^9\Pi^{-9/2}\iiint \exp\,[-\beta^2(r_{a1}^2 + r_{c2}^2 + r_{c3}^2)]/r_{12}r_{13} \times d\tau_1\,d\tau_2\,d\tau_3, \tag{50}$$

where I_{10} and I_{11} are special cases of I_8 and I_9, respectively.

Upon inspection of the volume integrals $I_1 - I_{11}$, it appears possible, by using (24), (25), and the following identities:

$$\int_{-1}^{1}(a^2 + b^2 - 2ab\zeta)^{-\frac{1}{2}}\,d\zeta = \begin{cases} 2/a, & b < a \\ 2/b, & a < b \end{cases}; \tag{51}$$

$$\int_0^\infty\int_{-1}^{1}(d^2 + u^2 - 2du\zeta)^{-1}u^2\exp\,(-u^2)\,d\zeta\,du = \Pi^{\frac{1}{2}}K(d)/2; \tag{52}$$

$$\int_0^d \exp\,(-u^2)\,\operatorname{erf} u\,du = (\Pi^{\frac{1}{2}}/4)d^2L^2(d); \tag{53}$$

$$\int_0^\infty \{\exp\,[-(u-d)^2] - \exp\,[-(u+d)^2]\}\,\operatorname{erf} u\,du = \Pi^{\frac{1}{2}}\operatorname{erf}\,(2^{-\frac{1}{2}}d); \tag{54}$$

$$\int_0^\infty \{\exp\,[-(u-d)^2] + \exp\,[-(u+d)^2]\}\,\operatorname{erf} u\,du = (\Pi^{\frac{1}{2}}/2)[1 + (\operatorname{erf} 2^{-\frac{1}{2}}d)^2], \tag{55}$$

to express these in terms of the nine basic integrals K to S, defined as

$$K(x) \equiv \frac{2}{x}e^{-x^2}\int_0^x e^{t^2}\,dt, \tag{56}$$

$$L(x) \equiv \frac{2}{x\Pi^{\frac{1}{2}}}\int_0^x e^{-t^2}\,dt = \frac{\operatorname{erf} x}{x}, \tag{57}$$

$$M(x) \equiv \frac{e^{-x^2}}{x}\int_0^x e^{u^2}\{\operatorname{erf}\,(2^{-\frac{1}{2}}u)\}^2\,du, \tag{58}$$

$$N(x) \equiv (1/x)\int_0^\infty \exp\,[-u^2 - (u-x)^2] - \exp\,[-u^2 - (u+x)^2]\,\operatorname{erf} iu\,du, \tag{59}$$

$$O(u,v,\Theta) \equiv \int_0^\infty\int_0^{2\Pi}\int_0^{\Pi} x^2\exp\,(-x^2) \times (u^2 + x^2 - 2ux\sin\alpha\sin\gamma)^{-\frac{1}{2}} \times [v^2 + x^2 - 2vx\sin\alpha\sin\,(\gamma+\Theta)]^{-\frac{1}{2}}\sin\alpha\,d\alpha\,d\gamma\,dx, \tag{60}$$

$$P(u,v,\Theta) \equiv \int_0^\infty\int_0^{2\Pi}\int_0^{\Pi} x^2\exp\,(-x^2) \times (v^2 + x^2 - 2vx\sin\alpha\sin\gamma)^{-\frac{1}{2}} \times (u^2 + x^2 - 2ux\sin\alpha\sin\,(\gamma+\Theta))^{-\frac{1}{2}}\operatorname{erf}\,[(v^2 + x^2 - 2vx\sin\alpha\sin\gamma)^{-\frac{1}{2}}]\sin\alpha\,d\alpha\,d\gamma\,dx, \tag{61}$$

$$Q(u,v,\Theta) \equiv \int_0^\infty\int_0^{2\Pi}\int_0^{\Pi} x^2\exp\,(-x^2) \times (u^2 + x^2 - 2ux\sin\alpha\sin\gamma)^{-\frac{1}{2}} \times [v^2 + x^2 - 2vx\sin\alpha\sin\,(\alpha+\Theta)]^{-\frac{1}{2}} \times \operatorname{erf}\,(u^2 + x^2 - 2ux\sin\alpha\sin\gamma)^{\frac{1}{2}} \times \operatorname{erf}\,[v^2 + x^2 - 2vx\sin\alpha\sin\,(\gamma+\Theta)]^{\frac{1}{2}} \times \sin\alpha\,d\alpha\,d\gamma\,dx, \tag{62}$$

$$R(x) \equiv \Pi^{-\frac{1}{2}}P(x,0,0^\circ) = 1 - x^2L^2(x) + \Pi^{-\frac{1}{2}}2[L(2^{\frac{1}{2}}x) - e^{-x^2}L(x)], \tag{63}$$

and

$$S(x) \equiv Q(x,x,0^\circ) = \frac{\Pi}{x}\int_0^x \{\exp\,[-(u-x)^2] - \exp\,[-(u+x)^2]\}\,\operatorname{erf}^2 u/u\,du. \tag{64}$$

It is seen that the integrals O and P are special cases of the general integral Q, namely, those cases in which one (or both) of the error functions occurring in the integrand of Q are replaced by 1.

The relations between the volume integrals I_2–I_{11} and the basic integrals K to S are as follows:

$$I_2 = \beta L(\beta R_{ab}), \tag{65}$$

$$I_3 = \beta 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}\beta R_{ab}), \quad [\text{see (23)}] \tag{66}$$

$$I_4 = \beta^2 N(\beta R_{ab}), \tag{67}$$

$$I_5 = \beta^2 K(\beta R_{ab}), \tag{68}$$

$$I_6 = \beta^2[\tfrac{1}{2}K(\beta R_{ab}) + M(\beta R_{ab})], \tag{69}$$

$$I_7 = \Pi^{-\frac{1}{2}}\beta^2 O(\beta R_{ab}, \beta R_{ac}, \measuredangle bac), \tag{70}$$

$$I_8 = \Pi^{-\frac{1}{2}}\beta^2 P(\beta R_{ac}, \beta R_{ab}, \measuredangle bac), \quad (71)$$

$$I_9 = \Pi^{-\frac{1}{2}}\beta^2 Q(\beta R_{ab}, \beta R_{ac}, \measuredangle bac), \quad (72)$$

$$I_{10} = \Pi^{-\frac{1}{2}}\beta^2 P(\beta R_{ac}, 0, 0°) = \beta^2 R(\beta R_{ac}), \quad (73)$$

and

$$I_{11} = \Pi^{-\frac{1}{2}}\beta^2 Q(\beta R_{ac}, \beta R_{ac}, 0°) = \Pi^{-\frac{1}{2}}\beta^2 S(\beta R_{ac}). \quad (74)$$

As the final step, we express the auxiliary functions $\mathfrak{A}$ to $\mathfrak{K}$ via the volume integrals I_1–I_{11} in terms of the basic integrals K to S. The results are

$$\mathfrak{A}(x) = 1/x^2 + 2L^2(x) + (2^{\frac{1}{2}}/x)L(2^{-\frac{1}{2}}x) + N(x) - 4L(x)/x - 4M(x); \quad (75)$$

$$\mathfrak{B}(x) = 1 + 1/x^2 + 2/x(2/\Pi^{\frac{1}{2}}) + 2K(x/2) + 2L^2(x/2) - 4/xL(x/2) - 4R(x/2); \quad (76)$$

$$\mathfrak{C}(x_1, x_2, \alpha) = [1/x_1 - L(x_1)][1/x_2 + 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_2) - 2L(x_2)] + [1/x_2 - L(x_2)][2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_1) - L(x_1)] + \Pi^{-\frac{1}{2}}[O(x_1, x_2, \alpha) - P(x_1, x_2, \alpha) - P(x_2, x_1, \alpha) + Q(x_1, x_2, \alpha)], \quad \text{where } \alpha = \measuredangle x_1, x_2; \quad (77)$$

$$\mathfrak{D}(x_1, x_2, \alpha) = 1/x_1^2 + K(x_1) + 2L(x_1)L(x_2) + (2^{\frac{1}{2}}/x_1)L(2^{-\frac{1}{2}}x_2) + N(x_2) - 2/x_1[L(x_1) + L(x_2)] - 2M(x_2) - 2/\Pi^{\frac{1}{2}}P(x_1, x_2, \alpha), \quad \text{where } \alpha = \measuredangle x_1, x_2; \quad (78)$$

$$\mathfrak{E}(x_1, x_2, x_3) = 1/x_1x_2 - 2^{-\frac{1}{2}}L(x_3)L(2^{-\frac{1}{2}}x_3) + L(x_1)[L(x_3) - 1/x_2] + L(x_2)[L(x_3) - 1/x_1] + [L(x_3) - (x_1 + x_2)/x_1x_2] \times [L(x_3) - 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_3)] + \Pi^{-\frac{1}{2}}[O(x_1, x_2, \measuredangle x_1, x_2) - P(x_1x_2, \measuredangle x_1, x_3) - P(x_2, x_3, \measuredangle x_2, x_3) + S(x_3)]; \quad (79)$$

$$\mathfrak{F}(x_1, x_2, x_3) = [1/x_2 - L(x_2)][1/x_1 - 2L(x_1/2) + (2/\Pi)^{\frac{1}{2}}] + [L(x_1/2) - 1/x_1][L(x_3) - 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_3)] - R(x_3) + \Pi^{-\frac{1}{2}}[O(x_1/2, x_3, \measuredangle x_1/2, x_3) - P(x_1/2, x_3; \measuredangle x_1/2, x_3) + Q(x_3, 0, 0°)]; \quad (80)$$

$$\mathfrak{G}(x_1, x_2, x_3) = 1/x_1^2 + K(x_1/2) + K(x_2) + N(x_3) + 2L(x_1/2)[L(x_2) - 1/x_1] + 2/x_1[2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_3) - L(x_2)] - (2/\Pi)^{\frac{1}{2}}[P(x_1/2, x_3; \measuredangle x_1/2, x_3) + P(x_2, x_3; \measuredangle x_2, x_3)]; \quad (81)$$

$$\mathfrak{K}(x_1, x_2, x_3, (x_4, x_5, x_6)) = [L(x_2/2) - 1/x_2][L(x_1/2) + L(x_6) - 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_5) - 1/x_1] + [L(x_6) - 1/x_1][L(x_3) - 2^{-\frac{1}{2}}L(2^{-\frac{1}{2}}x_4)] + \Pi^{-\frac{1}{2}}[O(x_1/2, x_3; \measuredangle x_1/2, x_3) - P(x_1/2, x_4; \measuredangle x_1/2, x_4) - P(x_3, x_5; \measuredangle x_3, x_5) + Q(x_4, x_5; \measuredangle x_4, x_5)]. \quad (82)$$

The variables $x_1, x_2, x_3, x_4, x_5, x_6$ have the following meaning:

$\mathfrak{K}(\beta R_{ac}, \beta R_{bc}, \beta R_{b(ac)})$

x_1	x_2	x_3	x_4	x_5	x_6
βR_{ac}	βR_{bc}	$\beta R_{b(ac)}$	$\beta R_{(ac)(bc)}$	$\beta R_{(ab)(ac)}$	$\beta R_{c(ab)}$

For the remaining five $\mathfrak{K}$ functions, the variables are found by permutations.

3. EVALUATION OF THE BASIC INTEGRALS

A. General

For small values of the parameters x, u, and $v(< 2, 5)$, the evaluation of the basic integrals is accomplished by means of electronic computation. For large values of $x(x \geq 2, 5)$, the functions $K(x)$, $L(x)$, $M(x)$, $N(x)$, $R(x)$, and $S(x)$ are evaluated by means of an asymptotic expansion, which gives an accuracy of 10^{-5} to 10^{-6} for $x = 2, 5$, whereas for the functions O, P, and Q, a double-series expansion is used.

We will give here the expansions used, and then discuss some aspects of their derivation. *The asymptotic series expansions* are:

$$\frac{1}{x} - L(x) = \frac{e^{-x^2}}{x^2\Pi^{\frac{1}{2}}} \sum_{n=1}^{N} \frac{(2n-3)!!}{(2x^2)^{n-1}} + O(x^{-2N-2}), \quad (83)$$

$$K(x) = \sum_{n=1}^{N} \frac{(2n-3)!!}{2^{n-1}x^{2n}} + O(x^{-2N-2}), \quad (84)$$

$$R(x) - \left(\frac{2}{\Pi}\right)^{\frac{1}{2}} \Big/ x = \frac{2e^{-x^2}}{x\Pi^{\frac{1}{2}}} \sum_{n=2}^{N} \frac{(-1)^{n-1}(2n-3)!!}{(2x^2)^{n-1}} + O\left(\frac{e^{-x^2}}{x^{2N+1}}\right), \quad (85)$$

$$M(x) = \tfrac{1}{2}K(x) - \Pi^{-\frac{1}{2}}2^{\frac{1}{2}} \frac{e^{-x^2/2}}{x^3} \times \left(1 + \frac{1}{x^2} + \frac{7}{x^4} + \frac{27}{x^6}\right) + O(e^{-x^2/2}/x^{11}), \quad (86)$$

$$N(x) = \sum_{n=1}^{N} \frac{(2n-3)!!}{x^{2n}} + O(x^{-2N-2}), \quad (87)$$

and

$$S(x) = \Pi^{\frac{1}{2}}K(x) - 2^{\frac{1}{2}}\Pi\frac{e^{-x^2/2}}{x^3} + O\left(\frac{e^{-x^2/2}}{x^5}\right). \quad (88)$$

For $Q(u, v, \Theta)$ the following double-series expansion is used:

$$Q(u,v,\Theta) \sim 2\sum_{(n+m)}\sum_{\text{even}}\frac{(2n-1)!!(2m-1)!!(n+m)!!}{(2n)!!(2m)!!(n+m+1)!!}$$
$$\times\int_0^{2\Pi}\sin^n\gamma\sin^m(\Theta+\gamma)\,d\gamma\left(\frac{2ux}{x^2+u^2}\right)^n\left(\frac{2vx}{x^2+v^2}\right)^m$$
$$\times\frac{x^2e^{-x^2}\,dx}{(u^2+x^2)^{\frac{1}{2}}(v^2+x^2)^{\frac{1}{2}}}\operatorname{erf}(u-x_i)\operatorname{erf}(v-x_i), \quad (89)$$

where $u \geq v$,

$$0 = x_0 < x_1 < \cdots < x_i < x_{i+1} < \cdots < x_l = v - a,$$

and a is a small fixed number.

The series expansions for P and O are particular cases of (89), in which one, (or both) of the error functions are replaced by unity.

B. Derivation of the Asymptotic Expansions

As each of the functions K, L, M, N, R, and S involves either erf x or erf ix, we give first the asymptotic expansions of these two functions, namely

$$1 - \operatorname{erf} x \equiv 1 - 2\Pi^{-\frac{1}{2}}\int_0^x e^{-t^2}\,dt$$
$$= \frac{e^{-x^2}}{x\Pi^{\frac{1}{2}}}\sum_{n=1}^{N}\frac{(-1)^{n-1}(2n-3)!!}{(2x^2)^{n-1}} + O\left(\frac{e^{-x^2}}{x^{2N+1}}\right), \quad (90)$$

and

$$\operatorname{erf} ix = 2\Pi^{-\frac{1}{2}}\int_0^x e^{t^2}\,dt$$
$$= \frac{e^{x^2}}{x\Pi^{\frac{1}{2}}}\sum_{n=1}^{N}\frac{(2n-3)!!}{(2x^2)^{n-1}} + O\left(\frac{e^{x^2}}{x^{2N+1}}\right). \quad (91)$$

The last two expansions are easily established by applying l'Hospital's rule. By using (90) and (91), the asymptotic expansions for $K(x)$, $L(x)$, and $R(x)$ follow directly. For the function $M(x)$, we apply first l'Hospital's rule, which gives

$$M(x)xe^{x^2} \equiv \int_0^x e^{t^2}[\operatorname{erf}(2^{-\frac{1}{2}}t)]^2\,dt$$
$$= \int_0^x e^{t^2}\,dt - 2(2/\Pi)^{\frac{1}{2}}\sum_{n=1}^{N}(-1)^{n-1}(2n-3)!!$$
$$\times\int_a^x\frac{e^{t^2/2}}{t^{2n-1}} + O\left(\frac{e^{x^2/2}}{x^{2(N+1)}}\right),$$

where a is a fixed small number. Then, by repeated application of the identity

$$\int_a^x\frac{e^{t^2/2}}{t^{2n-1}}\,dt = \frac{e^{x^2/2}}{x^{2n}} + 2n\int_a^x\frac{e^{t^2/2}}{t^{2n+1}}\,dt + O(1),$$
$$\text{for } n = 1, 2, \cdots, N-1,$$

we obtain Eq. (86). For the function $N(x)$, we divide the integral in two parts, the first one between the limits 0 and a, the second one between a and ∞; these partial integrals are denoted, respectively, by $N^*(x)$ and $N^{**}(x)$. Since we have

$$N^*(x) = O(e^{-(x-a)^2}/x),$$

it follows that

$$N^*(x) = N^{**}(x) + O(e^{-(x-a)^2}/x),$$

where

$$N^{**}(x) = \int_a^\infty\{\exp[-u^2-(x-u)^2]$$
$$-\exp[-u^2-(x+u)^2]\}\operatorname{erf} iu\,du.$$

We now replace erf iu in $N^{**}(x)$ by its asymptotic expansion (91), and obtain

$$xN^{**}(x) = \Pi^{-\frac{1}{2}}\sum_{k=1}^{N}2^{-(2k-1)}(2k-3)!!$$
$$\times N_k^{**}(x) + O(x^{-2N-1})$$

with

$$N_k^{**}(x) = \int_a^\infty u^{-(2k-1)}\{\exp[-(u-x)^2]$$
$$-\exp[-(u+x)^2]\}\,du, \quad k = 1, 2, \cdots, N.$$

By using for $N_1^{**}(x)$ the identity

$$\int_0^\infty\frac{e^{-(u-x)^2}-e^{-(u+x)^2}}{u}\,du = \Pi^{\frac{1}{2}}xK(x) \quad (92)$$

and the property

$$N_v^{**}(x) = \frac{1}{[2(v-1)]!!}\frac{d^{2(v-1)}}{dx^{2(v-1)}}[N_1^{**}(x)],$$
$$v = 1, 2, \cdots, n,$$

we find Eq. (87). For the function $S(x)$, we consider again only the integral between the limits a and ∞, where a is a fixed small number, since we have

$$\int_0^a\{\exp[-(u-x)^2]-\exp[-(u+x)^2]\}$$
$$\times\operatorname{erf}^2 u/u\,du = O(xe^{-x^2}).$$

Then we use (90), which leads to

$$\Pi^{-1}xS(x) = \int_a^\infty\frac{e^{-(u-x)^2}-e^{-(u+x)^2}}{u}\,du$$
$$+\sum_{\nu=1}^{N}I_\nu(x) + O(e^{-x^2/2}/x^{2N+1}),$$

where

$$I_\nu(x) = \frac{(-1)^\nu(2\nu-3)!!}{2^{\nu-2}\Pi^{\frac{1}{2}}} \times \int_0^\infty \frac{\{e^{-(u-x)^2} - e^{-(u+x)^2}\}e^{-u^2}}{u^{2\nu}}\,du, \quad \nu = 1, 2, \cdots, N.$$

By using the identity (92), and considering the fact that

$$\sum_{\nu=1}^{N} I_\nu(x) = o(1/x),$$

we obtain

$$\lim_{x\to\infty}\{S(x)/K(x)\} = \Pi^{\frac{1}{2}}.$$

To determine the second term of the asymptotic expansion of $S(x)$, we note first that

$$\sum_{\nu=2}^{n} I_\nu = o(I_1).$$

Then we write

$$-2^{-1}\Pi^{-\frac{1}{2}}\exp(x^2/2)I_1(x) = \int_a^\infty \{\exp[-2(u-x/2)^2] - \exp[-2(u+x/2)^2]\}/u\,du.$$

and differentiate the last integral with respect to x, which yields

$$I_1(x) = -2^{5/2}\exp(-\tfrac{1}{2}x^2)/x^2 + O[\exp(-\tfrac{1}{2}x^2)/x^4].$$

Consecutive terms are obtained by the same procedure.

C. Derivation of the Double-Series Development Used for the Functions O(u, v, Θ), P(u, v, Θ) and Q(u, v, Θ)

We sketch the derivation for the function $O(v, v, \Theta)$ only, since the method is similar for the general case $u \neq v$, as well as for the functions P and Q.

It is sufficient to consider only the integral between the limits $x = 0$ and $x = v - a$, where a is a fixed small number, since we note that

$$O(v, v, \Theta) \leq O_1 + 12\Pi v e^{-(v-a)^2}(1 + \tfrac{1}{6}v^2 a), \tag{93}$$

with

$$O_1 = \int_0^{v-a}\int_0^{2\Pi}\int_0^{\Pi} (x^2 + v^2 - 2xv\sin\alpha\sin\gamma)^{\frac{1}{2}} \times (x^2 + v^2 - 2xv\sin\alpha\sin(\gamma+\Theta))^{\frac{1}{2}} \times x^2 e^{-x^2}\sin\alpha\,d\alpha\,d\gamma\,dx. \tag{94}$$

By using the binomial series

$$(v^2 + x^2 - 2vx\sin\alpha\sin\gamma)^{-\frac{1}{2}} = (x^2+v^2)^{-\frac{1}{2}}\sum_{n=0}^{\infty}\frac{(2n-1)!!}{(2n)!!}\left(\frac{2vx}{x^2+v^2}\right)^n$$

we obtain, changing the orders of integration and summation,

$$O_1 = \sum_{(n+m)}\sum_{\text{even}} C_{n,m}J_{n+m}, \tag{95}$$

where

$$C_{n,m} = \frac{2(2n-1)!!(2m-1)!!(n+m)!!}{(2n)!!(2m)!!(n+m+1)!!}$$

and

$$J_{n+m} = \int_0^{v-a}\left(\frac{2vx}{x^2+v^2}\right)^{n+m}\frac{x^2e^{-x^2}}{x^2+v^2}\,dx, \qquad n+m = 0, 2, 4, 6, \cdots.$$

The coefficients $C_{n,m}$ can be evaluated on a desk calculator; J_{n+m} is determined by electronic computation. In (95), it appears that sufficient accuracy is obtained in terminating the double series at values of m and n equal to about 8. This can be seen from considering the remainder R_S of the series (95), with n or $m > S$, which satisfies the inequality

$$R_S \leq 4\Pi\frac{S!!}{(S+1)!!}\left[\frac{(2S+1)!!}{(2S+1)!!}\right]^3 \times \frac{J_{2(S+1)}}{\left[1 - \dfrac{2v(v+a)}{v^2+(v-a)^2}\right]^2}.$$

D. Particular Cases for the Basic Integrals

For $x = 0$ we have

$$K(0) = 2, \quad L(0) = 2\Pi^{-\frac{1}{2}}, \quad M(0) = 0,$$
$$N(0) = 1, \quad R(0) = 1, \quad \text{and} \quad S(0) = 2\Pi^{\frac{1}{2}}/3.$$

These values are obtained directly by using l'Hospital's rule. Other particular cases are

$$O(v, v, 180°) = \Pi^2 e^{v^2}v^{-1}[1 - vL(v)],$$
$$O(v, v, 0°) = 2[\Pi v^{-1}(1 - e^{-v^2}) + \Pi^{\frac{1}{2}}(1 - vL(v)],$$
$$P(v, 0, 0°) = \Pi^{\frac{1}{2}}R(v),$$
$$P(v, v, 0°) = \Pi^{\frac{1}{2}}[\tfrac{1}{2}K(v) + M(v)],$$

and

$$Q(v, v, 0°) = S(v).$$

The last identities are obtained with the help of Eqs. (24), (25), and (51)–(55).

4. NUMERICAL RESULTS

A. General

In this section we present tables containing numerical results for the basic integrals $K(x)$, $L(x)$, $M(x)$,

TABLE I. Numerical values for the basic integrals $K(x_1)$ to $S(x_1)$; $x = \beta R_{ab} = \beta R_{ac} = 2.5$.

$(x_1/x)^2$	$K(x_1)$	$L(x_1)$	$M(x_1)$	$N(x_1)$	$R(x_1)$	$S(x_1)$
0	2.0	1.128379	0	1.0	1.0	3.712219
1/24		1.037623				
1/12	1.431003	0.959653	0.081558	0.795128		
1/8		0.892313				
1/6		0.833800				
1/4	0.793322	0.738320	0.138294	0.607405	0.603990	2.404900
1/3	0.615730	0.664243	0.150726	0.480991		
3/8		0.633351				
11/24		0.580986				
1/2	0.401537	0.558660	0.140018	0.362737	0.448154	
5/8		0.503339				
2/3	0.287157	0.489707		0.284294	0.383076	
3/4	0.249742	0.460864	0.150145	0.271146	0.368128	1.218120
19/24		0.448817				
7/8		0.427215				
11/12	0.197250	0.417489		0.209192	0.333259	
1	0.178467	0.399837	0.083428	0.199248	0.319080	
9/8		0.377057				
5/4	0.138791	0.357743	0.067490	0.155003	0.285451	
4/3		0.340395				
3/2		0.326594				
19/12	0.107280	0.317885	0.053213	0.116012		
7/4	0.096396	0.302371	0.048177	0.104100	0.241257	0.534454
2	0.083700	0.282842				
25/12	0.080183	0.277128	0.040082	0.084989		
9/4	0.073976	0.266667	0.037105	0.078038	0.212762	0.411425
8/3	0.062004	0.244949				
3	0.054888	0.230940	0.027442	0.056856		
11/3	0.044680					
4	0.040854	0.2	0.020427	0.041849		

TABLE II. Numerical values of the basic integrals O, P, and Q.

$(u/2.5)^2$	$(v/2.5)^2$	$\cos\Theta$	$O(u,v,\Theta)$	$P(u,v,\Theta)$	$Q(u,v,\Theta)$	$(u/2.5)^2$	$(v/2.5)^2$	$\cos\Theta$	$O(u,v,\Theta)$	$P(u,v,\Theta)$	$Q(u,v,\Theta)$
0	1/4	1		4.097613	2.874890	3/4	1/4	$-3^{1/2}/2$		1.546731	
0	3/4	1			2.002423	11/12	1/4	$(11/12)^{1/2}$		1.561488	
0	5/4	1			1.582341	1	0	1	2.512953		
0	7/4	1			1.342051	1	1/12	$12^{-1/2}$		1.652784	
0	9/4	1			1.184667	1	1/4	1		1.513208	
1/12	1/4	$12^{-1/2}$		3.612911		1	1/4	1/2		1.449800	
1/4	1/4	1/2		2.756714	2.317396	1	1/4	-1		1.305177	
1/4	1/4	1/3		2.682352		1	1/3	$3^{-1/2}$		1.366500	
1/4	1/4	0		2.590675	2.443580	1	1/2	$2^{-1/2}$		1.228400	
1/4	1/4	$-1/3$		2.535872	2.197441	1	3/4	$3^{1/2}/2$		1.121595	
1/4	1/4	$-1/2$		2.500426	2.176713	1	1	1		1.776742	
1/4	1/4	$-5/6$		2.428994		1	1	1/2	0.920568	0.908411	0.896354
1/4	1/4	-1		2.404981	2.118723	1	1	$-1/2$	0.862465	0.854839	0.847225
1/4	1/2	$2^{-1/2}$		2.317859	1.942700	1	1	-1	0.832231	0.825495	0.818761
1/4	1/2	$-2^{-1/2}$		2.017603		1	5/4	$2(5)^{-1/2}$		0.849002	
1/4	2/3	$(2/3)^{1/2}$		2.143085	1.758387	1	19/12	$7(57)^{-1/2}$		0.755000	
1/4	2/3	$-(2/3)^{1/2}$		1.857811		1	7/4	$5(28)^{-1/2}$		0.717906	
1/4	3/4	$3^{1/2}/2$		2.087066	1.680937	1	5/12	$17/10.3^{1/2}$		0.657017	
1/4	3/4	0	1.837384	1.800251		1	9/4	1		0.631944	
1/4	3/4	$-3^{1/2}/2$		1.693078		1	3	$3^{1/2}/2$	0.537121	0.537106	0.528104
1/4	11/12	$(11/12)^{1/2}$		1.864405		1	4	1	0.466147	0.466146	0.458173
1/4	1	1		1.850083	1.490413	5/4	1/4	$2(5)^{-1/2}$		1.331747	
1/4	1	-1		1.614754		5/4	1/2	$3(10)^{-1/2}$		1.119067	
1/4	5/4	$5^{-1/2}$	1.602570			19/12	1/4	$7(57)^{-1/2}$		1.177939	
1/4	5/4	$-5^{-1/2}$	1.536950	1.530590		19/12	2/3	$6(38)^{-1/2}$		0.889531	
1/4	19/12	$5(57)^{-1/2}$		1.390239		7/4	1/4	$5(28)^{-1/2}$		1.118648	
1/4	19/12	$-5(57)^{-1/2}$	1.244082			7/4	3/4	$5(28)^{-1/2}$		0.804509	
1/4	7/4	$2(7)^{-1/2}$	1.337278	1.336076		2	5/4	$3(10)^{-1/2}$		0.589880	
1/4	7/4	$-2(7)^{-1/2}$	1.175596	1.174327		25/12	1/4	$17/10.3^{1/2}$		1.022714	
1/4	9/4	-1	1.196663	1.196574		25/12	11/12	$17/10.3^{1/2}$		0.671650	
1/3	1/4	$3^{-1/2}$		2.480120		9/4	1/4	1		0.983292	
1/2	1/4	$2^{-1/2}$		2.099467	1.942670	9/4	1	1		0.619564	
1/2	1/4	$-2^{1/2}$		1.847348		8/3	19/12	$6(38)^{-1/2}$		0.451	
1/2	1/2	0	1.710851			3	1	$3^{1/2}/2$	0.537121	0.528118	0.528104
$(2/3)^{1/2}$	1/4	$(2/3)^{1/2}$		1.842978		3	7/4	$9(84)^{-1/2}$		0.403154	
$(2/3)^{1/2}$	1/4	$-(2/3)^{1/2}$		1.513210		11/3	25/12	$(99/100)^{1/2}$		0.332393	
$(2/3)^{1/2}$	1/3	0	1.778815			4	1	1	0.466147	0.458174	0.458173
3/4	1/4	$3^{1/2}/2$		1.744611	1.680937	4	9/4	1		0.305211	
3/4	1/4	0	1.874103								

TABLE III (a). Numerical values for the auxiliary functions $\mathfrak{A}$ to $\mathfrak{K}$ Functions $\mathfrak{A}(x_1)$ and $\mathfrak{B}(x_1)$; $x = \beta R_{ab} = \beta R_{ac} = 2.5$.

Θ	$(x_1/x)^2$	$10^6\mathfrak{A}(x_1)$	$10^6\mathfrak{B}(x_1)$
60°	1	21561	38572
90°	2	1973	1031
109°28′	8/3	647	118
120°	3	420	38
146°27′	11/3	191	5
180°	4	142	1

$N(x)$, $R(x)$, and $S(x)$ for different values of the argument x. These values occur in the expression for six equilateral triangles with opening angles 60°, 90°, 109°28′, 120°, 146°27′, and 180°, for which we have evaluated the relative second-order three-body interactions. For values of $x > 2$, 5, the asymptotic expansions (83) to (88) were used; for smaller values of the variable, the results were obtained by means of electronic computation.

Tables containing numerical values for the remain-

TABLE III (b). Functions $\mathfrak{C}$ and $\mathfrak{D}$ [see Eqs. (77) and (78)]; $x = \beta R_{ab} = \beta R_{ac} = 2.5$.

Function	Θ	$(x_1/x)^2$	$(x_2/x)^2$	b^2 $b = \cos\alpha$	Numerical value $\times 10^6$
	60°	1	1	1/4	64
	90°	1	2	1/2	6
$4\mathfrak{C}(x_1, x_2, \alpha)$	109°28′	1	8/3	2/3	1
where					
$x_1 = \beta R_{ac}$	120°	1	3	3/4	<1
$x_2 = \beta R_{bc}$	146°27′	1	11/3	11/12	<1
$\alpha = \sphericalangle bca$	180°	1	2	1	<1
	60°	1	1	1/4	32
	90°	1	1	0	7
$2\mathfrak{C}(x_1, x_2, \alpha)$	109°28′	1	1	1/9	4
where					
$x_1 = \beta R_{ab}$	120°	1	1	1/4	3
$x_2 = \beta R_{ac}$	146°27′	1	1	25/36	<1
$\alpha = \sphericalangle cab$	180°	1	1	1	<1
	60°	1	3/4	3/4	3052
	90°	1	5/4	4/5	1607
$2\Delta^2\cdot(x)\mathfrak{D}(x_1, x_2, \alpha)$	109°28′	1	19/12	49/57	938
where					
$x_1 = \beta R_{ac}$	120°	1	7/4	25/28	884
$x_2 = \beta R_{c(ab)}$	146°27′	1	25/12	289/300	791
$\alpha = \sphericalangle ac(ab)$	180°	1	9/4	1	760
	90°	2	5/4	5/4	1163
$2\Delta^2(x)\mathfrak{D}(x_1, x_2, \alpha)$	109°28′	8/3	19/12	18/19	442
where					
$x_1 = \beta R_{bc}$	120°	3	7/4	3/28	354
$x_2 = \beta R_{c(ab)}$	146°27′	11/3	25/12	33/100	195
$\alpha = \sphericalangle bc(ab)$	180°	4	9/4	1	150
	60°	1	3/4	3/4	3052
	90°	1	1/2	1/2	300
$2\Delta^2(\beta R_{bc})\mathfrak{D}(x_1, x_2, \alpha)$	109°28′	1	1/3	1/3	86
where					
$x_1 = \beta R_{ac}$	120°	1	1/4	1/4	56
$x_2 = \beta R_{a(bc)}$	146°27′	1	1/12	1/12	12
$\alpha = \sphericalangle ca(bc)$	180°	1	0	1	7

TABLE III (c). Functions $\mathfrak{E}$, $\mathfrak{F}$, $\mathfrak{G}$, and $\mathfrak{H}$ [see Eqs. (79)–(82)].

Function	Θ	$(x_1/x)^2$	$(x_2/x)^2$	$(x_3/x)^2$	Numerical value $\times 10^6$
	60°	1	1	3/4	−624
	90°	1	2	5/4	−360
$4\Delta^2(x)\mathfrak{E}(x_1, x_2, x_3)$	109°28′	1	8/3	19/12	−340
where					
$x_1 = \beta R_{ac}$	120°	1	3	7/4	−330
$x_2 = \beta R_{bc}$	146°27′	1	11/3	25/12	−324
$x_3 = \beta R_{c(ab)}$	180°	1	4	9/4	−320

TABLE III (c) (continued).

Function	Θ	$(x_1/x)^2$	$(x_2/x)^2$	$(x_3/x)^2$	Numerical value $\times 10^6$
	60°	1	1	3/4	−312
	90°	1	1	1/2	+30
$2\Delta^2(\beta R_{bc})\mathfrak{S}(x_1, x_2, x_3)$	109°28′	1	1	1/3	+12
where					
$x_1 = \beta R_{ac}$	120°	1	1	1/4	+4
$x_2 = \beta R_{ab}$	146°27′	1	1	1/12	1
$x_3 = \beta R_{a(bc)}$	180°	1	1	0	<1
	60°	1	1	3/4	441
	90°	1	1	5/4	76
$4\Delta^2(x)\mathfrak{F}(x_1, x_2, x_3)$	109°28′	1	1	19/12	18
where					
$x_1 = \beta R_{ac}$	120°	1	1	7/4	7
$x_2 = \beta R_{ab}$	146°27′	1	1	25/12	2
$x_3 = \beta R_{b(ac)}$	180°	1	1	9/4	−4
	60°	1	1	3/4	441
	90°	1	2	5/4	81
$4\Delta^2(x)\mathfrak{F}(x_1, x_2, x_3)$	109°28′	1	8/3	19/12	24
where					
$x_1 = \beta R_{ab}$	120°	1	3	7/4	13
$x_2 = \beta R_{bc}$	146°27′	1	11/3	25/12	3
$x_3 = \beta R_{c(ab)}$	180°	1	4	9/4	2
	60°	1	1	3/4	441
	90°	1/2	1	1/2	40
$4\Delta^2(\beta R_{bc})\mathfrak{F}(x_1, x_2, x_3)$	109°28′	8/3	1	1/3	13
where					
$x_1 = \beta R_{bc}$	120°	3	1	1/4	6
$x_2 = \beta R_{ac}$	146°27′	11/3	1	1/12	1
$x_3 = \beta R_{a(bc)}$	180°	4	1	0	<1
	60°	1	3/4	1/4	6032
	90°	1	1/2	1/4	2510
$2\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{G}(x_1, x_2, x_3)$	109°28′	1	1/3	1/4	1140
where					
$x_1 = \beta R_{ac}$	120°	1	1/4	1/4	712
$x_2 = \beta R_{a(bc)}$	146°27′	1	1/12	1/4	396
$x_3 = \beta R_{(bc)(ac)}$	180°	1	0	1/4	339
	60°	1	3/4	1/4	6032
	90°	1	5/4	1/2	1228
$2\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{G}(x_1, x_2, x_3)$	109°28′	1	19/12	2/3	409
where					
$x_1 = \beta R_{ac}$	120°	1	7/4	3/4	222
$x_2 = \beta R_{c(ab)}$	146°27′	1	25/12	11/12	74
$x_3 = \beta R_{(ac)(ab)}$	180°	1	9/4	1	41
	60°	1	3/4	1/4	6032
	90°	2	5/4	1/4	1120
$2\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{G}(x_1, x_2, x_3)$	109°28′	8/3	19/12	1/4	354
where					
$x_1 = \beta R_{bc}$	120°	3	7/4	1/4	178
$x_2 = \beta R_{c(ab)}$	146°27′	11/3	25/12	1/4	59
$x_3 = \beta R_{(ab)(bc)}$	180°	4	9/4	1/4	34
	60°	1	1	3/4	1225
	90°	1	1	5/4	488
$4\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{K}(x_1, x_2, x_3)$	109°28′	1	1	19/12	250
where					
$x_1 = \beta R_{ac}$	120°	1	1	7/4	155
$x_2 = \beta R_{ab}$	146°	1	1	25/12	73
$x_3 = \beta R_{b(ac)}$	180°	1	1	9/4	51
	60°	1	1	3/4	1225
	90°	1	2	5/4	232
$4\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{K}(x_1, x_2, x_3)$	109°28′	1	8/3	19/12	−13
where					
$x_1 = \beta R_{ac}$	120°	1	3	7/4	−41
$x_2 = \beta R_{bc}$	146°27′	1	11/3	25/12	−51
$x_3 = \beta R_{b(ac)}$	180°	1	4	9/4	−57

TABLE III (c) (continued).

Function	Θ	$(x_{1/x})^2$	$(x_{2/x})^2$	$(x_{3/x})^2$	Numerical value $\times 10^6$
	60°	1	1	3/4	1225
	90°	2	1	1/2	−24
$4\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{K}(x_1, x_2, x_3)$ where	109°28′	8/3	1	1/3	−65
$x_1 = \beta R_{bc}$	120°	3	1	1/4	−115
$x_2 = \beta R_{ac}$	146°27′	11/3	1	1/12	−77
$x_3 = \beta R_{a(bc)}$	180°	4	1	0	−67
$x_1 = \beta R_{ac}$	120°	1	3	7/4	−41
$x_2 = \beta R_{bc}$	146°27′	1	11/3	25/12	−51
$x_3 = \beta R_{b(ac)}$	180°	1	4	9/4	−57
	60°	1	1	3/4	1225
	90°	2	1	1/2	−24
$4\Delta^2(x)\Delta(\beta R_{bc})\mathfrak{K}(x_1, x_2, x_3)$ where	109°28′	8/3	1	1/3	−65
$x_1 = \beta R_{bc}$	120°	3	1	1/4	−115
$x_2 = \beta R_{ac}$	146°27′	11/3	1	1/12	−77
$x_3 = \beta R_{a(bc)}$	180°	4	1	0	−67

TABLE IV. Final results for relative first- and second-order three-body interactions, as functions of opening Θ of isoceles triangles; $\beta R_{ab} = \beta R_{ac} = 2.5$.

Θ	$\Delta E_1/E_1^{(0)}$	$\Delta E_2/E_2^{(0)}$
60°	−0.2008	−0.1612
90°	−0.0612	−0.0378
109°28′	+0.0187	+0.0197
120°	+0.0209	+0.0432
146°27′	+0.0339	+0.0539
180°	+0.0374	+0.0557

ing three basic integrals $O(u, v, \Theta)$, $P(u, v, \Theta)$, and $Q(u, v, \Theta)$ are also given as functions of the three variables, again corresponding to the six triangles considered. These basic integrals were evaluated by electronic computation for u or $v < 2$, 5 and by using the double-series expansions (89) for the remaining values of u and v. It was possible to avoid excessive machine calculations by making use of some theoretical relations between the values of O, P, or Q for different values of u and v; i.e., if $Q(u_i, v_i, \Theta)$ is known for a set of values of u_i and v_i, then $Q(u', v', \Theta)$ can be determined theoretically with a certain given precision. In some cases, general asymptotic expansions were used for direct evaluation of the auxiliary functions, instead of via the basic integrals.

Numerical values for $K(x)$, $L(x)$, $M(x)$, $N(x)$, $R(x)$ and $S(x)$ are given in Table I, those for $O(u, v, \Theta)$; $P(u, v, \Theta)$ and $Q(u, v, \Theta)$ in Table II, and those for the auxiliary functions $\mathfrak{A}$ to $\mathfrak{K}$ in Table III (a–c). The values of Table III (a–c) follow directly from the relations (75)–(82). Finally, numerical results for the relative first- and second-order three-body interactions are given for $x = \beta R = 2{,}5$, which corresponds to the case of solid argon (see Table IV). These results have been obtained directly by using Eqs. (38) and (39).

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Quantum Statistics of Multicomponent Systems

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Methods of quantum statistics are applied to the general multicomponent system and explicit rules for the calculation of thermodynamic quantities and distribution functions in terms of the basic particle interactions are derived. Particular attention is given to the nonrelativistic system of charged particles, and several inherent difficulties are investigated and treated. Included are the renormalization, by the Λ transformation, of charged-particle energy contributions due to the emission and reabsorption of photons and the formal sum over all long-range Coulomb effects wherever (diagrammatically) they give divergent expressions. The latter sum is shown to result in the familiar Debye–Hückel theory in the high-temperature, low-density limit.

INTRODUCTION

ALTHOUGH most of the macroscopic systems in nature are comprised of more than one kind of particle, the quantum-mechanical microscopic theory of multicomponent systems has hardly been developed at all.[1] Part of the reason for this is that the important physical consequences of a theory are usually exhibited by simple models, so that theoretical efforts in the many-body problem have been largely concentrated on single-component systems. Unfortunately, this particular simplifying feature is no longer present when there are charges in the system, and the primary purpose of this paper is to present a complete and usable theory for the study of charged-particle systems.

Several other formalisms have been developed and applied to a quantum-mechanical system of charge particles.[2-6] However, almost all of these studies have been confined to an electron gas in a uniform background of positive charge, and have been examined only in the limits of high temperature and low density (classical), or high density and low temperature (ground state). The majority of these calculations have considered only the ring diagram, or random-phase approximation, although Abe[7] and others[8,9] have made some progress in understanding nonring terms in the classical case, and DeWitt[10] has considered some of the quantum corrections.

In order to understand the general ionized gas in thermal equilibrium, one must be able to calculate thermodynamic quantities beyond these approximations, and for finite temperature and density. Furthermore, Baxter[11] has recently shown in the one-dimensional case that there are indeed differences between the thermodynamics of true multicomponent systems and those with uniform background of positive charge, so that the need is evident for a developable theory of multicomponent systems. In principle, the formalisms mentioned above may be extended to multicomponent systems and developed further, but this further development has not taken place, despite the intervening length of time, and it is not clear with what ease they can be extended so as to explicitly calculate thermodynamic quantities. We must note, however, that DeWitt[12] and others[13] have made some probings in this direction.

Our exposition is based on the original work of Lee and Yang,[14] as further developed by Mohling,[15,16] and can be considered as a natural extension of that work. The success in understanding low-temperature Bose and Fermi systems from this point of view leads us to believe that the same success can be obtained with charged-particle systems, but in the

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final analysis this can only be decided, of course, after making suitable applications. Thus, the quantum-statistical theory which is presented here is actually very flexible, in that it can include all possible kinds of particles and their interactions, provided only that the number of each kind of particle considered is very large. The essentials of such a theory are well known, and therefore Sec. I on the Ursell expansion of the grand partition function for a multicomponent system contains no novel features.

In order to formulate the detailed rules for explicitly calculating thermodynamic functions, it is useful to study a particular set of interactions. Hence, in Sec. II the notation of the Fock representation is reviewed and applied to the case of nonrelativistic electromagnetic interactions. Some of the consequences of electromagnetic interactions are pursued in the remainder of the paper along with the development of the general theory.

The most important steps in the development of the general theory are contained in Sec. III, where the Ursell functions $U_N^{(S)}$ are expressed in terms of the basic interactions of the system. The final result of this section is Eq. (41), which provides a diagrammatic prescription for the calculation of the $U_N^{(S)}$ in terms of wiggly-line cluster graphs.

One of the inherent difficulties associated with electromagnetic interactions is the self-energy problem due to the emission and reabsorption of photons by a single charged particle. In Sec. IV, it is shown that one-particle cluster graphs contain this self-energy problem. Moreover, it is demonstrated that the (divergent) self-energy terms are completely independent of any thermodynamic parameters of the many-body system. It is therefore physically acceptable that they be removed by canceling them against counterterms in the single-particle energy–momentum relations. This is formally achieved by the Λ_S transformation [Eqs. (52)–(65)], under which one-particle cluster graphs retain their system-dependent, nondivergent parts.

A principle result of this paper is the linked-pair expansion of the grand potential (the logarithm of the grand partition function). Equations (71) and (77) in Sec. V denote this expansion as a sum over all linked-pair 0 graphs, whose prescription represents a concise formulation of quantum statistics in terms of the basic particle interactions. Furthermore, in the derivation of this prescription from results in the preceding sections most of the tedious combinatorial problems of the theory are solved by the use of symmetry numbers. The linked-pair expansion given here, which includes photon interaction terms, is a generalization of the first author's previous result for the grand potential of a single-component system.[15]

In Sec. VI, the momentum distribution $\langle n_\alpha(\mathbf{k})\rangle$ and the pair correlation function $P(\mathbf{k}_\alpha, \mathbf{k}'_\beta)$ are investigated. It is shown whenever momentum-space ordering becomes important, that the equations of quantum statistics can be rewritten so that each solid-line factor in the grand potential and the distribution functions is given by a function $N_\alpha(\mathbf{k})$, which is related to $\langle n_\alpha(\mathbf{k})\rangle$ by Eq. (81). Thus, the momentum distribution plays a central role in quantum statistics. This aspect of the theory is further displayed in Sec. VII, where the master graph formulation of quantum statistics is written down. In this formulation, all "many-body self-energy parts" (defined to have only one incoming and one outgoing line) of graphs have been summed and included as the vertex factors $\mathcal{G}_\alpha(\mathbf{k})$ of Eqs. (98). The intimate relation between these self-energy parts and momentum space ordering has been previously shown explicitly for a very low temperature Fermi system.[16] Equations (99) and (105) show the close connection between $\mathcal{G}_\alpha(\mathbf{k})$ and $\langle n_\alpha(\mathbf{k})\rangle$.

Sections VIII and IX deal specifically with the Coulomb interaction. The long range of the Coulomb potential results in a momentum space singularity which is iterated by the "ring structure" of Fig. 5, thereby exhibiting an apparent divergence of the theory. The purpose of Sec. VIII is to sum such ring structures wherever they occur in the graphs of quantum statistics by means of integral equations. The hope is that the solutions to these integral equations will no longer exhibit a momentum-space singularity, or, in other words, that the solutions will correspond to a screened Coulomb potential. Such a behavior is, in fact, deduced in Sec. IX in the high-temperature, low-density limit, where the well-known Debye–Hückel expression for the pressure of an ionized gas is obtained. It is only to exhibit this behavior and to illustrate the methods that this expression is derived, and the future application to other temperature-density regions, along with quantum-mechanical corrections, is also briefly discussed in this section.

I. URSELL EXPANSION FOR MULTICOMPONENT SYSTEMS

In the general multicomponent system, there will be different kinds of particles (α, β, η, $\cdots$) interacting among themselves as well as with each other. We let N_α be the number of α-type particles, N_β be the number of β-type particles, etc. It is

assumed that these particle numbers are all very much greater than unity, in which case, we may determine the properties of the system by computing ensemble averages. In particular, we assume that the method of the most probable distribution[17] applied to a grand canonical ensemble can be used to calculate average values of the system at equilibrium. For the case when the particle numbers $(N_\alpha, N_\beta, N_\eta, \cdots)$ are each separately conserved, one obtains for the grand partition function

$$e^{\Omega f} = \sum_{N_\alpha, N_\beta, \cdots = 0}^{\infty} \exp \beta(N_\alpha g_\alpha + N_\beta g_\beta + \cdots) \times \sum_{i\{N_\alpha\}} \exp(-\beta E_i), \quad (1)$$

where the sum over i, corresponding to the system energies E_i, is performed for each different set $\{N_\alpha\}$ of particle numbers $(N_\alpha, N_\beta, N_\eta, \cdots)$. The identification of the Lagrange multipliers $(\beta, g_\alpha, g_\beta, \cdots)$ is made with the aid of thermodynamics, and one finds

$$\beta = 1/kT, \quad (2)$$

where T is the temperature of the system and k = Boltzmann's constant;

$$G = \sum_\alpha \langle N_\alpha \rangle g_\alpha = (\langle N_\alpha \rangle g_\alpha + \langle N_\beta \rangle g_\beta + \cdots), \quad (3)$$

where G is the thermodynamic potential; and that

$$g_\alpha = (\partial G / \partial \langle N_\alpha \rangle)\,|_{\mathcal{P},T} \quad (4)$$

is the partial thermodynamic potential for the α-type particles. The quantity Ω is the volume of the system.

We assume for very large systems that the grand potential $f(\beta, g_\alpha, \Omega)$ is an intensive quantity, and this assumption is made physically reasonable by the Ursell expansion as well as by inspection of the following set of equations. Thus, the thermodynamic properties of a system can be calculated by performing certain partial derivatives of the grand potential. For example, the probability for finding the system in the ith energy state, for fixed $(N_\alpha, N_\beta, \cdots)$, is

$$P_i = e^{-\Omega f} e^{\beta(G - E_i)} = -\beta^{-1} \partial(\Omega f)/\partial E_i. \quad (5)$$

Thermodynamic properties of the system can be calculated using the following equations:

Pressure

$$\mathcal{P} = \beta^{-1} \partial(\Omega f)/\partial \Omega. \quad (6)$$

Particle number

$$\langle N_\alpha \rangle = \beta^{-1} \partial(\Omega f)/\partial g_\alpha. \quad (7)$$

Particle density

$$\rho = \frac{\langle N \rangle}{\Omega} = \sum_\alpha \frac{\langle N_\alpha \rangle}{\Omega} = \beta^{-1} \sum_\alpha \frac{\partial f}{\partial g_\alpha}. \quad (8)$$

Energy

$$\langle E \rangle = G - \partial(\Omega f)/\partial \beta. \quad (9)$$

Entropy

$$\langle S \rangle = \partial(\beta^{-1} \Omega f)/\partial T. \quad (10)$$

We have so far written down the grand partition function for the special case in which the particle numbers $(N_\alpha, N_\beta, \cdots)$ are each separately conserved. Other cases may be easily included, however, by simply making the following observations:

(i) The partial thermodynamic potential vanishes $(g = 0)$ for components, such as photons, for which the particle number is not conserved.

(ii) When α particles can transform into β particles, then one must set $g_\alpha = g_\beta$. This situation could occur if one wished to treat the different phases, e.g., vapor and liquid, of a substance as different components.

(iii) When chemical reactions can take place in a system, then one obtains fewer Lagrange multipliers than appear in Eq. (1). One is thereby able to deduce the equilibrium conditions for chemical reactions, which are relations among the partial thermodynamic potentials. For example, if the reversible reaction $\alpha = \beta + \eta$ can take place, then one can derive the equilibrium condition $g_\alpha = g_\beta + g_\eta$ from the fact that $(2N_\alpha + N_\beta + N_\eta)$ and $(N_\beta - N_\eta)$ are conserved quantities. In this example, one may further deduce that $g_\beta = g_\eta$ if $\langle N_\beta \rangle = \langle N_\eta \rangle$ in the system of interest.

After making the observations of the preceding paragraph, one concludes that Eq. (1) is the most general expression for the grand partition function of a system at rest. This expression can also be written as

$$e^{\Omega f} = \sum_{N_\alpha, N_\beta, \cdots = 0}^{\infty} \exp \beta(N_\alpha g_\alpha + N_\beta g_\beta + \cdots) \times [\mathrm{Tr}\,(e^{-\beta H})]_{\{N_\alpha\}}, \quad (11)$$

where $\mathrm{Tr}\,[\ ]_{\{N_\alpha\}}$ indicates that the trace of $\exp(-\beta H)$ is to be taken over a complete set of states for a system with the particle numbers $(N_\alpha, N_\beta, \cdots)$ and Hamiltonian H. Upon comparing Eqs. (11) and (5), we conclude that the density matrix for this system is

$$\rho = e^{-\Omega f} e^{\beta(G - H)}. \quad (12)$$

We next introduce the interaction representation

[17] E. Schrödinger, *Statistical Mechanics*, (Cambridge University Press, New York, 1960), Chaps. II and VI.

into Eq. (11) by means of the operator $W(\beta)$.

$$W(\beta) \equiv e^{\beta H_0} e^{-\beta H}, \tag{13}$$

where H_0 is the free-particle Hamiltonian.[18] We also use the momentum, or free-particle representation to evaluate the trace in Eq. (11). With these notations, the grand partition function can be written as

$$e^{\Omega/} = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\mathbf{k}_1 \cdots \mathbf{k}_N} e^{\beta G} \exp\left[-\beta \sum_{i=1}^{N} \omega_i^{(0)}\right] \times W^{(S)}\begin{pmatrix} \mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N \\ \mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N \end{pmatrix}, \tag{14}$$

where the $\omega_i^{(0)}$ are single-particle energies, in the momentum representation, of the Hamiltonian H_0, and where *each* $\mathbf{k}_i$ ranges over all of the free-particle states of all the different kinds of particles.[19] The last factor in Eq. (14) is defined in terms of the matrix elements of $W(\beta)$ by the relation (S stands for symmetrized)

$$W^{(S)}\begin{pmatrix} 1 & 2 & \cdots & N \\ 1' & 2' & \cdots & N' \end{pmatrix} = \sum_{P'} \left(\prod_{\alpha} \epsilon_\alpha^{P_\alpha'}\right) P' \langle 12 \cdots N | \, W(\beta) \, | 1' \, 2' \cdots N' \rangle, \tag{15}$$

where $\sum_{P'}$ denotes the sum over all permutations *among identical particles* of the primed indices, and P' can always be written as a product of permutations each of which refers to a different kind of particle. Thus, there are $\prod_\alpha (N_\alpha!)$ terms in this sum. The quantity ϵ_α refers to the statistics of the α particles and it is $(+1)$ for Bose–Einstein statistics and (-1) for Fermi–Dirac statistics.

Application of the Ursell Method

The sum over all states in the grand partition function includes states in which N particles are divided into two noninteracting clusters with N_1 particles in one cluster and N_2 particles in the other cluster. The contribution of such states to the grand partition function has an Ω^2 dependence. Similarly, states for which there are M noninteracting clusters of particles have a volume dependence Ω^M. The method of Ursell exploits this property of the sum over all states and leads to an expression for the grand potential in which factorizing or clustering does not occur. The final expression (19), therefore, exhibits the intensive character of the grand potential directly.

Clustering in quantum systems occurs not only because particles are dynamically interacting, but it can also arise from purely quantum mechanical effects. Thus, the effect of wavefunction overlap of identical particles may result in an appreciable contribution to the grand partition function from exchange integrals when the sum over permutations in Eq. (15) is performed. This contribution from exchange integrals is a "quantum clustering." It occurs for any representation, and must not necessarily be thought of as occurring in position space. Furthermore, it also occurs for free particles and results in the well-known free-particle grand potential (77) for degenerate systems. A measure of the effect of "quantum clustering" is given by the parameter $\rho\lambda_\alpha^3$, where

$$\lambda_\alpha = (2\pi\hbar^2\beta/M_\alpha)^{\frac{1}{2}} \tag{16}$$

is the thermal wavelength for α particles, and M_α is the mass of an α particle. Thus, when $\rho\lambda_\alpha^3 \gtrsim 1$, then quantum clustering occurs for α particles.

The method of Ursell consists of defining "cluster functions" $U_N^{(S)}$ in terms of the $W_N^{(S)}$ of Eq. (15) by the following set of equations:

$$\begin{aligned}
W^{(S)}\begin{pmatrix} 1 \\ 1' \end{pmatrix} &= U^{(S)}\begin{pmatrix} 1 \\ 1' \end{pmatrix}, \\
W^{(S)}\begin{pmatrix} 1 & 2 \\ 1' & 2' \end{pmatrix} &= U^{(S)}\begin{pmatrix} 1 \\ 1' \end{pmatrix} U^{(S)}\begin{pmatrix} 2 \\ 2' \end{pmatrix} + U^{(S)}\begin{pmatrix} 1 & 2 \\ 1' & 2' \end{pmatrix}, \\
W^{(S)}\begin{pmatrix} 1 & 2 & 3 \\ 1' & 2' & 3' \end{pmatrix} &= U^{(S)}\begin{pmatrix} 1 \\ 1' \end{pmatrix} U^{(S)}\begin{pmatrix} 2 \\ 2' \end{pmatrix} U^{(S)}\begin{pmatrix} 3 \\ 3' \end{pmatrix} \\
&\quad + U^{(S)}\begin{pmatrix} 1 \\ 1' \end{pmatrix} U^{(S)}\begin{pmatrix} 2 & 3 \\ 2' & 3' \end{pmatrix} + U^{(S)}\begin{pmatrix} 2 \\ 2' \end{pmatrix} U^{(S)}\begin{pmatrix} 3 & 1 \\ 3' & 1' \end{pmatrix} \\
&\quad + U^{(S)}\begin{pmatrix} 3 \\ 3' \end{pmatrix} U^{(S)}\begin{pmatrix} 1 & 2 \\ 1' & 2' \end{pmatrix} + U^{(S)}\begin{pmatrix} 1 & 2 & 3 \\ 1' & 2' & 3' \end{pmatrix},
\end{aligned} \tag{17}$$

etc.

These equations are such that the Nth equation connects $W_N^{(S)}$ with all of the $U_1^{(S)}, U_2^{(S)}, \cdots, U_N^{(S)}$. From the preceding discussion, it should be clear that each $U_M^{(S)}$ can be made to correspond to a physical cluster of M particles, i.e., a group of M particles which cannot be broken into two or more noninteracting groups.[20]

[18] When there are external applied fields, then their effect can be included in H_0, but we are not concerned with such situations in this paper.

[19] We are excluding in what follows the fact that the composite particles of the system can have internal, or excited states. In this connection, see A. I. Larkin, Zh. Eksperim. i Teor. Fiz. 38, 1896 (1960) [English transl.: Soviet Phys.—JETP 11, 1363 (1960)], and M. Girardeau, J. Math. Phys. 4, 1096 (1963).

[20] In this connection, see D. ter Haar, *Elements of Statistical Mechanics*, (Rinehart and Company, New York, 1954), Chap. VIII.

We now define an N-particle cluster integral $b_N(\beta, g_\alpha, \Omega)$ by the relation[21]

$$b_N(\beta, g_\alpha, \Omega) = (\Omega N!)^{-1} \sum_{\mathbf{k}_1 \cdots \mathbf{k}_N} e^{\beta G} \exp\left[-\beta \sum_{i=1}^{N} \omega_i^{(0)}\right] \times U^{(S)}\begin{pmatrix}\mathbf{k}_1 \cdots \mathbf{k}_N \\ \mathbf{k}_1 \cdots \mathbf{k}_N\end{pmatrix}. \quad (18)$$

After substituting the Ursell equations (17) into the grand partition function (14), and gathering together identical terms, one finds that the grand potential can be written directly as a sum over the b_N.

$$f(\beta, g_\alpha, \Omega) = \sum_{N=1}^{\infty} b_N(\beta, g_\alpha, \Omega) = \Omega^{-1} \sum_{N=1}^{\infty} (N!)^{-1} \sum_{\mathbf{k}_1 \cdots \mathbf{k}_N} e^{\beta G} \exp\left[-\beta \sum_{i=1}^{N} \omega_i^{(0)}\right] \times U^{(S)}\begin{pmatrix}\mathbf{k}_1 \cdots \mathbf{k}_N \\ \mathbf{k}_1 \cdots \mathbf{k}_N\end{pmatrix}. \quad (19)$$

By their definition, the b_N are volume independent for a very large system ($N \gg 1$), and therefore, the grand potential has been exhibited as an intensive quantity. It is to be emphasized that *each* $\mathbf{k}_i$ in the single-particle sums of (18) and (19) ranges over all of the free-particle states (including spin) of *all* of the different kinds of particles.

II. USE OF THE FOCK REPRESENTATION

The presence of interactions in the general multicomponent system gives rise to the continual annihilation and creation of certain particles, subject to the conservation laws of the system. In order to describe such processes with a Hamiltonian formulation, we shall resort to the Fock, or number, representation.[22] In this representation, Eq. (15) for $W_N^{(S)}$ becomes

$$W^{(S)}\begin{pmatrix}\mathbf{k}_1\, \mathbf{k}_2 \cdots \mathbf{k}_N \\ \mathbf{k}_1'\, \mathbf{k}_2' \cdots \mathbf{k}_N'\end{pmatrix} = \langle \mathbf{k}_1\, \mathbf{k}_2 \cdots \mathbf{k}_N |\, W^{(S)}(\beta)\, | \mathbf{k}_1'\, \mathbf{k}_2' \cdots \mathbf{k}_N' \rangle, \quad (20)$$

where the normalization used in Eq. (15) implies that the state vectors have the form.

$$|\mathbf{k}_1\, \mathbf{k}_2 \cdots \mathbf{k}_N\rangle = \prod_{\mathbf{k}} (a_{\mathbf{k}}^\dagger)^{n_{\mathbf{k}}} |0\rangle. \quad (21)$$

In Eq. (21), $n_{\mathbf{k}}$ is the number of particles in the state $\mathbf{k}$ and $|0\rangle$ is the vacuum state. We have again adopted the notation that the product over states $\mathbf{k}$ ranges over all of the free-particle states (including spin) of all the different kinds of particles. The creation operator $a_{\mathbf{k}}^\dagger$, therefore, can represent any kind of particle in any free-particle state. We must, of course, maintain the proper commutation relations for fermions and bosons. Thus

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0, \qquad [a_i, a_j^\dagger] = \delta_{ij} \quad (22a)$$

for any two bosons, whereas

$$[a_i, a_j]_+ = [a_i^\dagger, a_j^\dagger]_+ = 0, \quad [a_i, a_j^\dagger]_+ = \delta_{ij} \quad (22b)$$

for any two fermions.

In the Fock representation, the Hamiltonian is written as

$$H = H_0 + V, \quad (23)$$

where

$$H_0 = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \omega_{\mathbf{k}}^{(0)}, \quad (24)$$

and where V gives the explicit interactions of the system. The general form of V for two-particle interactions is

$$V_2 = \tfrac{1}{2} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4} a_1^\dagger a_2^\dagger \langle \mathbf{k}_1 \mathbf{k}_2 |\, V_2\, | \mathbf{k}_3 \mathbf{k}_4 \rangle a_4 a_3. \quad (25)$$

For identical fermions it is important to observe the order of the annihilation and creation operators in (25).

Of particular interest are systems in which electromagnetic interactions must be considered. We only consider nonrelativistic charged particles, in which case their interaction with photons arises from the prescription

$$\frac{p^2}{2M} \rightarrow \frac{(\mathbf{p} - e\mathbf{A}/c)^2}{2M}.$$

When the vector potential $\mathbf{A}$ is expanded in canonical variables, the second quantization form (27) of the electromagnetic interaction represents the annihilation or creation of zero, one, or two photons.[23] The interaction of photons with charged particles will be written as follows:

$$V_\gamma = V_{1\gamma} + V_{2\gamma} + V_{1\gamma}^\dagger + V_{2\gamma}^\dagger, \quad (26)$$

where

$$V_{1\gamma} = \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} a_1^\dagger \langle \mathbf{k}_1 |\, V_{1\gamma}\, | \mathbf{k}_2, \mathbf{k}_3 \rangle a_2 a_3^{(\gamma)}, \quad (27a)$$

$$V_{2\gamma} = \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4} a_1^\dagger \langle \mathbf{k}_1 |\, V_{2\gamma}\, | \mathbf{k}_2, \mathbf{k}_3 \mathbf{k}_4 \rangle a_2 a_3^{(\gamma)} a_4^{(\gamma)} + \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4} a_1^\dagger a_2^{(\gamma)\dagger} \langle \mathbf{k}_1, \mathbf{k}_2 |\, V_{2\gamma}\, | \mathbf{k}_3, \mathbf{k}_4 \rangle a_3 a_4^{(\gamma)}. \quad (27b)$$

We do not include the second term of $V_{2\gamma}$ in the

[21] It should be observed that the b_N reduce in the classical limit to the cluster integrals originally defined by Mayer. See E. E. Salpeter, Ann. Phys. 5, 183 (1958).

[22] V. Fock, Z. Physik 75, 622 (1932).

[23] In the remainder of the paper, the particle-type-label γ will be used only for photons, in both equations and figures.

category of terms in V_2, Eq. (25), but we assume that this second term must be written in "normal" form with the photon annihilation operator $a^{(\gamma)}$ always appearing to the right of the photon creation operator $a^{(\gamma)\dagger}$. Finally, we assume that each photon momentum sum excludes the value $\mathbf{k} = 0$, which corresponds to a vacuum interaction, and implicitly includes a sum over polarization indices.

In the case of the interaction of elementary charged particles with photons, we write the (real) matrix elements of $V_{1\gamma}$ and $V_{2\gamma}$ using standard notation.[24]

$$\langle \mathbf{k}_1|\ V_{1\gamma}\ |\mathbf{k}_2, \mathbf{k}_3\rangle = -Z_1(\hbar^2/M)k_1(2\pi\alpha/\Omega k_3)^{\frac{1}{2}}(\hat{\mathbf{k}}_1\cdot\hat{\mathbf{e}}_3) \times \delta_{[\mathbf{k}_1,(\mathbf{k}_2+\mathbf{k}_3)]}\delta_{(m_1,m_2)} \quad (28a)$$

$$\langle \mathbf{k}_1|\ V_{2\gamma}\ |\mathbf{k}_2, \mathbf{k}_3\mathbf{k}_4\rangle = Z_1^2(\hbar^2/M)(\pi\alpha/\Omega)k_3^{-\frac{1}{2}}k_4^{-\frac{1}{2}}(\hat{\mathbf{e}}_3\cdot\hat{\mathbf{e}}_4) \times \delta_{[\mathbf{k}_1,(\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4)]}\delta_{(m_1,m_2)} \quad (28b)$$

$$\langle \mathbf{k}_1, \mathbf{k}_2|\ V_{2\gamma}\ |\mathbf{k}_3, \mathbf{k}_4\rangle = Z_1^2(\hbar^2/M)(\pi\alpha/\Omega)k_2^{-\frac{1}{2}}k_4^{-\frac{1}{2}}(\hat{\mathbf{e}}_2\cdot\hat{\mathbf{e}}_4) \times \delta_{[(\mathbf{k}_1+\mathbf{k}_2),(\mathbf{k}_3+\mathbf{k}_4)]}\delta_{(m_1,m_3)}. \quad (28c)$$

In Eqs. (28), $\delta(a, b)$ is a Kronecker δ function of a and b, Z_1 is the charge of the particle (1) in units of $|e|$, m_1 is the spin projection quantum number, and $\alpha = e^2/\hbar c$ is the fine-structure constant. The Lorentz condition makes possible the elimination of longitudinal photons, resulting in the condition on Eqs. (28)

$$(\hat{\mathbf{k}}_i\cdot\hat{\mathbf{e}}_i) = 0, \quad (29)$$

where $\hat{\mathbf{e}}_i$ is the polarization vector of the photon in the ith state.

Two remarks concerning the interactions of photons with charged particles must be made. The first is that Eqs. (28) can be used for atomic and molecular ions only when second-order processes, such as the photoelectric effect, are unimportant in the many-body system. A similar restriction holds with respect to particle spins, which we have assumed to remain "unflipped" in photon interactions. Actually, photons are not "transverse," but instead have two possible helicity states. One must go to a relativistic treatment of photon–particle interactions, however, in order to deal with the spin projections properly.

We assume that the most general interaction in the multicomponent system is of the form

$$V = V_2 + V_\gamma. \quad (30)$$

If there are other important types of interactions, such as pair production, then these can easily be included in the general formalism of the next section.

As a final matter for this section, we shall write down the interaction Hamiltonian V in the interaction representation

$$V(\beta) \equiv e^{\beta H_0}Ve^{-\beta H_0} = V_2(\beta) + V_\gamma(\beta). \quad (31)$$

If one makes use of the identities[25]

$$\begin{aligned} a_{\mathbf{k}}(\beta) &\equiv e^{\beta H_0}a_{\mathbf{k}}e^{-\beta H_0} = a_{\mathbf{k}}\exp[-\beta\omega_{\mathbf{k}}^{(0)}] \\ a_{\mathbf{k}}^\dagger(\beta) &\equiv e^{\beta H_0}a_{\mathbf{k}}^\dagger e^{-\beta H_0} = a_{\mathbf{k}}^\dagger\exp[\beta\omega_{\mathbf{k}}^{(0)}], \end{aligned} \quad (32)$$

then one can readily verify the following expressions:

$$\begin{aligned} V_2(\beta) &= \tfrac{1}{2}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_1^\dagger a_2^\dagger\langle \mathbf{k}_1\mathbf{k}_2|\ V_2(\beta)\ |\mathbf{k}_4\mathbf{k}_3\rangle a_3a_4 \\ &= \tfrac{1}{2}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_1^\dagger a_2^\dagger\langle \mathbf{k}_1\mathbf{k}_2|\ V_2\ |\mathbf{k}_4\mathbf{k}_3\rangle a_3a_4 \\ &\quad\times\exp\beta[\omega_1^{(0)} + \omega_2^{(0)} - \omega_3^{(0)} - \omega_4^{(0)}] \end{aligned} \quad (33)$$

and

$$V_\gamma(\beta) = V_{1\gamma}(\beta) + V_{2\gamma}(\beta) + V_{1\gamma}^\dagger(-\beta) + V_{2\gamma}^\dagger(-\beta), \quad (34)$$

where

$$V_{1\gamma}(\beta) = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} a_1^\dagger\langle \mathbf{k}_1|\ V_{1\gamma}(\beta)\ |\mathbf{k}_2, \mathbf{k}_3\rangle a_2a_3^{(\gamma)} \quad (35)$$

$$\begin{aligned} V_{2\gamma}(\beta) &= \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_1^\dagger\langle \mathbf{k}_1|\ V_{2\gamma}(\beta)\ |\mathbf{k}_2, \mathbf{k}_3\mathbf{k}_4\rangle a_2a_3^{(\gamma)}a_4^{(\gamma)} \\ &\quad+\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_1^\dagger a_2^{(\gamma)\dagger}\langle \mathbf{k}_1, \mathbf{k}_2|\ V_{2\gamma}(\beta)\ |\mathbf{k}_3, \mathbf{k}_4\rangle a_3a_4^{(\gamma)}. \end{aligned}$$

III. DETERMINATION OF THE CLUSTER FUNCTIONS $U_N^{(S)}$

The determination of the cluster functions $U_N^{(S)}$, which are defined by the Ursell equations (17), follows from a study of the matrix elements of the operator $W(\beta)$ of Eq. (13). This operator satisfies the differential equation

$$\partial W(\beta)/\partial\beta = -V(\beta)W(\beta), \quad (36)$$

where $V(\beta)$ is defined by Eq. (31). By using the "initial" condition $W(0) = 1$, one can rewrite (36) as an integral equation,

$$\begin{aligned} W(\beta) &= 1 - \int_0^\beta dtV(t)W(t) \\ &= 1 - \int_0^\beta dtV(t) + \int_0^\beta dt_2\int_0^{t_2} dt_1V(t_2)V(t_1) \\ &\quad - \int_0^\beta dt_3\int_0^{t_3} dt_2\int_0^{t_2} dt_1V(t_3)V(t_2)V(t_1) + O(V^4). \end{aligned} \quad (37)$$

[24] *Quantum Theory*, edited by D. R. Bates (Academic Press, Inc., New York, 1962), Vol. III, Chap. II.

[25] S. S. Schweber, H. A. Bethe, and F. de Hoffmann, *Mesons and Fields* (Row, Peterson and Company, Evanston, Illinois, 1956), Vol. I, p. 170.

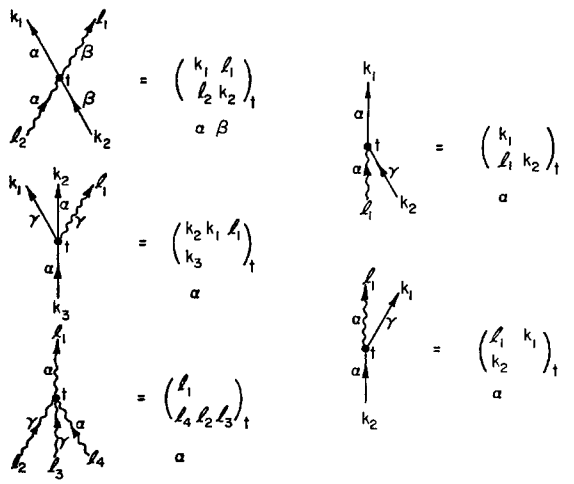


FIG. 1. Examples of cluster vertices. The explicit expressions for these symbols are given in Eqs. (38).

The identification of the $U_N^{(S)}$ then proceeds by exhibiting the matrix elements of the iterated form of (37) in the form of the Ursell equations.

The prescription for calculating the cluster functions $U_N^{(S)}$ in terms of the basic particle interactions can be conveniently expressed in terms of wiggly-line cluster graphs. We therefore first define these graphs and then give the prescription and its proof.

Wiggly-Line Cluster Graphs[26]

The basic units of a cluster graph are symbols for the matrix elements in Eqs. (33) and (35), and we call such symbols *cluster vertices*. At any cluster vertex there are *incoming* and *outgoing* lines, equipped with arrows, which correspond to the momentum (and spin) states of the vertex function. In these symbols, we distinguish between *internal* (**l**) and *external* (**k**) momenta by drawing the internal momentum lines as wiggly lines and the external momentum lines as solid lines. The type of particle represented by the line is indicated with an additional Greek letter. Examples of cluster vertices are given in Fig. 1. The explicit expressions for the bracket symbols used in this figure are

$$\begin{aligned}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{l}_2\mathbf{k}_2\end{pmatrix}_t &= -[\langle \mathbf{k}_1\mathbf{l}_1|\ V_2(t)\ |\mathbf{l}_2\mathbf{k}_2\rangle + \epsilon_\alpha\langle \mathbf{k}_1\mathbf{l}_1|\ V_2(t)\ |\mathbf{k}_2\mathbf{l}_2\rangle] \\ &\qquad \text{for identical particles } (\alpha = \beta) \\ &= -\epsilon_\alpha\epsilon_\beta\langle \mathbf{k}_1\mathbf{l}_1|\ V_2(t)\ |\mathbf{l}_2\mathbf{k}_2\rangle \\ &\qquad \text{for nonidentical particles } (\alpha \neq \beta) \\ &= -2\epsilon_\alpha\langle \mathbf{k}_1, \mathbf{l}_1|\ V_{2\gamma}(t)\ |\mathbf{l}_2, \mathbf{k}_2\rangle \\ &\qquad \text{for } \beta = \text{photon and } \alpha = \text{charged particle,}\end{aligned} \tag{38}$$

$$\begin{aligned}\begin{pmatrix}\mathbf{k}_2\mathbf{k}_1\mathbf{l}_1\\ \mathbf{k}_3\end{pmatrix}_t &= -\epsilon_\alpha[\langle \mathbf{k}_2, \mathbf{k}_1\mathbf{l}_1|\ V_{2\gamma}(t)\ |\mathbf{k}_3\rangle \\ &\qquad + \langle \mathbf{k}_2, \mathbf{l}_1\mathbf{k}_1|\ V_{2\gamma}(t)\ |\mathbf{k}_3\rangle], \\ \begin{pmatrix}\mathbf{l}_1\\ \mathbf{l}_4\mathbf{l}_2\mathbf{l}_3\end{pmatrix}_t &= -\epsilon_\alpha[\langle \mathbf{l}_1|\ V_{2\gamma}(t)\ |\mathbf{l}_4, \mathbf{l}_2\mathbf{l}_3\rangle \\ &\qquad + \langle \mathbf{l}_1|\ V_{2\gamma}(t)\ |\mathbf{l}_4, \mathbf{l}_3\mathbf{l}_2\rangle], \\ \begin{pmatrix}\mathbf{k}_1\\ \mathbf{l}_1\mathbf{k}_2\end{pmatrix}_t &= -\epsilon_\alpha\langle \mathbf{k}_1|\ V_{1\gamma}(t)\ |\mathbf{l}_1, \mathbf{k}_2\rangle, \\ \begin{pmatrix}\mathbf{l}_1\mathbf{k}_1\\ \mathbf{k}_2\end{pmatrix}_t &= -\epsilon_\alpha\langle \mathbf{l}_1, \mathbf{k}_1|\ V_{1\gamma}(t)\ |\mathbf{k}_2\rangle.\end{aligned}$$

A Qth order *wiggly-line cluster graph* is defined to be a set of Q cluster vertices which are entirely interconnected by wiggly lines. We let R equal the number of outgoing external lines, R' equal the number of incoming external lines, and I equal the number of internal (wiggly) lines. Since photons are created and destroyed by electromagnetic interactions it can happen that $R \neq R'$. The rules for connecting the Q vertices of a wiggly-line cluster graph together with the prescriptions for writing down the corresponding expression are as follows:

(1) It must not be possible to complete a loop in a cluster graph by following the arrows on wiggly lines. Cluster graphs therefore always have a braided structure, as shown in Fig. 5 of I.

(2) Every wiggly line is attached to a cluster vertex at each end, so that the temperature variable t_i at the tail end is less than the temperature variable t_j at the head end.

(3) Associate with each of the I internal lines and the $(R + R')$ external lines an integer i ($i = 1, 2, \cdots, I + R + R'$) and a corresponding momentum $\mathbf{l}_i$, $\mathbf{k}_i$, or $\mathbf{k}_i'$ according to whether the line is internal, outgoing external, or incoming external

(4) Two wiggly-line cluster graphs are different if they cannot be topologically (including the relative positions of the *particle-type* labels and the *external-momentum* labels) deformed into each other.

(5) Temperature integrations for the Q temperature variables are performed over the associated product of vertex functions according to rules (6) and (7) for wiggly-line cluster graphs in I. These two rules are somewhat more general than is necessary when one considers wiggly-line cluster graphs in perturbation theory [because $V(t)$ depends only on *one* temperature label]. However, after summing over certain types of double bonds (see Rule 6 and the beginning of Sec. V) the full prescription for the integration limits becomes essential, as in I.

[26] These graphs are a generalization for a multicomponent system of the wiggly-line cluster graphs defined in I.

(6) A factor of $\frac{1}{2}$ is included for each *identical-particle* double bond, where a *double bond* is defined to be a structure in which two *wiggly* lines connect the same two vertices (there may even be a third, different line in the case of photon double bonds).

(7) When the cluster graph is written in terms of its associated vertex functions (using the bracket notation of Fig. 1), then a factor of $\prod_\alpha (\epsilon^{P_B})_\alpha$ is included, where $(P_B)_\alpha$ is the total permutation for the α-particles of the bottom-row momenta (both external and internal) with respect to the top-row momenta. In this connection, a convention for the identical permutation of the $\mathbf{k}_i'$-momenta with respect to the $\mathbf{k}_i$-momenta must be adopted and remembered for later use. Of course, this rule is only necessary for fermions.

(8) The sum over the I internal momentum (and spin) coordinates is performed. (It may also be necessary to sum over internal states for some of the particles; see Footnote 19.)

(9) When $I = 0$, we define the cluster graph to be

$$\begin{pmatrix} \mathbf{k} \\ \mathbf{k}' \end{pmatrix}_\alpha = \epsilon_\alpha \delta_{\mathbf{k},\mathbf{k}'} \qquad (\text{with} \quad R = R' = 1).$$

We next define a function $T_{RR'}(\beta)$ by the equation

$$T\begin{pmatrix} \mathbf{k}_1 \cdots \mathbf{k}_R \\ \mathbf{k}_1' \cdots \mathbf{k}_{R'}' \end{pmatrix} \equiv \sum_{Q=0}^{\infty} \left[\begin{array}{l} \text{all different } Q\text{th-order wiggly-line} \\ \text{cluster graphs with outgoing exter-} \\ \text{nal lines } \mathbf{k}_1 \cdots \mathbf{k}_R \text{ and incoming} \\ \text{external lines } \mathbf{k}_1' \cdots \mathbf{k}_{R'}' \end{array} \right]. \tag{39}$$

The quantity $T_{RR'}$ is a generalization of the quantity T_N given by Eq. (I-54). It will be zero if the particles represented by the $\mathbf{k}_i$ and the $\mathbf{k}_i'$ are not all connected by interactions. Moreover, when $R \neq R'$, then $T_{RR'} = 0$ unless some of the particles are photons or other nonconserved particles.

Consider next the partitions $\{n_i\}$ of N as a sum of postive integers such that each $n_i = R$ corresponds to a $T_{RR'}$ function. We show below that the function $W_N^{(S)}(\beta)$ of Eq. (20) can be written (assuming that $\mathbf{k}_i$ and $\mathbf{k}_i'$ refer to the same kind of particle) as

$$\prod_\alpha (\epsilon_\alpha^{N_\alpha}) W^{(S)}\begin{pmatrix} \mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N \\ \mathbf{k}_1' \mathbf{k}_2' \cdots \mathbf{k}_N' \end{pmatrix} = \sum_{\{n_i\},\{n_i'\}} \prod_\alpha (\epsilon^{P_B})_\alpha \times [T_{n_1 n_1'} T_{n_2 n_2'} \cdots T_{n_S n_S'}], \tag{40}$$

$$\sum_{i=1}^{S} n_i = \sum_{i=1}^{S} n_i' = \sum_\alpha N_\alpha = N.$$

The sum on the right-hand side of Eq. (40) is to be extended: (1) over all possible partions $\{n_i\}$ of N as a sum of positive integers, and similarly for $\{n_i'\}$, and (2) for each partition $\{n_i\}$ and $\{n_i'\}$, over all different ways in which *both* the N $\mathbf{k}_i$ *and* the N $\mathbf{k}_i'$ can be divided into groups of $(n_1, n_2, \cdots n_S)$- and $(n_1', n_2', \cdots n_S')$-momenta. Thus for $N = 4$, $\binom{1}{1'}\binom{2}{2'}$ and $\binom{1}{1'}\binom{2}{3'}$ must both be included. Each factor $(\epsilon^{P_B})_\alpha$ in Eq. (40) is the sign of the total permutation for the α-particles of the bottom row $\mathbf{k}_i'$ with respect to the top row $\mathbf{k}_i$, using the ordering convention given at the end of Rule (7) for wiggly-line cluster graphs.

The cluster functions $U_N^{(S)}$, which are required for the evaluation of the grand potential by Eq. (19), can be identified by placing Eq. (40) in one-to-one correspondence with the Nth of the Ursell equations (17). Clearly, the general expression for $U_N^{(S)}$ is

$$\prod_\alpha (\epsilon_\alpha^{N_\alpha}) U^{(S)}\begin{pmatrix} \mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N \\ \mathbf{k}_1' \mathbf{k}_2' \cdots \mathbf{k}_N' \end{pmatrix} = \sum_{\{n_i\},\{n_i'\}} \prod_\alpha (\epsilon^{P_B})_\alpha \times [T_{n_1 n_1'} T_{n_2 n_2'} \cdots T_{n_S n_S'}]_{\text{connected}}, \tag{41}$$

$$\sum_{i=1}^{S} n_i = \sum_{i=1}^{S} n_i' = \sum_\alpha N_\alpha = N,$$

where a *connected* product of T functions is one which *cannot* be separated into two factors with no coordinates in common when one sets $\mathbf{k}_i' = \mathbf{k}_i$.

We now turn our attention to the proof of Eq. (40), which we briefly outline in three parts. To facilitate this discussion, we introduce dashed-line cluster graphs, which are defined to be wiggly-line cluster graphs with the following changes:

(a) All wiggly lines are replaced by dashed lines.

(b) Rule (2) also includes the statement: The Q temperature variables are labeled so that

$$0 < t_1 < t_2 < \cdots < t_Q < t_{Q+1} \equiv \beta.$$

(c) Rule (4) is changed to: Two dashed-line cluster graphs are different if they cannot be topologically (including the relative positions of the *temperature labels*, particle-type labels, and the external-momentum labels) deformed into each other.

(d) Rule (5) is changed to: For any given assignment of the temperature labels, the temperature integrations

$$\int_0^\beta dt_Q \int_0^{t_Q} dt_{Q-1} \cdots \int_0^{t_2} dt_1$$

must be performed over the corresponding vertex functions. We finally distinguish between *unconnected* cluster graphs for which the Q cluster vertices are not entirely interconnected by dashed lines and the *connected* cluster graphs defined above. The three parts in the proof of Eq. (40) are then as follows:

Part A

In Part A one must determine the general prescription for the N-particle matrix elements of an arbitrary term in the iterated form of Eq. (37). The procedure for accomplishing this objective is to first (Step A1) express this arbitrary term as a sum over other terms each of which is in normal form; i.e., with all creation operators appearing to the left of all annihilation operators. Step A1 is analogous to the method of Wick,[27] but somewhat simpler because one only requires Eqs. (22) to carry through the analysis. An important aspect to Step A1 is to *adopt the sign convention of rule* (7) for cluster graphs (noting that each annihilation and each creation operator corresponds to a variable in some vertex function), when determining the sign factor for each of the normal products. Becuase of Step A2 below, one may discard all normal products for which the number R_α of α-particle creation operators (α = any component of system) differs from the number of α-particle annihilation operators. The resulting sign factor is then that of rule (7) *times* $\prod_\alpha(\epsilon_\alpha^{R_\alpha+V_\alpha})$, where V_α is the number of α-particle creation (or annihilation) operators in the original arbitrary term. [The V_α factors of ϵ_α are included in the vertex functions of Eqs. (38).]

The second step (A2) in accomplishing the objective of Part A is to determine the N-particle matrix elements of a normal product of creation and annihilation operators, assuming that $\mathbf{k}_i$ and $\mathbf{k}_i'$ always refer to the same kind of particle. Such a matrix element will clearly vanish unless $R_\alpha \leqq N_\alpha$, where $\sum_\alpha N_\alpha = N$. When the results of Steps A1 and A2 are combined, one finds that the matrix elements of $W(\beta)$ can be written as a sum over terms which are in one-to-one correspondence with those in the sum over all possible dashed-line cluster graphs.

In the final step (A3) of Part A, one shows that

$$\prod_\alpha (\epsilon_\alpha)^{N_\alpha} W^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_2 \cdots \mathbf{k}_N \\ \mathbf{k}_1'\mathbf{k}_2' \cdots \mathbf{k}_N'\end{pmatrix} = \sum_{Q=0}^{\infty}\left[\begin{array}{l}\text{all different } Q\text{th-order connected} \\ \textit{and} \text{ unconnected dashed-line} \\ \text{cluster graphs with } N \text{ external} \\ \text{incoming and } N \text{ external outgoing} \\ \text{lines}\end{array}\right]. \tag{42}$$

In all of the cluster graphs of Eq. (42), $\mathbf{k}_i'$ and $\mathbf{k}_i$ both refer to the same kind of particle. Equation (42) is fairly simple to verify from the preceding two steps. The essential point is to show that the numerical factor associated with each of the terms identified in the isomorphism of the preceding paragraph is $(\frac{1}{2})^D$, where D is the number of identical particle double-bonds in the corresponding cluster graph.

[27] G. C. Wick, Phys. Rev. 80, 268 (1950).

Part B

In Part B, one separates the various connected parts of unconnected dashed-line cluster graphs. These connected parts are interrelated through their temperature variables, after all temperature integrations are performed. They can be separated, however, by summing over *all possible ways* of ordering the temperature variables in the unconnected parts. Since Rule (2) for cluster graphs does not apply to unconnected parts, it should be clear that the result of this sum will be to *remove* all temperature interrelations between unconnected parts. One then obtains Eq. (40) from Eq. (42), except that each of the $T_{RR'}(\beta)$ is given as a sum over (connected) dashed-line cluster graphs instead of wiggly-line cluster graphs.

Part C

In Part C, one proves that the sum over all (connected) dashed-line cluster graphs is equal to the sum over all wiggly-line cluster graphs for given external lines. The first step is to define a *proper cluster part* as a part of a cluster graph which is connected to the rest of the cluster graph by only one incoming and/or outgoing dashed line. (There may be any number of solid-line connections.) One then proves that the temperature interrelations of proper cluster parts can be removed, except for the endpoints, by summing over all possible orderings of the temperature variables as in Part B. As a consequence of this sum, one achieves the objective of Part C by deriving rule (5) for wiggly-line cluster graphs. The proof of Eq. (40) is then complete.

IV. ONE-PARTICLE PROBLEM

The one-particle problem in multicomponent systems is to identify and remove self-energy terms due to the electromagnetic interactions of charged particles with the radiation field. If fields involving other kinds of nonconserved particles are important in a system, then the techniques of this section can be generalized to include these fields. In Eq. (24), we have written the free-particle Hamiltonian H_0 as a sum over single-particle number operators each multiplied by the eigenvalue $\omega^{(0)}(k)$. We now write these eigenvalues as

$$\omega_\alpha^{(0)}(k) = \omega_\alpha(k) + \epsilon_\alpha S_\alpha(k), \tag{43}$$

where for particles with mass, $\omega_\alpha(k) = \hbar^2k^2/2M_\alpha$, and for photons $\omega_\alpha(k) = \hbar ck$. The quantity $S(k)$ is a counterterm which has been included for charged particles, and it is defined subsequently so as to exactly cancel all electromagnetic self-energy terms.

As will be seen, these self-energy terms have only to do with interaction between a charged particle and its own radiation field; they have no dependence on the temperature of the system nor on other external conditions. These terms are therefore unmeasurable and unphysical, and it is a consistent procedure to cancel them by a counterterm in $\omega_\alpha^{(0)}(k)$. The fact that the terms are infinite has no bearing on this procedure. For uncharged particles, we take $S(k) = 0$.

Although the analysis which we make is very general, it is important to see how it applies to a given particle and its associated cluster graphs. For this reason we write down four of the simpler *one-particle cluster-graphs* using the notation of Fig. 2 and the explicit interactions (28). One-particle cluster graphs are characterized by one incoming line, coming from a vertex labeled t_0, and one outgoing line, going to a vertex labeled t_2. If the incoming line is solid, then we define $t_0 = 0$, and if the outgoing line is solid, then we define $t_2 \equiv \beta$. Either or both lines may be wiggly lines, however, because one-particle cluster graphs may be parts of larger wiggly-line cluster graphs. From Fig. 2 we have

$$T_1(t_2 - t_0, l_1) = \epsilon \frac{2\pi Z^2\alpha}{\Omega}\left(\frac{\hbar^2}{M}\right)^2 l_1^2 \sum_{l_3} (\hat{l}_1\cdot\hat{e}_3)^2 l_3^{-1} \times \int_{t_0}^{t_2} ds_2 \int_{t_0}^{s_2} ds_1 \exp(s_2 - s_1)[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)}], \tag{44a}$$

where $(l_2 = l_1 - l_3)$;

$$T_2(t_2 - t_0, l_1) = \epsilon(2\pi Z^2\alpha/\Omega)^2(\hbar^2/M)^4 l_1^4 \sum_{l_3, l_5} (\hat{l}_1\cdot\hat{e}_3)^2(\hat{l}_1\cdot\hat{e}_5)^2 \times l_3^{-1} l_4^{-1} \int_{t_0}^{t_2} ds_4 \int_{t_0}^{s_4} ds_3 \int_{t_0}^{s_2} ds_2 \int_{t_0}^{s_2} ds_1 \times \exp(s_4 - s_3)[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)}] \times \exp(s_2 - s_1)[\omega_1^{(0)} - \omega_4^{(0)} - \omega_5^{(0)}], \tag{44b}$$

where $(l_2 = l_1 - l_3,\ l_4 = l_1 - l_5)$;

$$T_3(t_2 - t_0, l_1) = \epsilon\left(\frac{2\pi Z^2\alpha}{\Omega}\right)^2\left(\frac{\hbar^2}{M}\right)^4 l_1^2 \sum_{l_3, l_5} l_2^2(\hat{l}_1\cdot\hat{e}_3)^2 \times (\hat{l}_2\cdot\hat{e}_5)^2 l_3^{-1} l_5^{-1} \int_{t_0}^{t_2} ds_4 \int_{t_0}^{s_4} ds_3 \int_{t_0}^{s_2} ds_2 \int_{t_0}^{s_2} ds_1 \times \exp(s_4 - s_1)[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)}] \times \exp(s_3 - s_2)[\omega_2^{(0)} - \omega_4^{(0)} - \omega_5^{(0)}], \tag{44c}$$

where $(l_2 = l_1 - l_3,\ l_4 = l_2 - l_5 = l_1 - l_3 - l_5)$;

$$T_4(t_2 - t_0, l_1) = 2\epsilon\left(\frac{\pi Z^2\alpha}{\Omega}\right)^2\left(\frac{\hbar^2}{M}\right)^2 \sum_{l_3, l_4} (\hat{e}_3\cdot\hat{e}_4)^2 l_3^{-1} l_4^{-1} \times \int_{t_0}^{t_2} ds_2 \int_{t_0}^{s_2} ds_1 \{(\exp(s_2 - s_1) \times [\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)} - \omega_4^{(0)}])_f, \tag{44d}$$

where $(l_2 = l_1 - l_3 - l_4)$.

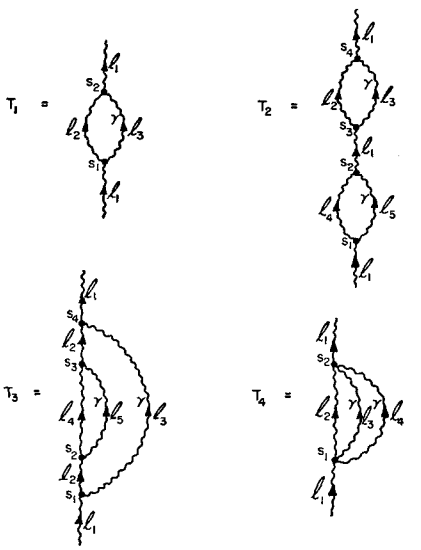


FIG. 2. Four of the simplest one-particle cluster graphs, in which the charged particle line labels have been omitted for convenience. Physically, these graphs represent the simplest ways in which a charged particle can emit or reabsorb one or two virtual photons.

It is important to observe that except for the end-point temperature variables t_0 and t_2, the terms of Eq. (44) have been written down completely independently from the rest of the wiggly-line cluster graphs of which they may be part. This could not have been done in the dashed-line formulation described below Eq. (41). It is this essential feature of wiggly-line cluster graphs which makes possible the analysis of self-energy effects that we now make. Proceeding then, let us make the nature of the above equations more transparent by rearranging the right sides of them with some straightforward algebra. Thus, we write

$$T_1(t_2 - t_0, l_1) = \int_{t_0}^{t_2} ds_1 [T_1'(t_2 - s_1, l_1) + S_1(l_1)], \tag{45}$$

$$T_2(t_2 - t_0, l_1) = \epsilon \int_{t_0}^{t_2} ds_1 \int_{s_1}^{t_2} ds_3 \times [T_1'(t_2 - s_3, l_1) + S_1(l_1)] \times [T_1'(s_3 - s_1, l_1) + S_1(l_1)],$$

$$T_3(t_2 - t_0, l_1) = \int_{t_0}^{t_2} ds_1 \int_{s_1}^{t_2} ds_4 \int_{s_1}^{s_4} ds_2 \times \frac{2\pi Z^2\alpha}{\Omega}\left(\frac{\hbar^2}{M}\right)^2 l_1^2 \sum_{l_3} (\hat{l}_1\cdot\hat{e}_3)^2 l_3^{-1}$$

$$\times \exp(s_4 - s_1)[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)}]$$
$$\times [T_1'(s_4 - s_2, l_2) + S_1(l_2)],$$

$$T_4(t_2 - t_0, l_1) = \int_{t_0}^{t_2} ds_1 [T_4'(t_2 - s_1, l_1) + S_4(l_1)],$$

where

$$T_1'(t_2 - s_1, l_1) \equiv \epsilon\left(\frac{2\pi Z^2\alpha}{\Omega}\right)\left(\frac{\hbar^2}{M}\right)^2 l_1^2$$
$$\times \sum_{\mathbf{l}_3} (\hat{\mathbf{l}}_1 \cdot \hat{\mathbf{e}}_3)^2 l_3^{-1}[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)}]^{-1}$$
$$\times \exp(t_2 - s_1)[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)}],$$

$$T_4'(t_2 - s_1, l_1) \equiv 2\epsilon\left(\frac{\pi Z^2\alpha}{\Omega}\right)^2\left(\frac{\hbar^2}{M}\right)^2 \sum_{\mathbf{l}_3,\mathbf{l}_4} (\hat{\mathbf{e}}_3 \cdot \hat{\mathbf{e}}_4)^2$$
$$\times l_3^{-1} l_4^{-1}[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)} - \omega_4^{(0)}]^{-1}$$
$$\times \exp(t_2 - s_1)[\omega_1^{(0)} - \omega_2^{(0)} - \omega_3^{(0)} - \omega_4^{(0)}], \tag{46}$$

and

$$S_1(l_1) \equiv \epsilon\left(\frac{2\pi Z^2\alpha}{\Omega}\right)\left(\frac{\hbar^2}{M}\right)^2 l_1^2 \sum_{\mathbf{l}_3} (\hat{\mathbf{l}}_1 \cdot \hat{\mathbf{e}}_3)^2 l_3^{-1}$$
$$\times [\omega_2^{(0)} + \omega_3^{(0)} - \omega_1^{(0)}]^{-1}, \tag{47}$$

$$S_4(l_1) \equiv 2\epsilon\left(\frac{\pi Z^2\alpha}{\Omega}\right)^2\left(\frac{\hbar^2}{M}\right)^2 \sum_{\mathbf{l}_3,\mathbf{l}_4} (\hat{\mathbf{e}}_3 \cdot \hat{\mathbf{e}}_4)^2 l_3^{-1} l_4^{-1}$$
$$\times [\omega_3^{(0)} + \omega_4^{(0)} + \omega_2^{(0)} - \omega_1^{(0)}]^{-1}.$$

One now observes that each of the quantities in Eqs. (44) has been written in terms of two distinct functions. [T_3 has not been completely rewritten in this manner, but is so exhibited in Eq. (66).] The functions T_1' and T_4' are temperature dependent and will be interpreted as "structure parts" of one-particle cluster graphs. That is, they represent the contribution from self-emission and absorption of virtual photons which produce a finite effect. The quantities $S_1(l_1)$ and $S_4(l_1)$, on the other hand, are temperature independent[28] and become divergent integrals in the limit $\Omega \to \infty$. The interpretation of these terms as "self-energy parts," as well as the identification of T_1' and T_4', can really only be justified by the subsequent analysis. We note, also, that there are other divergent terms [including $S_3(l_1)$, Eqs. (66) and (68)], which occur in other one-particle cluster graphs and which are also temperature independent. We have encountered no divergent terms which have a temperature dependence, and it is almost certain that there are none.

[28] By temperature independent is meant that these parts do not depend on any temperature integration variables, such as s_1.

We wish to treat terms of the type S_1 and S_4 in a systematic manner, because they are divergent. The systematic treatment which we make will then result in the classification of these terms as self-energy terms, and therefore, we will be able to discard them. In order to account for all possible self-energy terms, it is necessary to calculate for each charged particle all possible ways to emit and reabsorb virtual photons, as illustrated partially in Fig. 2. We begin then by defining a quantity $L_S(t_2, t_1, l_1)$ to be

$$L_S(t_2, t_1, l_1) \equiv \sum [\text{all different one-particle } L\text{-graphs}], \tag{48}$$

where a *one-particle L-graph* is defined to be a one-particle cluster graph for which: (1) the temperature integration over the variable t_1 at which the incoming line is attached is *not* performed, (2) the step-function factor[29] $\theta(t_2 - s)$ is associated with the vertex s to which the outgoing line attaches (at its tail end), and (3) a factor $\theta(s_i' - s_i)$ is associated with each of the other vertices s_i, where s_i' is the temperature variable at the vertex where the outgoing *particle* line attaches at its head end. (Note that $\mathbf{l}_1$ implicitly includes a particle-type label.) It is easy to write down the L-graphs of Fig. 2 from Eqs. (45), because the step-function factors do not affect the value of a one-particle cluster graph. The introduction of the step-function factors is useful, because it makes it possible to extend all of the temperature integrations in the expressions for L-graphs to the full temperature range 0 to β without changing their values.

We next define a quantity $G_S(t_2, t_1, 1)$:

$$G_S(t_2, t_1, 1) \equiv \delta(t_2 - t_1) + \epsilon L_S(t_2, t_1, 1). \tag{49}$$

With the aid of this function it is possible to write down an integral equation for $L_S(t_2, t_1, 1)$ as follows:

$$L_S(t_2, t_1, 1) \equiv \int_0^\beta dt\, G_S(t_2, t, 1) P_S(t, t_1, 1, G_S), \tag{50}$$

where

$$P_S(t_2, t_1, 1, G_S) \equiv \sum \left[\begin{array}{l}\text{all different one-particle } L\text{-graphs} \\ \text{which cannot be separated into two} \\ \text{parts by cutting one or two non-} \\ \text{photon (wiggly) lines, and in which} \\ \int_0^\beta ds\, G_S(s_2, s, 1') \text{ is substituted for} \\ \text{each internal line characterized by} \\ s_2, s_1, \text{ and } 1'\end{array}\right]. \tag{51}$$

The introduction of the integral equation (50) is an essential ingredient for the following treatment of the self-energy difficulties associated with the one-particle problem.

[29] The step function $\theta(t - s)$ is defined to be unity when $t > s$, and to be zero when $t \leq s$.

Λ_S Transformation

We must now systemically remove from L_S and P_S all divergent terms of the form S_1 and S_4, Eqs. (47), *wherever* such terms occur in one-particle L graphs. An elegant method for accomplishing this objective is that of the Λ transformation of II. The simpler version of this transformation presented here will be called the Λ_S *transformation*. It makes use of two functions

$$\Lambda_S(t_2 - t_1, 1) \equiv S(1)\theta(t_2 - t_1), \tag{52}$$

where $S(1)$ will be defined later, and

$$G_0(t_2 - t_1, 1) \equiv \delta(t_2 - t_1) + \epsilon\Lambda_S(t_2 - t_1, 1) \times \exp[\epsilon(t_2 - t_1)S(1)]$$
$$= \delta(t_2 - t_1) + \epsilon\int_0^\beta ds\, \Lambda_S(t_2 - s, 1)G_0(s - t_1, 1). \tag{53}$$

The Λ_S transformation is then defined to be a transformation involving the quantities G_S, L_S, P_S, and the particle–photon vertex functions. The two basic transformation equations are

$$L'_S(t_2, t_1, 1) \equiv \exp[-\epsilon(t_2 - t_1)S(1)] \times \left\{L_S(t_2, t_1, 1) - \int_0^\beta dt\, G_S(t_2, t, 1)\Lambda_S(t - t_1, 1)\right\} \tag{54}$$

and

$$\begin{pmatrix}1_1\\1_2\end{pmatrix}'_{t_1}\theta(t_2 - t_1) = \int_0^\beta dt\, G_0(t_2 - t, 1_1)\begin{pmatrix}1_1\\1_2\end{pmatrix}_{t_1}\theta(t - t_1) \times \exp[-\epsilon t_2 S(1_1) + \epsilon t_1 S(1_2)], \tag{55}$$

where the unprimed bracket symbol can be any of the particle–photon vertex functions of Fig. 1, with the photon momentum dependences suppressed.

We now wish to prove the following two theorems:

I. The sum over all possible one-particle cluster graphs can be expressed in terms of the primed quantities (54) and (55) instead of the corresponding unprimed quantities.

II. If one-particle cluster graphs are calculated using only primed quantities, then all self-energy terms can be eliminated with the proper choice of $S(1)$.

After substituting the first line of Eq. (53) into Eq. (55), one can carry out the integration over t in (55). Then, upon identifying the $S(1)$ of (52) with the counterterm in Eq. (43), one finds the simple result

$$\begin{pmatrix}1_1\\1_2\end{pmatrix}'_{t_1} = \left[\begin{pmatrix}1_1\\1_2\end{pmatrix}_{t_1}\right]_{S=0}. \tag{56}$$

Thus, the transformation equation (55) leads to the cancellation of the counterterm in Eq. (43).

We next invert the first of the transformation equations (54) with the aid of the integral equation for $G_0(t_2 - t_1, 1)$ [second line of (53)]. This gives the result

$$G_S(t_2, t_1, 1) = \int_0^\beta dt \exp[\epsilon(t_2 - t)S(1)] \times G'_S(t_2, t, 1)G_0(t - t_1, 1), \tag{57}$$

where

$$G'_S(t_2, t_1, 1) \equiv \delta(t_2 - t_1) + \epsilon L'_S(t_2, t_1, 1). \tag{58}$$

Now, according to Eqs. (48)–(51), the sum over all possible one-particle cluster graphs is given by $\int_{t_0}^{t_0} dt\, G_S(t_2, t_1, 1)$. With the aid of Eqs. (53) and (57), one can show that

$$\int_{t_0}^{t_0} dt_1 G_S(t_2, t_1, 1) = \exp[\epsilon(t_2 - t_0)S(1)]\int_{t_0}^{t_0} dt_1 G'_S(t_2, t_1, 1), \tag{59}$$

which demonstrates that $G'_S(t_2, t_1, 1)$ also leads to a correct calculation of the sum over all possible one-particle cluster graphs, thereby proving the first theorem.

The explicit prescription for calculating $L'_S(t_2, t_1, 1)$ can be determined from Eq. (54) by substituting Eq. (57). This gives

$$L'_S(t_2, t_1, 1) = \exp[-\epsilon(t_2 - t_1)S(1)]L_S(t_2, t_1, 1) - \int_0^\beta dt\, G'_S(t_2, t, 1)\Lambda_S(t - t_1, 1), \tag{60}$$

a result which is true for any function $S(1)$. In order to see how to choose $S(1)$ in a useful manner, we use Eqs. (55) and (57) to prove that

$$\int_0^\beta dt\, G_S(t_2, t, 1_1)\begin{pmatrix}1_1\\1_2\end{pmatrix}_{t_1}\theta(t - t_1) = \exp[\epsilon t_2 S(1_1)] \times \int_0^\beta dt\, G'_S(t_2, t, 1_1)\begin{pmatrix}1_1\\1_2\end{pmatrix}'_{t_1}\theta(t - t_1)\exp[-\epsilon t_1 S(1_2)]. \tag{61}$$

Therefore, if we define $\mathfrak{L}'(t_2, t_1, 1)$ in analogy with the integral equations (50) and (51) as

$$\mathfrak{L}'(t_2, t_1, 1) \equiv \int_0^\beta dt\, G'_S(t_2, t, 1)P'_S(t, t_1, 1, G'_S), \tag{62}$$

where $P'_S(t_2, t_1, 1, G'_S)$ is defined in the same way as $P_S(t_2, t_1, 1, G_S)$ except that primed functions are used, then we may conclude from (61) that

$$\mathfrak{L}'(t_2, t_1, 1) = \exp[-\epsilon(t_2 - t_1)S(1)]L_S(t_2, t_1, 1). \tag{63}$$

Upon substituting this result into Eq. (60), we obtain the final expression

$$L'_S(t_2, t_1, 1) = \mathcal{L}'(t_2, t_1, 1) - \int_0^\beta dt\, G'_S(t_2, t, 1)\Lambda_S(t - t_1, 1) = \int_0^\beta dt\, G'_S(t_2, t, 1) \times [P'_S(t, t_1, 1, G'_S) - \Lambda_S(t - t_1, 1)]. \quad (64)$$

Equations (56), (59), and (64) are the important results of the Λ_S transformation. They show that for *any* function $S(1)$, one may calculate the sum over all one-particle cluster graphs using primed quantities instead of unprimed quantities. Moreover, they show that the counterterm $S(1)$ can be cancelled by performing the Λ_S transformation. It now only remains to define $S(1)$ as

$$S(1) \equiv \text{the temperature-independent part of } P'_S(t_2, t_1, 1, G'_S). \quad (65)$$

With this definition, together with the expression (52) for $\Lambda_S(t_2 - t_1, 1)$, it should be clear that all terms of the form $S_1(l)$ and $S_4(l)$, Eqs. (47), are explicitly subtracted away in the prescription (64) for calculating $L'_S(t_2, t_1, 1)$, which proves Theorem II. We may now justifiably call such terms *self-energy terms*, because their sum cancels the counterterm of Eq. (43).

We next observe that the exponential factor in Eq. (59) is exactly the factor which is needed to cancel the counterterm $S(1)$ *wherever* it appears in the entire formalism for calculating the grand potential via Eqs. (19) and (41). Therefore, all charged-particle self-energy terms due to the occurrence of electromagnetic interactions are eliminated from the theory, and we have carried out a complete renormalization program for this nonrelativistic theory.[30]

It is important to observe that after the Λ_S transformation there is a nonvanishing contribution from one-particle cluster graphs. The nonvanishing terms must be due to the structure of a charged particle which arises when it interacts with the electromagnetic field. The prescription which results from the Λ_S transformation for calculating this effect is, as follows:

(1) Replace all particle energies $\omega^{(0)}(k)$ by $\omega(k)$.
(2) Calculate one-particle cluster graphs using Eqs. (64) and (58).

Thus, one obtains for the one-particle cluster graphs of Fig. 2, using Eqs. (45),

$$\begin{aligned}
T_1(t_2 - t_0, l_1) &= \int_{t_0}^{t_2} ds\, T'_1(t_2 - s, l_1), \\
T_2(t_2 - t_0, l_1) &= \epsilon \int_{t_0}^{t_2} ds_1 \int_{s_1}^{t_2} ds_3 \times T'_1(t_2 - s_3, l_1)T'_1(s_3 - s_1, l_1), \\
T_3(t_2 - t_0, l_1) &= \int_{t_0}^{t_2} ds_1 \int_{s_1}^{t_2} ds_4 \int_{s_1}^{s_4} ds_2 \times \left(\frac{2\pi Z^2\alpha}{\Omega}\right)\left(\frac{\hbar^2}{M}\right)^2 l_1^2 \sum_{l_3} (\hat{\mathbf{l}}_1\cdot\hat{\mathbf{e}}_3)^2 l_3^{-1} \\
&\quad \times \exp[(s_4 - s_1)(\omega_1 - \omega_2 - \omega_3)] \times T'_1(s_4 - s_2, l_2) - \int_{t_0}^{t_2} ds_1 S_3(l_1), \\
T_4(t_2 - t_0, l_1) &= \int_{t_0}^{t_2} ds_1 T'_4(t_2 - s_1, l_1),
\end{aligned} \quad (66)$$

where one must refer to Eqs. (44) for the various definitions of $\mathbf{l}_2$ and $\mathbf{l}_4$, and where T'_1 and T'_4 are given by Eqs. (46) with the replacements $\omega_i^{(0)} \to \omega_i$.

The electromagnetic self-energy term $S(1)$ which has been eliminated from the theory is given by

$$S(1) = S_1(l) + S_3(l) + S_4(l) + \cdots, \quad (67)$$

where $S_1(l)$ and $S_4(l)$ are given by Eqs. (47) with the replacements $\omega_i^{(0)} \to \omega_i$. The term $S_3(l_1)$ is

$$\begin{aligned}
S_3(l_1) &= \epsilon\left(\frac{2\pi Z^2\alpha}{\Omega}\right)^2\left(\frac{\hbar^2}{M}\right)^4 l_1^2 \sum_{l_3, l_5} l_2^2(\hat{\mathbf{l}}_1\cdot\hat{\mathbf{e}}_3)^2 \\
&\quad \times (\hat{\mathbf{l}}_2\cdot\hat{\mathbf{e}}_5)^2 l_3^{-1} l_5^{-1}(\omega_2 - \omega_4 - \omega_5)^{-2} \\
&\quad \times [(\omega_1 - \omega_2 - \omega_3)^{-1} - (\omega_1 - \omega_3 - \omega_4 - \omega_5)^{-1}],
\end{aligned} \quad (68)$$

where $\mathbf{l}_2 = \mathbf{l}_1 - \mathbf{l}_3$ and $\mathbf{l}_4 = \mathbf{l}_1 - \mathbf{l}_3 - \mathbf{l}_5$). This term is a divergent integral in the limit $\Omega \to \infty$, as are $S_1(l_1)$ and $S_4(l_1)$, but the Λ_S transformation has shown that such infinities are of no consequence to the physical theory.

V. LINKED-PAIR EXPANSION OF THE GRAND POTENTIAL

The linked-pair expansion of the grand potential is derived by substituting Eq. (41) for the cluster functions of quantum statistics into Eq. (19). It is a prescription for calculating the grand potential directly in terms of the basic vertex functions of Fig. 1 using the expressions (38) with the single-

[30] A renormalization program in quantum statistics has also been conducted by I. A. Akhiezer and S. V. Peletminskii, Zh. Eksperim. i Teor. Fiz. **38**, 1829 (1960) [English transl. Soviet Phys.—JETP **11**, 1316 (1960)]. These authors use the methods of conventional field theory and apply them to the relativistic theory of a system composed of electrons, positrons, and photons.

particle energies $\omega(k)$ [not $\omega^{(0)}(k)$], and diagrammatically it corresponds to connecting together the solid external lines of wiggly-line cluster graphs in all possible ways. The procedure for handling one-particle cluster graphs will always be to use Eq. (64).

Before deriving the linked-pair expansion of the grand potential, we make a brief study of the two-particle problem. When the forces between two particles can be represented by a short-range potential V_2 (local *or* nonlocal), then the "effective" interaction is obtained by a repetition of the matrix elements of $V_2(t)$ for various possible intermediate states, as in ordinary perturbation theory. Diagrammatically this is equivalent to inserting double bonds in wiggly-line cluster graphs (see Rule 6 in Sec. III). The sum over all possible ways of including such double bonds for two particles leads to the conclusion that one may replace the short-range $V_2(t_1)$ by

$$\begin{aligned} R(t_2, t_1) \equiv & -\Big\{1 - \int_{t_1}^{t_2} ds V_2(s) \\ & + \int_{t_1}^{t_2} ds_2 \int_{t_1}^{s_2} ds_1 V_2(s_2) V_2(s_1) \cdots \Big\} V_2(t_1) \\ & = -(\partial/\partial t_1)\{\exp(t_2 H_0^{(2)}) \exp[-(t_2 - t_1)H^{(2)}] \\ & \times \exp(-t_1 H_0^{(2)}) - 1\}, \end{aligned} \tag{69}$$

where it is not necessary to use the Fock representation for $V(t)$ in this case. The reason why the sum of Eq. (69) occurs independently of the rest of the wiggly-line cluster graph has already been discussed after Eqs. (44) in connection with one-particle cluster graphs. The function $R(t_2, t_1)$ is discussed in detail in I; however, we note here that its matrix elements can be expressed completely in terms of two-body wavefunctions, thereby admitting the realistic situation obtaining when the two-body interaction contains a hard core.

We call a matrix element of $R(t_2, t_1)$ a *pair function*, and we use square-bracket symbols for pair functions:

$$\begin{aligned} {}^{t_2}\begin{bmatrix} \mathbf{k}_1\mathbf{k}_2 \\ \mathbf{k}_3\mathbf{k}_4 \end{bmatrix}_{t_1} \equiv & \langle \mathbf{k}_1\mathbf{k}_2 | R(t_2, t_1) | \mathbf{k}_3\mathbf{k}_4 \rangle \\ & + \epsilon_\alpha \langle \mathbf{k}_1\mathbf{k}_2 | R(t_2, t_1) | \mathbf{k}_4\mathbf{k}_3 \rangle \\ & \text{for identical particles } (\alpha = \beta), \\ = & \epsilon_\alpha \epsilon_\beta \langle \mathbf{k}_1\mathbf{k}_2 | R(t_2, t_1) | \mathbf{k}_3\mathbf{k}_4 \rangle \\ & \text{for nonidentical particles } (\alpha \neq \beta). \end{aligned} \tag{70}$$

The "upper" temperature variable t_i associated with a pair function is determined graphically by the outgoing lines at the vertex t_i. The determination of t_i in the possible cases which can arise is shown in Fig. 3. We henceforth assume that all two-particle cluster vertices which correspond to short-range interactions represent pair functions (see Rule 5 in Sec. III for remarks concerning integrations over temperature variables in this case). The only remaining double bonds in wiggly-line cluster graphs are therefore those which involve one or two photons and those connecting vertices at least one of which represents the long-range Coulomb potential.

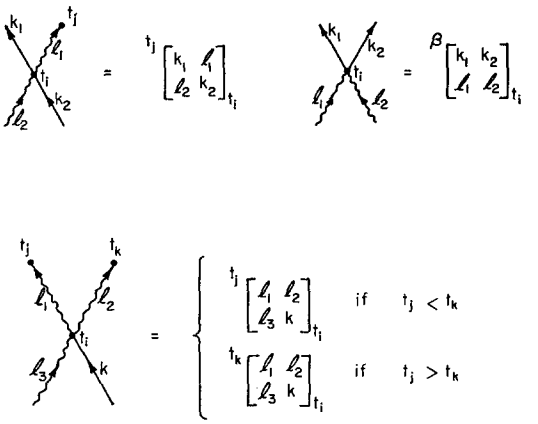


FIG. 3. Cluster vertices for pair functions. The upper temperature variable of a pair function is determined by the nature of the outgoing lines and the labels of the other vertices where the wiggly lines (if any) attach.

We now state the general result for the grand potential which one obtains when Eq. (41) is substituted into Eq. (19) and all terms are gathered together which become identical after relabeling of **k**-momenta.

$$\begin{aligned} \Omega f(\beta, g_\alpha, \Omega) = & \Omega \sum_\alpha f_0(\beta, g_\alpha, \Omega) \\ & + \sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order linked-pair 0-graphs}], \end{aligned} \tag{71}$$

where the first, or free particle, term is given by Eq. (77). The proof of Eq. (71) will be given after we have defined Qth-order linked-pair 0-graphs.

Linked-Pair ζ-Graphs

For the purpose of studying the distribution functions of a system, such as the momentum distribution, it is necessary to define not only linked-pair 0-graphs, but also linked-pair ζ-graphs for $\zeta > 0$. We, therefore, define a *Qth-order, linked-pair ζ-graph* ($\zeta = 0, 1, 2 \cdots$) to be a collection of Q cluster vertices (see Figs. 1 and 3), which are entirely interconnected by m solid lines and n wiggly lines, and which have ζ incoming external solid lines and ζ outgoing external solid lines. The type of particle represented by the line is indicated by a Greek letter (α, β, $\cdots$). Linked-pair 0-graphs

which can be separated into two parts by cutting a single photon line are excluded, because in this case the photon always has zero momentum [see comment below Eqs. (27)]. The rules for connecting the Q cluster vertices by the $(m + n)$ internal lines of a linked-pair ζ-graph, and the procedures for determining the corresponding expression are as follows:

(i) When connecting the $(m + n)$ internal lines to the Q vertices, the n wiggly lines must be connected according to Rules (1) and (2) for wiggly-line cluster graphs (Sec. III).

(ii) The only wiggly-line double bonds which can occur are those which involve an electromagnetic interaction vertex. A factor of $\frac{1}{2}$ is included for each identical particle (wiggly-line) double bond.

(iii) If $\zeta \neq 0$, then associate the external lines with certain pregiven momenta, such that the incoming lines refer to the same set of particles as the outgoing lines.

(iv) Two linked-pair ζ-graphs are different if their topological structures, including line types, line directions, and particle-type labels, are different. External lines with different momentum labels are regarded as being distinguishable when they leave (or enter) different vertices.

(v) Associate with each internal line a different integer $i (i = 1, 2, \cdots, m + n)$ and a corresponding momentum $\mathbf{k}_i$ or $\mathbf{l}_i$ according to whether the line is solid or wiggly.

(vi) According to Rules (i)–(v), every linked-pair ζ-graph consists of interconnected wiggly-line cluster graphs. For each cluster graph, perform the integrations over the temperature variables of its cluster vertices according to Rules (6) and (7) in I for wiggly-line cluster graphs.

(vii) Assign a factor S^{-1} to the entire linked-pair graph, where

$$S = \text{symmetry number}. \tag{72}$$

The symmetry number S is defined to be the total number of permutations of the m integers associated with the *solid* internal lines that leave the graph topologically (including the positions of these numbers relative to the m solid internal lines and their particle type labels) unchanged.

(viii) Assign a factor $\prod_\alpha (\epsilon^{P_B})_\alpha$ to the graph, where $(P_B)_\alpha$ is the total permutation for the α-particles of the bottom-row momenta of the Q vertex functions with respect to the top-row momenta.

(ix) Assign a factor $(\epsilon\nu_k)_\alpha$ to each solid internal α-particle line, where

$$\nu_k \equiv \exp \beta(g - \omega_k)/[1 - \epsilon \exp \beta(g - \omega_k)]. \tag{73}$$

(x) Finally, sum over all $(m + n)$ internal momentum (and spin) coordinates according to the particle type labels of these lines. (It may also be necessary to sum over internal states for some of the particles; see Footnote 19.)

The above rules are equivalent to those of I for a single-component system. The one-and two-vertex linked-pair ζ-graphs of a single-component system for $\zeta = 0$ and $\zeta = 1$, are shown in Fig. 10 of I.

The general proof that Eq. (71) is correct proceeds as follows. We first define *numbered 0-graphs* to be linked-pair 0-graphs with the following changes:

(a) One-particle cluster vertices, i.e., vertices with one line in and one line out, corresponding to $\epsilon\delta_{\mathbf{k}\mathbf{k}'}$ are allowed (see Rule 9 for wiggly-line cluster graphs).

(b) Rule ix is changed to: Assign a factor

$$[\epsilon \exp \beta(g - \omega_k)]_\alpha$$

to each solid internal α-particle line.

(c) Rule (vii) is changed to: The numerical factor associated with each number 0-graph is $\prod_\alpha (N_\alpha!)^{-1}$, where N_α is the number of solid (internal) α-particle lines and $\sum_\alpha N_\alpha = m$. [This factor can be verified from Eq. (19).]

(d) The m solid-line integers of Rule v are *assigned* to the solid (internal) lines.

(e) Rule (iv) is changed to: Two numbered 0-graphs are different if they have different topological structures, including the positions of the m numbers of (d) relative to the solid lines and their particle type labels.

With the aid of the concept of numbered 0-graphs, it is easy to see that substituting Eq. (41) into Eq. (19) (and using the results of Sec. IV) gives

$$\Omega f(\beta, g_\alpha, \Omega) = \sum_{Q=0}^{\infty} [\substack{\text{all different } Q\text{th-order} \\ \text{numbered 0-graphs}}]. \tag{74}$$

Let D be the total number of different numbered 0-graphs which correspond to the same linked-pair 0-graph, where for the present we include among the latter 0-graphs those with one-particle cluster vertices $\epsilon\delta_{\mathbf{k}\mathbf{k}'}$. From the definition of the symmetry number below (72), it is easy to see that

$$D = S^{-1} \prod_\alpha (N_\alpha!); \qquad (\sum_\alpha N_\alpha = m). \tag{75}$$

But after properly relabeling k-momenta, the D numbered 0-graphs are seen to be equal. We may therefore deduce the following result:

$$\Omega f(\beta, g_\alpha, \Omega) = \sum_{Q=0}^{\infty} \left[\substack{\text{all different } Q\text{th-order linked-pair} \\ \text{0-graphs, including those with one-} \\ \text{particle cluster vertices}}\right], \tag{76}$$

where the internal solid-line factors of the 0-graphs on the right-hand side of (76) are still those corresponding to (b) above.

We now observe that the free-particle grand potential

$$\sum_\alpha f_0(\beta, g_\alpha, \Omega) = -\Omega^{-1} \sum_\alpha \epsilon_\alpha \sum_{\mathbf{k}} \ln [1 - \epsilon_\alpha \exp \beta(g - \omega_k)_\alpha] \quad (77)$$

can be easily derived from (76) by summing over those linked-pair 0-graphs constructed entirely from one-particle cluster vertices. We finally consider all those linked-pair 0-graphs in (76) which do not include any one-particle cluster vertices. This set of terms is in one-to-one correspondence with those in the second term of (71). By summing over all possible ways of including one-particle cluster vertices in the set of terms from (76), one obtains the solid-line factors $(\epsilon\nu_k)_\alpha$ of (73) for linked-pair 0-graphs. Moreover, after performing this sum, there are no longer any 0-graphs with one-particle cluster vertices in (76), and the proof of (71) is completed.

VI. DISTRIBUTION FUNCTIONS

In this section we show how to calculate distribution functions in terms of the linked-pair ζ-graphs of the previous section. In particular, we are interested in the momentum distribution and the pair-correlation function, which are the probabilities for finding one and two particles in momentum states. The momentum distribution has been studied in detail in II. Thus, Eq. (II.4) for $\langle n(\mathbf{k})\rangle$ remains valid for a multicomponent system provided the notation of Eq. (14) is used:

$$\langle n_\alpha(\mathbf{k}_\alpha)\rangle = e^{-\Omega f} \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\mathbf{k}_1 \cdots \mathbf{k}_N} e^{\beta G} \exp\left[-\beta \sum_{i=1}^{N} \omega_i^{(0)}\right] \times W^{(S)}\begin{pmatrix}\mathbf{k}_1 & \cdots & \mathbf{k}_N \\ \mathbf{k}_1 & \cdots & \mathbf{k}_N\end{pmatrix}\left(\sum_{i=1}^{N} \delta_{\mathbf{k}_i, \mathbf{k}_\alpha}\right). \quad (78)$$

Equation (78) gives the probability for finding an α particle with momentum (and spin) $\mathbf{k}_\alpha$ in the system, where the subscript indicates the type of particle so that only those $\mathbf{k}_i$ referring to α particles contribute to the final Kronecker δ of (78).

By referring to Eqs. (14) and (43), one can readily see that the momentum distribution (78) can be obtained by a simple functional differentiation of the grand partition function

$$\langle n_\alpha(\mathbf{k})\rangle = -\beta^{-1} e^{-\Omega f}\{[\delta/\delta\omega_\alpha(\mathbf{k})] e^{\Omega f}\}_W, \quad (79)$$

where the matrix elements of $W(\beta)$ are to be held *fixed* during the differentiation. We have *chosen* to differentiate with respect to $\omega_\alpha(k)$ instead of $\omega_\alpha^{(0)}(k)$, because after carrying through the renormalization program of Sec. IV the quantity $S_\alpha(k)$ is eliminated from the grand potential f. Thus, one may reduce Eq. (79) to a calculable form by the following three steps:

$$\begin{aligned}\langle n_\alpha(\mathbf{k})\rangle &= -\beta^{-1}\{[\delta/\delta\omega_\alpha(\mathbf{k})]\Omega f\}_V \\ &= \nu_\alpha(\mathbf{k}) + \nu_\alpha(\mathbf{k})[1 + \epsilon_\alpha\nu_\alpha(\mathbf{k})] \\ &\quad \times \{[\delta/\delta\nu_\alpha(\mathbf{k})] \sum^{(\text{all linked-pair 0-graphs})}\}_V, \\ &= \nu_\alpha(\mathbf{k}) + \epsilon_\alpha\nu_\alpha(\mathbf{k})[1 + \epsilon_\alpha\nu_\alpha(\mathbf{k})] \\ &\quad \times \sum_{(\text{all linked-pair 1-graphs})\mathbf{k}_\alpha}. \end{aligned} \quad (80)$$

We have used Eqs. (71) and (73) to obtain the second line of (80), and the subscripts V indicate that the vertex functions of Figs. 1 and 3 are to be held constant during the functional differentiation. Finally, one can modify a proof due to Lee and Yang[31] to verify the third line of (80). Linked-pair 1-graphs were defined in the preceding section.

The third line of Eq. (80) expresses the momentum distribution of the α particles in a multicomponent system in a form which is suitable for calculation for some systems. But as we have shown in II, Eq. (80) is not in a suitable form for calculating the momentum distributions of very low temperature systems. Therefore, it is of value to carry through the following steps in the analysis of $\langle n_\alpha(\mathbf{k})\rangle$, which are *essential* for low-temperature systems and which do not complicate the calculations for other systems. Thus, as in II, we define a quantity $N_\alpha(\mathbf{k})$,

$$\begin{aligned}N_\alpha(\mathbf{k}) &\equiv \exp[\beta(g - \omega_k)_\alpha][1 + \epsilon_\alpha\langle n_\alpha(\mathbf{k})\rangle] \\ &= \nu_\alpha(\mathbf{k})[1 + \nu_\alpha(\mathbf{k}) \sum^{(\text{all linked-pair 1-graphs})\mathbf{k}_\alpha}]. \end{aligned} \quad (81)$$

The second line of (81) can be rewritten as an integral equation for $N_\alpha(\mathbf{k})$ after introducing the concept of reducible and irreducible graphs.

Definitions

A linked-pair ζ-graph is called *reducible* if by cutting two of its solid internal lines open the entire graph can be separated into two (or three) disconnected ζ-graphs one of which is a 1-graph. An *irreducible* ζ-graph is a linked-pair ζ-graph which is not reducible, with its solid internal lines representing factors $\epsilon_\alpha N_\alpha(\mathbf{k})$ instead of $\epsilon_\alpha\nu_\alpha(\mathbf{k})$. Examples of reducible and irreducible 0-graphs for a single component system are shown in Fig. 1 of II.[32]

With the above definitions of reducible and

[31] See the end of Appendix C in T. D. Lee and C. N. Yang, Phys. Rev. 117, 22 (1960).

[32] The second reducible 0-graph in Fig. 1 of II is missing a line and one of the lines in the next to last irreducible 0-graph should be wiggly.

irreducible graphs, one can readily verify that the second line of (81) can be rewritten as

$$N_\alpha(\mathbf{k}) = \nu_\alpha(\mathbf{k})[1 + N_\alpha(\mathbf{k}) \sum^{(\text{all irreducible linked-pair 1-graphs})_{\mathbf{k}\alpha}}]. \quad (82)$$

Equation (82) represents a set of coupled integral equations for the functions $N_\alpha(\mathbf{k})$ of a multicomponent system. When substituted into the first line of Eq. (81), the solution for $N_\alpha(\mathbf{k})$ yields the momentum distribution $\langle n_\alpha(\mathbf{k})\rangle$. If the steps of Eqs. (81) and (82) are unnecessary for a particular system, then the solution of (82) by iteration yields the third line of (80). Therefore Eqs. (81) and (82) can be used to calculate the momentum distribution for any system. [Here we encounter an essential difference from other formalisms, e.g., that of Bloch and De Dominicis,[3] which employ the functions $\nu_\alpha(\mathbf{k})$ of Eq. (73) throughout. When particle interactions are included, these functions are unphysical at low temperatures and in the present formulation are replaced, after resummations, by the functions $N_\alpha(\mathbf{k})$. Thus, while other authors[33] obtain expressions similar to Eq. (83) for the grand potential, say, these expressions do not contain this essential analysis of the distribution functions.] We return to a further analysis of these last two equations in the next section.

Grand Potential

When the considerations of Eqs. (81) and (82) are important for a calculation of the momentum distribution, then it is important to also express the grand potential in terms of irreducible graphs. The correct expression is

$$\Omega f(\beta, N_\alpha, \Omega) = \sum_\alpha \epsilon_\alpha \sum_{\mathbf{k}} \ln[1 + \epsilon_\alpha \langle n_\alpha(\mathbf{k})\rangle]$$
$$- \sum_\alpha \epsilon_\alpha \sum_{\mathbf{k}} [\nu_\alpha^{-1}(\mathbf{k}) N_\alpha(\mathbf{k}) - 1] + \sum^{\substack{(\text{all irreducible linked-pair} \\ 0\text{-graphs})}} \quad (83)$$

In order to verify that Eqs. (83) and (71) for the grand potential are equivalent, it is simplest to calculate the average number of particles $\langle N_\alpha\rangle$ by substituting (83) into Eq. (7) [$\langle N_\alpha\rangle$ should not be confused with the function $N_\alpha(\mathbf{k})$ defined by Eq. (81)]. One then verifies that (83) yields $\langle N_\alpha\rangle = \Sigma_{\mathbf{k}}\langle n_\alpha(\mathbf{k})\rangle$, which shows that both expressions (83) and (71) satisfy the same linear partial differential equations in the variables (βg_α) [Eq. (71) satisfies Eqs. (7) by definition]. Therefore, the expressions (71) and (83) can differ at most by a temperature-dependent constant. Investigation of the high-temperature limits of these expressions then leads to the conclusion that this constant is zero. Q.E.D.

[33] For example, J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

Pair-Correlation Function

The pair-correlation function $P(\mathbf{k}_\alpha, \mathbf{k}'_\beta)$ is defined to be the probability that an α particle in a system has momentum (and spin) $\mathbf{k}$, while a β particle has momentum $\mathbf{k}'$. (We may, of course, also be interested in the case $\alpha = \beta$),

$$P(\mathbf{k}_\alpha, \mathbf{k}'_\beta) \equiv \langle n_\alpha(\mathbf{k}) n_\beta(\mathbf{k}')\rangle - \langle n_\alpha(\mathbf{k})\rangle \delta_{\mathbf{k},\mathbf{k}'} \delta_{\alpha,\beta}. \quad (84)$$

It is related to the fluctuation in particle number

$$\langle \Delta n_\alpha(\mathbf{k}) \Delta n_\beta(\mathbf{k}')\rangle \equiv \langle n_\alpha(\mathbf{k}) n_\beta(\mathbf{k}')\rangle - \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle \quad (85)$$

by the equation

$$\langle \Delta n_\alpha(\mathbf{k}) \Delta n_\beta(\mathbf{k}')\rangle = P(\mathbf{k}_\alpha, \mathbf{k}'_\beta) - \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle + \langle n_\alpha(\mathbf{k})\rangle \delta_{\mathbf{k},\mathbf{k}'} \delta_{\alpha,\beta}. \quad (86)$$

In analogy with the derivation of Eqs. (80) from Eq. (78) for the momentum distribution, one may verify that the general expression for the pair-correlation function is given by

$$\begin{aligned}
&P(\mathbf{k}_\alpha, \mathbf{k}'_\beta) \\
&= \beta^{-2} e^{-\Omega f}\left[e^{-\beta\omega_\alpha(\mathbf{k})} \frac{\delta}{\delta\omega_\beta(\mathbf{k}')} e^{\beta\omega_\alpha(\mathbf{k})} \frac{\delta}{\delta\omega_\alpha(\mathbf{k})} e^{\Omega f}\right]_W \\
&= \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle \\
&\quad + \beta^{-2} e^{-\beta\omega_\alpha(\mathbf{k})}\left[\frac{\delta}{\delta\omega_\beta(\mathbf{k}')} e^{\beta\omega_\alpha(\mathbf{k})} \frac{\delta}{\delta\omega_\alpha(\mathbf{k})} \Omega f\right]_V \\
&= \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle \\
&\quad - \beta^{-1} e^{-\beta\omega_\alpha(\mathbf{k})}\left[\frac{\delta}{\delta\omega_\beta(\mathbf{k}')} e^{\beta\omega_\alpha(\mathbf{k})}\langle n_\alpha(\mathbf{k})\rangle\right]_V \\
&= \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle - \langle n_\alpha(\mathbf{k})\rangle \delta_{\mathbf{k},\mathbf{k}'} \delta_{\alpha,\beta} \\
&\quad + \nu_\beta(\mathbf{k}')[1 + \epsilon_\beta \nu_\beta(\mathbf{k}')]\{[\delta/\delta\nu_\beta(\mathbf{k}')]\langle n_\alpha(\mathbf{k}')\rangle\}_V \\
&= \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle(1 + \epsilon_\alpha \delta_{\mathbf{k},\mathbf{k}'} \delta_{\alpha,\beta}) \\
&\quad + \epsilon_\alpha \epsilon_\beta \nu_\alpha(\mathbf{k})[1 + \epsilon_\alpha \nu_\alpha(\mathbf{k})]\nu_\beta(\mathbf{k}')[1 + \epsilon_\beta \nu_\beta(\mathbf{k}')] \\
&\quad \times \sum^{(\text{all linked-pair 2-graphs})_{\mathbf{k}\alpha,\mathbf{k}\beta'}}. \quad (87)
\end{aligned}$$

We have used the first line of Eq. (80) to derive the third line of (87), and Eq. (73) to derive the fourth line. The last line of Eq. (87) can be verified by substituting the third line of Eq. (80) into the fourth line of (87) and then using the identity

$$\epsilon_\beta[\delta/\delta\nu_\beta(\mathbf{k}')] \sum^{(\text{all linked-pair 1-graphs})_{\mathbf{k}\alpha}} = \epsilon_\alpha \delta_{\mathbf{k},\mathbf{k}'} \delta_{\alpha,\beta} \times [\sum^{(\text{all linked-pair 1-graphs})_{\mathbf{k}\alpha}}]^2 + \sum^{(\text{all linked-pair 2-graphs})_{\mathbf{k}\alpha,\mathbf{k}\beta}}. \quad (88)$$

In deriving this identity, it has been assumed that the basic interactions of the multicomponent system do not permit 1-graphs in which the incoming and outgoing external lines refer to different particles.

The last line of (Eq. (87) expresses the pair-

correlation function of a multicomponent system in a form which is suitable for calculation for some systems. As with the momentum distribution, however, we must incorporate the analysis of Eqs. (81) and (82) in order to calculate the pair-correlation function for low-temperature systems. We are, therefore, led to use the concept of reducible and irreducible 2-graphs, introduced below Eq. (81).

It is a simple matter to generate the sum over all linked-pair 2-graphs from the sum over all irreducible linked-pair 2-graphs. Thus, one may readily verify that the following identity is true:

$$[N_\alpha(\mathbf{k})]^2[N_\beta(\mathbf{k}')]^2 \sum^{\text{(all irreducible linked-pair 2-graphs)}_{\mathbf{k}_\alpha,\mathbf{k}'_\beta}} = [\nu_\alpha(\mathbf{k})]^2[\nu_\beta(\mathbf{k}')]^2 \sum^{\text{(all linked-pair 2-graphs)}_{\mathbf{k}_\alpha,\mathbf{k}'_\beta}} \tag{89}$$

If this identity is substituted into the last line of Eq. (87) and if the last lines of Eqs. (80) and (81) are used, then one obtains the following expression for the pair-correlation function:

$$P(\mathbf{k}_\alpha, \mathbf{k}'_\beta) = \langle n_\alpha(\mathbf{k})\rangle\langle n_\beta(\mathbf{k}')\rangle(1 + \epsilon_\alpha\delta_{\mathbf{k},\mathbf{k}'}\delta_{\alpha,\beta}) + \epsilon_\alpha\epsilon_\beta[1 + \epsilon_\alpha\langle n_\alpha(\mathbf{k})\rangle][1 + \epsilon_\beta\langle n_\beta(\mathbf{k}')\rangle]N_\alpha(\mathbf{k})N_\beta(\mathbf{k}') \times \sum^{\text{(all irreducible linked-pair 2-graphs)}_{\mathbf{k}_\alpha,\mathbf{k}'_\beta}}. \tag{90}$$

We see from this equation that once the solution to the coupled integral equations (82) is known, then one may calculate $P(\mathbf{k}_\alpha, \mathbf{k}'_\beta)$. Alternatively, use of the iterated forms of Eqs. (82) in Eq. (90) is equivalent to the calculation of the pair-correlation function by the last line of (87).

Our purpose in this section has been twofold. In the first place, we wished to show that the distribution functions of a many-body system can be expressed in terms of the linked-pair ζ-graphs of Sec. V. In the second place, we wished to show that the momentum distribution occupies a central role in the theory and that the other distribution functions and the grand potential can all be expressed in terms of the functions $N_\alpha(\mathbf{k})$, instead of $\nu_\alpha(\mathbf{k})$, which are directly related to the momentum distributions $\langle n_\alpha(\mathbf{k})\rangle$ by Eq. (81). We are not interested any further in the pair-correlation function in this paper.

VII. MASTER GRAPHS

In Sec. VI, we expressed the grand potential and the distribution functions in terms of irreducible ζ-graphs. In irreducible ζ-graphs, there are no constituent parts which consist of only one solid line in, one solid line out, and no connecting wiggly lines. Such graphical parts do appear in the linked-pair ζ-graphs of Sec. V, but in the irreducible ζ-graph formulation they are all contained in the functions $N_\alpha(\mathbf{k})$ of Eq. (81). The importance of collecting together these parts has to do with the momentum-space ordering associated with low-temperature systems. Thus, we have shown in II that the functions $\nu_\alpha(\mathbf{k})$ which appear in Eqs. (80) are not very closely related to the momentum distribution $\langle n_\alpha(\mathbf{k})\rangle$ for very low temperature Fermi systems with particle interactions. In order to extract the dominant low-temperature behavior of $\langle n_\alpha(\mathbf{k})\rangle$, one is forced to analyze the integral equation (82) in considerable detail.

Now, in the irreducible ζ-graphs, there may still occur graphical parts with one line in, one line out, and no other connecting lines, where either or both of these lines are wiggly. Moreover, it was shown in the investigations of Sec. II in II, that these graphical parts were just as important for understanding low-temperature momentum-space ordering as those with two solid lines. It was therefore necessary to collect together these graphical parts by deriving a second integral equation which was written down graphically in terms of master ζ-graphs.

We now derive the master-graph formulation for a multicomponent system. Since this formulation is really only a prescription for writing down integral equations in temperature variables [just as Eqs. (82) are integral equations in momentum variables], it becomes convenient to formally eliminate the complicated rules for temperature integrations [see Rule (vi) of Sec. V]. This objective is accomplished by introducing step functions into the vertex functions of (38) and (70) as follows:

$$^{t_1}(\ )_{t_0} = (\ )_{t_0}\theta(t_1 - t_0) \quad \text{if one outgoing line,}$$

$$^{t_1t_2}(\ )_{t_0} = (\ )_{t_0}\theta(t_1 - t_0)\theta(t_2 - t_0) \quad \text{if two outgoing lines,}$$

$$^{t_1t_2t_3}(\ )_{t_0} = (\ )_{t_0}\theta(t_1 - t_0)\theta(t_2 - t_0)\theta(t_3 - t_0) \quad \text{if three outgoing lines,}$$

$$^{t_1t_2}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0} = \begin{cases} \theta(t_1 - t_2)\,^{t_2}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\theta(t_2 - t_0) \\ \quad + \theta(t_2 - t_1)\,^{t_1}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\theta(t_1 - t_0) & \text{if } t_1 \neq t_2, \\ ^{t_1}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\theta(t_1 - t_0) & \text{if } t_1 = t_2. \end{cases} \tag{91}$$

The variables t_1, t_2, and t_3 are the temperature labels

at the heads of outgoing wiggly lines from the vertex t_0, and for a solid outgoing line i, $t_i = \beta$. When we use the vertex functions (91) in a linked-pair ζ-graph, we may extend the range of integration of the temperature variables at all of the vertices to the entire interval 0 to β. For this reason, we assume in what follows that the vertex functions (91) are being used in linked-pair ζ-graphs.

Corresponding to each irreducible linked-pair 1-graph, we next introduce an *L-graph* with exactly the same structure, but subject to the condition that we do not integrate over the temperature variable t_1 at the vertex to which the incoming line attaches. These L-graphs are generalizations of the "one-particle L-graphs" of Sec. IV. Thus if we define

$$L_\alpha(\beta, t_1, \mathbf{k}) \equiv \sum^{(\text{all } L\text{-graphs with solid external lines})_{\mathbf{k}\alpha}}, \tag{92}$$

then Eq. (82) may be replaced by

$$N_\alpha(\mathbf{k}) = \nu_\alpha(\mathbf{k})\left[1 + N_\alpha(\mathbf{k}) \int_0^\beta dt_1 L_\alpha(\beta, t_1, \mathbf{k})\right]. \tag{93}$$

The advantage of the L-graphs over the irreducible linked-pair 1-graphs is that the former permit a simple generalization which is useful for generating more complicated graphs from simpler graphs. We next define L-graphs with one or both of the solid external lines replaced by wiggly lines by merely specifying the temperature variable t_2 at the vertex to which the outgoing line is directed if that line is wiggly:

$$L_\alpha(t_2, t_1, \mathbf{k}) \equiv \sum^{(\text{all } L\text{-graphs with given external lines})_{\mathbf{k}\alpha}}. \tag{94}$$

Equation (94) reduces to Eq. (92) for L-graphs with external solid lines. For L-graphs with outgoing wiggly lines, we note that we may have $t_2 < t_1$ as well as $t_2 > t_1$.

We next define a quantity $P_\alpha(t_2, t_1, \mathbf{k})$:

$$P_\alpha(t_2, t_1, \mathbf{k}) \equiv \sum \left[\begin{array}{l}\text{all } L\text{-graphs with given external lines which cannot be separated into two } L\text{-graphs by cutting one wiggly line}\end{array}\right]_{\mathbf{k}\alpha}, \tag{95}$$

in terms of which we can write down a simple integral equation [see remark below Eq. (88)]

$$L_\alpha(t_2, t_1, \mathbf{k}) = \int_0^\beta ds G_\alpha(t_2, s, \mathbf{k}) P_\alpha(s, t_1, \mathbf{k}), \tag{96}$$

where

$$G_\alpha(t_2, t_1, \mathbf{k}) \equiv \delta(t_2 - t_1) + \epsilon_\alpha L_\alpha(t_2, t_1, \mathbf{k}). \tag{97}$$

Note that Eqs. (92)–(97) apply to each component of a multicomponent system, and that the various components are still only coupled together by the integral equations (93). Equations (96) and (97) are represented graphically in Fig. 2 of II.

Master graphs are expressed in terms of *generalized vertex functions*, which are defined in terms of the vertex functions (91) as follows:

$$^{t_1}\langle\ \rangle_{t_0} \equiv \int_0^\beta ds_1 \mathcal{G}_\alpha(t_1, s_1, \mathbf{k}_1)\, ^{s_1}\langle\ \rangle_{t_0}$$

if one outgoing line: $(\mathbf{k}_1)_\alpha$;

$$^{t_1 t_2}\langle\ \rangle_{t_0} \equiv \int_0^\beta ds_1\, ds_2 \mathcal{G}_\alpha(t_1, s_1, \mathbf{k}_1)\mathcal{G}_\beta(t_2, s_2, \mathbf{k}_2)\, ^{s_1 s_2}\langle\ \rangle_{t_0}$$

if two outgoing lines: $(\mathbf{k}_1)_\alpha$, $(\mathbf{k}_2)_\beta$;

$$^{t_1 t_2 t_3}\langle\ \rangle_{t_0} \equiv \int_0^\beta ds_1\, ds_2\, ds_3 \mathcal{G}_\alpha(t_1, s_1, \mathbf{k}_1) \times \mathcal{G}_\beta(t_2, s_2, \mathbf{k}_2)\mathcal{G}_\eta(t_3, s_3, \mathbf{k}_3)\, ^{s_1 s_2 s_3}\langle\ \rangle_{t_0}$$

if three outgoing lines: $(\mathbf{k}_1)_\alpha$, $(\mathbf{k}_2)_\beta$, $(\mathbf{k}_3)_\eta$;

$$^{t_1 t_2}\left\{\begin{matrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{matrix}\right\}_{t_0} \equiv \int_0^\beta ds_1\, ds_2 \{\mathcal{G}_\alpha(t_1, s_1, \mathbf{k}_1)\mathcal{G}_\beta(t_2, s_2, \mathbf{k}_2) - \delta(t_2 - s_1)\,\delta(t_1 - s_1)\,\delta_{t_1 t_2}\}\, ^{s_1 s_2}\left[\begin{matrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{matrix}\right]_{t_0}, \tag{98}$$

where

$$\mathcal{G}_\alpha(t, s, \mathbf{k}) \equiv G_\alpha(t, s, \mathbf{k}) + \epsilon_\alpha \mathfrak{N}_\alpha(t, \mathbf{k}) G_\alpha(\beta, s, \mathbf{k}), \tag{99}$$

and

$$\mathfrak{N}_\alpha(t, \mathbf{k}) \equiv N_\alpha(\mathbf{k}) \int_0^\beta ds' G_\alpha(t, s', \mathbf{k}). \tag{100}$$

The quantity $G_\alpha(t, s, \mathbf{k})$ is defined by Eq. (97), and if an outgoing line at the vertex t_0 is an *external* line, then in Eq. (98) we must make the replacement.

$$\mathcal{G}_\alpha(t, s, \mathbf{k}) \to G_\alpha(t, s, \mathbf{k})$$

(for an outgoing external line), (101)

where $\mathbf{k}$ is the momentum variable associated with the external line. The difference between the second and fourth of Eqs. (98) lies in the fact that the latter vertex function applies to the case of the two-particle interactions (25) which have been treated especially by the sum of Eq. (69). Thus, the subtracted term in the fourth generalized vertex function corresponds to the fact that in linked-pair ζ-graphs there are no wiggly-line double bonds between vertices which represent short-range interactions. In the third of Eqs. (98), it will be the case for nonrelativistic systems that two of the outgoing lines will always be photon lines [see Eqs. (38)]. In order to indicate in a graph that vertices represent generalized vertex functions, we shall use the usual vertex symbols of Figs. 1 and 3 with circles around them. Such a symbol will be called a *generalized*

vertex. The definition (98) is illustrated in Fig. 4 for the case of two outgoing internal lines with $t_1 \neq t_2$.

A Qth-order *master* ζ*-graph*($\zeta = 0, 1, 2, \cdots$) is defined to be a collection of Q generalized vertices which are entirely interconnected by m directed lines called *internal* lines, and to which are attached ζ *outgoing external* lines and ζ *incoming external* lines. The type of particle represented by the line is indicated by a Greek letter ($\alpha, \beta, \cdots$). All of the lines in master ζ-graphs are solid lines, and each master ζ-graph is *not reducible*. Two master ζ-graphs are different if their topological structures, including line directions and particle-type labels, are different.

To each master ζ-graph, we assign a term which is determined by the following procedures:

(i) Associate with each internal line a different integer $i (i = 1, 2, \cdots, m)$ and a corresponding momentum $\mathbf{k}_i$.

(ii) If $\zeta \neq 0$, then associate the external lines with certain pregiven momenta, such that the incoming lines refer to the same set of particles as the outgoing lines. External lines with different momentum labels are regarded as being distinguishable when they leave (or enter) different vertices.

(iii) Assign a factor S^{-1} to the entire graph, where S is the symmetry number defined below (72).

(iv) Associate with each generalized vertex a temperature variable t_i, and assign as a factor a corresponding generalized vertex function whose "upper temperature variables" are those at the vertices to which the outgoing lines from the vertex t_i are directed. The upper temperature variable for an outgoing external line is β.

(v) Assign a factor $\prod_\alpha (\epsilon^{P_B})_\alpha$ to the graph, where $(P_B)_\alpha$ is the total permutation for the α-particles of the bottom-row momenta of the Q vertex functions with respect to the top-row momenta.

(vi) Integrate over all of the temperature variables from 0 to β, and sum over the m internal momentum coordinates (and spin or other internal states) according to the particle-type labels of the lines.

A *master L-graph* is defined to be a master 1-graph in which (1) the integration over the temperature variable t_1 at the vertex to which the incoming external line attaches *is not* performed; (2) the last sentence of Rule (iv) is changed to read: "The upper temperature variable for an outgoing external line is $t_2 (< \beta)$;" and (3) the external lines may be wiggly or solid.

We can now realize the power of introducing the function $L_\alpha(t_2, t_1, \mathbf{k})$, for at this point an integral

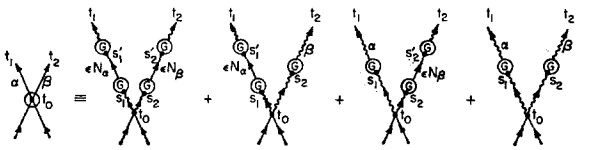


FIG. 4. The definition of the generalized vertex symbol for the case of two incoming lines, and two outgoing internal lines with $t_1 \neq t_2$; see Eqs. (98), (99), and (100).

equation in the temperature variables can be immediately deduced from Eqs. (94) and (96).

$$L_\alpha(t_2, t_1, \mathbf{k}) = \int_0^\beta ds G_\alpha(t_2, s, \mathbf{k}) \times [P_\alpha(s, t_1, \mathbf{k}, G) - \theta(s - t_1) S_\alpha(\mathbf{k})] = \sum \left(\begin{smallmatrix}\text{all master } L\text{-graphs with} \\ \text{given external lines}\end{smallmatrix}\right)_{\mathbf{k}\alpha}. \quad (102)$$

In the first line of Eq. (102), we have explicitly indicated that P_α is a functional of all of the G_α, G_β, G_η, $\cdots$ by the letter G. It should be clear that the various components of the multicomponent system are now coupled by *two* sets of integral equations; namely, (93) and (102). We have also now explicitly included the prescription of Eqs. (64) and (52) for the renormalization of the one-particle problem, where $S_\alpha(\mathbf{k})$ is defined by Eq. (65). In order to verify that Eq. (102) is correct, a straightforward procedure is to check that its iterated form is equivalent to Eq. (96).

According to (101) and the first line of (102), the function $P_\alpha(s, t, \mathbf{k}, G)$ is the sum over all master L-graphs with no external line factors. We now introduce two new quantities $L_\alpha^{(\tau)}(t_2, t_1)$ and $G_\alpha^{(\tau)}(t_2, t_1)$, which are slight modifications of the functions $L_\alpha(t_2, t_1)$ and $G_\alpha(t_2, t_1)$. These new functions are defined, for $\beta > \tau$, as follows:

$$L_\alpha^{(\tau)}(t_2, t_1, \mathbf{k}) \equiv \int_0^\tau ds\, G_\alpha^{(\tau)}(t_2, s, \mathbf{k}) \times [P_\alpha(s, t_1, \mathbf{k}, G^{(\beta)}) - \theta(s - t_1) S_\alpha(\mathbf{k})] \underset{\tau \to \beta}{\to} L_\alpha^{(\beta)}(t_2, t_1, \mathbf{k}) = L_\alpha(t_2, t_1, \mathbf{k}), \quad (103)$$

$$G_\alpha^{(\tau)}(t_2, t_1, \mathbf{k}) \equiv \delta(t_2 - t_1) + \epsilon_\alpha L_\alpha^{(\tau)}(t_2, t_1, \mathbf{k}) \underset{\tau \to \beta}{\to} G_\alpha^{(\beta)}(t_2, t_1, \mathbf{k}) = G_\alpha(t_2, t_1, \mathbf{k}).$$

It is to be emphasized that the definitions (103) do not entail any modifications of the *internal* line factors of G in $P_\alpha(s, t_1)$. The functions (103) occur in the expression for the grand potential given below.

Momentum Distribution

It is clear from Eq. (102) and the definition of master L graphs that Eq. (93) for the quantity

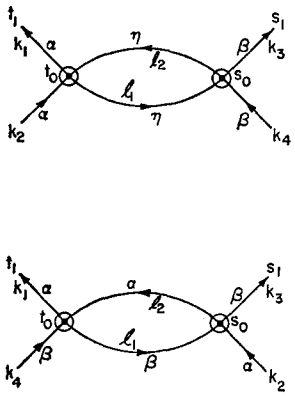


FIG. 5. The two basic ring structures. Only the first of these structures is associated with a q^{-4} singularity.

$N_\alpha(\mathbf{k})$ may be written as

$$N_\alpha(\mathbf{k}) = \nu_\alpha(\mathbf{k})[1 + N_\alpha(\mathbf{k}) \sum (^{\text{all master}}_{\text{1-graphs}})]. \quad (104)$$

Thus, by means of Eqs. (81) and (104), the momentum distribution $\langle n_\alpha(\mathbf{k})\rangle$ is given explicitly in terms of master 1-graphs. By combining Eqs. (81) and (93), one can also show that the momentum distribution is equal to the function $\mathfrak{N}_\alpha(\beta, \mathbf{k})$ of Eq. (100):

$$\mathfrak{N}_\alpha(\beta, \mathbf{k}) = \langle n_\alpha(\mathbf{k})\rangle. \quad (105)$$

Equation (105) shows that the weighting factors $\mathfrak{N}_\alpha(t, \mathbf{k})$ in master ζ-graphs are very closely related to the true momentum distribution of the system, which indicates that the master-graph formulation of quantum statistics is a very physical formulation.

Grand Potential

The grand potential (83) can also be written in the master-graph formulation. A straightforward generalization of the derivation given in II for a one-component system yields the result

$$\begin{aligned}
&\Omega f(\beta, N_\alpha, \Omega) \\
&= \sum_\alpha \epsilon_\alpha \sum_{\mathbf{k}} \ln [1 + \epsilon_\alpha \langle n_\alpha(\mathbf{k})\rangle] + \Omega F(\beta, N_\alpha, \Omega) \\
&- \sum_\alpha \epsilon_\alpha \sum_{\mathbf{k}} \int_0^\beta dt\, L_\alpha(\beta, t, \mathbf{k}) \mathfrak{N}_\alpha(t, \mathbf{k}) - \sum_\alpha \sum_{\mathbf{k}} \\
&\times \int_0^\beta dt_1 \left\{ \int_0^\beta dt_2 G_\alpha^{(\beta)}(t_1, t_2, \mathbf{k}) - \int_0^{t_1} dt_2 G_\alpha^{(t_1)}(t_1, t_2, \mathbf{k}) \right\} \\
&\times [P_\alpha(t_2, t_1, \mathbf{k}) - \theta(t_2 - t_1) S_\alpha(\mathbf{k})], \quad (106)
\end{aligned}$$

where

$$\Omega F(\beta, N_\alpha, \Omega) \equiv \sum (^{\text{all master}}_{\text{0-graphs.}}). \quad (107)$$

In Eq. (106) all quantities are expressed in terms of the generalized vertex functions (98), except the last term which involves a modified external line factor as defined by Eqs. (103). With Eqs. (104) and (106), we have achieved the goal of expressing both the momentum distribution and the grand potential in terms of master graphs.

VIII. COULOMB INTERACTIONS AND RING DIAGRAMS

The preceding sections constitute the main structure of the formalism required to achieve our major objective for any real system; namely, to calculate the grand potential via either (71) or (106). However, the existence of charged particles in a system leads to several difficulties in such calculations, the first of which was treated carefully in Sec. IV. Another major problem in fully ionized gases arises from the long-range nature of the Coulomb interaction.

The Ursell equations (17) presume the existence of clustering in the many-body system. It might seem then that the infinite range of the Coulomb force would allow only one large cluster to form in a charged-particle system. However, any neutral aggregate of particles has only a net short-range interaction with other particles, and we see [e.g., below Eq. (159)] that clusters with nonzero charge can probably always be combined to give finite results for systems with zero total charge.

The momentum-space matrix elements of the Coulomb interaction are

$$\begin{aligned}
&\langle \mathbf{k}_1^{(\alpha)} \mathbf{k}_3^{(\beta)} | \, V_C(\beta) \, | \mathbf{k}_2^{(\alpha)} \mathbf{k}_4^{(\beta)} \rangle \\
&= (2\pi)^3 \Omega^{-2} \delta^{(3)}(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_2 - \mathbf{k}_4) \\
&\times (4\pi Z_\alpha Z_\beta e^2) \delta_{m_1 m_2} \delta_{m_3 m_4} q^{-2} \\
&\times \exp \beta[\omega_\alpha(k_1) + \omega_\beta(k_3) - \omega_\alpha(k_2) - \omega_\beta(k_4)], \quad (108)
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{q} &= (M_\alpha + M_\beta)^{-1}[M_\beta(\mathbf{k}_1 - \mathbf{k}_2) + M_\alpha(\mathbf{k}_4 - \mathbf{k}_3)] \\
&= \mathbf{k}_1 - \mathbf{k}_2. \quad (109)
\end{aligned}$$

The q^{-2} singularity in (108) is due to the infinite range of the Coulomb potential, and it results in an apparent divergence of the grand potential. Thus, if one considers the *ring* structure of Fig. 5, then one can readily verify that a factor of q^{-4} occurs in part of the corresponding expression. Clearly, the iteration of this structure is associated with an extremely divergent expression. We call such an iterated structure a *ring chain*. Moreover, it will be a basic assumption of our approach that the sum over all possible ring chains is not divergent, but rather leads to a screened Coulomb interaction.

Ring Chains

We now write down two integral equations which generate the sum over all possible ring chains

corresponding to the two kinds of rings in Fig. 5:

$$L_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv {}^{t_1s_1}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{t_0}{}_{\alpha\beta}\delta(t_0-s_0)$$
$$+\sum_{\eta}\epsilon_\eta\sum_{l_1,l_2}\int_0^\tau dt_2\,{}^{t_1t_2}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{k}_2\mathbf{l}_2\end{matrix}\right\rangle_{t_0}{}_{\alpha\eta}L_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3\\ \mathbf{l}_1\mathbf{k}_4\\ \eta\beta\end{pmatrix}\begin{matrix}t_0s_1\\ t_2s_0\end{matrix}$$
$$\underset{\tau\to\beta}{\to}L_{\mathrm{C},(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix},\qquad(110)$$

$$L_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv {}^{t_1s_1}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{t_0}{}_{\alpha\beta}\delta(t_0-s_0)$$
$$+\epsilon_\alpha\epsilon_\beta\sum_{l_1,l_2}\int_0^\tau ds_2\,{}^{t_1s_2}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{l}_2\mathbf{k}_4\end{matrix}\right\rangle_{s_0}{}_{\alpha\beta}L_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3\\ \mathbf{k}_2\mathbf{l}_1\\ \alpha\beta\end{pmatrix}\begin{matrix}s_0s_1\\ t_0s_2\end{matrix}$$
$$\underset{\tau\to\beta}{\to}L_{\mathrm{E},(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv L_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix},\qquad(111)$$

where the generalized vertex functions are those of Eq. (98) using the Coulomb interaction (108), and we require these functions for $\tau \neq \beta$ as well as $\tau = \beta$. [The use of the Greek letter β for both $(kT)^{-1}$ and a particle-type label should not be confusing.] It is to be emphasized that each generalized vertex function in L_{E} corresponds to a single matrix element. So long as $\alpha \neq \beta$ there can be no confusion about this point; however, this point must be remembered when the case $\alpha = \beta$ occurs, as in Eqs. (138)–(143). Likewise, it is to be noted that, even though the analysis of the present section is completely in terms of master graphs, we have included all reducible diagrams, in order that these equations may also be valid in the linked-pair formulation of Sec. V [provided one uses Eq. (154) for the function $\mathcal{G}_\alpha(t_2, t_1, \mathbf{k})$]. The diagrammatic representations of these integral equations are given in Fig. 6.

We must next introduce two functions which are closely related to L_{C} and L_{E}, namely:

$$L^{(2)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}$$
$$\equiv L_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}-{}^{t_1s_1}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{t_0}{}_{\alpha\beta}\delta(t_0-s_0)$$
$$\underset{\tau\to\beta}{\to}L^{(2)}_{\mathrm{C},(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv L^{(2)}_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix},\qquad(112)$$

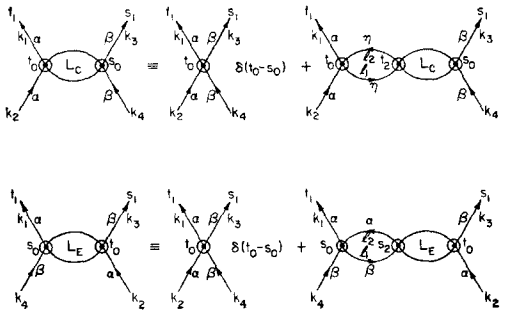


FIG. 6. The diagrammatic representations of the two integral equations (110) and (111).

$$L^{(2)}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv \epsilon_\alpha\delta_{\alpha\beta}L^{(2)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_4\mathbf{k}_2\\ \alpha\alpha\end{pmatrix}\begin{matrix}t_1s_1\\ s_0t_0\end{matrix}$$
$$+(1-\delta_{\alpha\beta})\left[L_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}-{}^{t_1s_1}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{t_0}{}_{\alpha\beta}\delta(t_0-s_0)\right]$$
$$\underset{\tau\to\beta}{\to}L^{(2)}_{\mathrm{E},(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\equiv L^{(2)}_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\\ \alpha\beta\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}.\qquad(113)$$

Both $L^{(2)}_{\mathrm{C}}$ and $L^{(2)}_{\mathrm{E}}$ are sums over all possible ring chains in which (diagrammatically) either $\mathbf{k}_2$ is the left incoming line $[L^{(2)}_{\mathrm{C}}]$ or $\mathbf{k}_4$ is the left incoming line $[L^{(2)}_{\mathrm{E}}]$. In these functions the single vertex term has been explicitly subtracted, because then these functions are suitable elements for the most-general ring diagrams discussed below. Note that for $L^{(2)}_{\mathrm{E}}$ a distinction must be made between the cases $\alpha = \beta$ and $\alpha \neq \beta$. We henceforth refer to the four functions L_{C}, L_{E}, $L^{(2)}_{\mathrm{C}}$, and $L^{(2)}_{\mathrm{E}}$ as *eggs*.

Ring Diagrams

If one appropriately connects combinations of the functions L_{C}, L_{E}, $L^{(2)}_{\mathrm{C}}$, and $L^{(2)}_{\mathrm{E}}$ in all possible ways, then one obtains, among other things, all possible *ring diagrams*. In order to specify the structure of ring diagrams more precisely, we define a *contraction* procedure to be used for their identification. Thus, in order to qualify as a ring diagram, it must be possible to identify a ring (Fig. 5) when all eggs are replaced by generalized vertices (i.e., points). Then, when the identified ring is replaced by a point, it must be possible to identify another ring. The continual contraction of rings to points must eventually result in a single generalized vertex. We note that in ring diagrams two lines never connect the *same* two ends of two eggs, for such a structure is already included in a single egg.

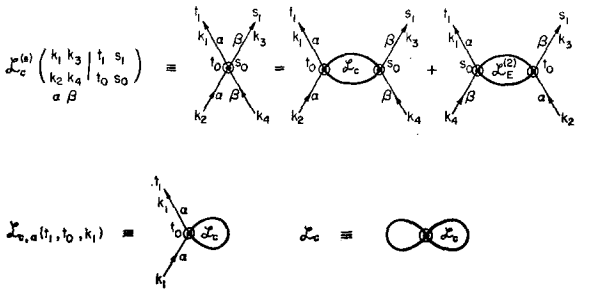


FIG. 7. The diagrammatic representations of the three functions $\mathcal{L}_C^{(S)}$, $\mathcal{L}_{C,\alpha}$, and $\mathcal{L}_C$ of Eqs. (120), (116), and (117) respectively. Note that the vertex which represents $\mathcal{L}_C^{(S)}$ is associated with *two* temperature labels.

The occurrence of the singular ring structure is not limited to the simple ring chains of L_C, but occurs in all possible combinations of the two functions L_C and L_E. Thus, it is essential that we have a systematic procedure for determining such combinations, and sums over these combinations. It is probably unnecessary to carry out a complete analysis of the most-general ring diagram in order to understand the physics of a real charged-particle system by an approximate calculation. However, as we show below, it is easy to formally write down the sum over all possible ring diagrams, thereby facilitating the systematic treatment of the Coulomb interactions for any given problem.

We now define the sum of all possible ring diagrams for four possible cases:

$$\mathcal{L}_{C,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \sum \left[\begin{matrix}\text{All ways of connecting eggs such}\\ \text{that } \mathbf{k}_3 \text{ is the } \textit{left} \text{ incoming line.}\end{matrix}\right]$$

$$\underset{\tau\to\beta}{\longrightarrow} \mathcal{L}_{C,(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \mathcal{L}_C\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}, \tag{114}$$

$$\mathcal{L}_{E,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \sum \left[\begin{matrix}\text{All ways of connecting eggs such that}\\ \mathbf{k}_3 \text{ is the } \textit{right} \text{ incoming line and } \beta \neq \alpha\end{matrix}\right]$$

$$\underset{\tau\to\beta}{\longrightarrow} \mathcal{L}_{E,(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \mathcal{L}_E\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}, \tag{115}$$

$$\mathcal{L}_{C,\alpha}(t_1, t_0, \mathbf{k}_1) \equiv \sum \left[\begin{matrix}\text{All ways of connecting eggs such that}\\ \text{there is only one incoming (and one}\\ \text{outgoing) external line}\end{matrix}\right], \tag{116}$$

$$\mathcal{L}_C \equiv \sum \left[\begin{matrix}\text{All ways of connecting eggs such}\\ \text{that there are } \textit{no} \text{ external lines}\end{matrix}\right], \tag{117}$$

where the single egg is included with both $\mathcal{L}_{C,(\tau)}$ and $\mathcal{L}_{E,(\tau)}$. We also define three functions which are closely related to $\mathcal{L}_{C,(\tau)}$ and $\mathcal{L}_{E,(\tau)}$.

$$\mathcal{L}_{C,(\tau)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}$$

$$\equiv \mathcal{L}_{C,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} - {}^{t_1s_1}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{t_0}{}_{\alpha\beta}\delta(t_0 - s_0)$$

$$\underset{\tau\to\beta}{\longrightarrow} \mathcal{L}_{C,(\beta)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \mathcal{L}_C^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}, \tag{118}$$

$$\mathcal{L}_{E,(\tau)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \epsilon_\alpha\delta_{\alpha\beta}\mathcal{L}_{C,(\tau)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_4\mathbf{k}_2\end{pmatrix}\begin{matrix}t_1s_1\\ s_0t_0\end{matrix}\Big)_{\alpha\alpha}$$

$$+ (1 - \delta_{\alpha\beta})\Big[\mathcal{L}_{E,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}$$

$$- {}^{t_1s_1}\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{t_0}{}_{\alpha\beta}\delta(t_0 - s_0)\Big]$$

$$\underset{\tau\to\beta}{\longrightarrow} \mathcal{L}_{E,(\beta)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \mathcal{L}_E^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}, \tag{119}$$

$$\mathcal{L}_{C,(\tau)}^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}$$

$$\equiv \mathcal{L}_{C,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} + \mathcal{L}_{E,(\tau)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}$$

$$\underset{\tau\to\beta}{\longrightarrow} \mathcal{L}_{C,(\beta)}^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta} \equiv \mathcal{L}_C^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}. \tag{120}$$

The diagrammatic representation of the three functions $\mathcal{L}_C^{(S)}$, $\mathcal{L}_{C,\alpha}$, and $\mathcal{L}_C$ is shown in Fig. 7. These functions may be used either in master graphs or in linked-pair graphs, in which case we must stipulate that *no* rings (Fig. 5) can occur which involve two Coulomb interaction vertices, because the functions $\mathcal{L}_C^{(S)}|_{\tau=\beta}$, $\mathcal{L}_{C,\alpha}$, and $\mathcal{L}_C$ represent all possible ways of including such rings. We note that $\mathcal{L}_{C,\alpha}$ is that part of L_α, Eqs. (96) or (102), which is due entirely to ring diagrams, and that $\mathcal{L}_C$ is the ring-diagram contribution to the sum over all linked-pair 0-graphs, or master 0-graphs, depending on whether (71) or (107) is used.

We now write down explicit coupled integral equations for $\mathcal{L}_{C,(\tau)}$ and $\mathcal{L}_{E,(\tau)}$, equations which can be verified by iteration to leading orders as well as by careful analysis of the general structure of ring diagrams.

$$\mathcal{L}_{C,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\Big)_{\alpha\beta}$$

$$= L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta} + \mathcal{L}^{(L-)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}$$

$$+ \sum_{\eta}\epsilon_\eta \sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta ds_2\int_0^\tau dt_2 L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{pmatrix}\begin{matrix}t_1t_2 \\ t_0s_2\end{matrix}_{\alpha\eta}$$

$$\times\left[\mathcal{L}^{(L-)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}\begin{matrix}s_2s_1 \\ t_2s_0\end{matrix}_{\eta\beta} + \mathcal{L}^{(2)}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}\begin{matrix}s_2s_1 \\ t_2s_0\end{matrix}_{\eta\beta}\right], \quad (121)$$

$$\mathcal{L}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}$$

$$\equiv L_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta} + \mathcal{L}^{(L-)}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}$$

$$+ \epsilon_\alpha\epsilon_\beta\sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta dt_2\int_0^\tau ds_2 L_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{l}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1t_2 \\ s_2s_0\end{matrix}_{\alpha\beta}$$

$$\times\left[\mathcal{L}^{(2)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{l}_1\end{pmatrix}\begin{matrix}s_2s_1 \\ t_0t_2\end{matrix}_{\alpha\beta} + \mathcal{L}^{(L-)}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{l}_1\end{pmatrix}\begin{matrix}s_2s_1 \\ t_0t_2\end{matrix}_{\alpha\beta}\right], \quad (122)$$

where

$$\mathcal{L}^{(L-)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}$$

$$\equiv \sum_{\eta}\epsilon_\eta\sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta ds_2\int_0^\tau dt_2\mathcal{L}^{(2)}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{pmatrix}\begin{matrix}t_1t_2 \\ t_0s_2\end{matrix}_{\alpha\eta}$$

$$\times\,\mathcal{L}^{(S)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}\begin{matrix}s_2s_1 \\ t_2s_0\end{matrix}_{\eta\beta}$$

$$\underset{\tau\to\beta}{\longrightarrow}\mathcal{L}^{(L-)}_{\mathrm{C},(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta} \equiv \mathcal{L}^{(L-)}_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}, \quad (123)$$

$$\mathcal{L}^{(L-)}_{\mathrm{E},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta} \equiv \epsilon_\alpha\epsilon_\beta\sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta dt_2\int_0^\tau ds_2$$

$$\times\,\mathcal{L}^{(2)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{l}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1t_2 \\ s_2s_0\end{matrix}_{\alpha\beta}\mathcal{L}^{(S)}_{\mathrm{C},(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{l}_1\end{pmatrix}\begin{matrix}s_2s_1 \\ t_0t_2\end{matrix}_{\alpha\beta}$$

$$\underset{\tau\to\beta}{\longrightarrow}\mathcal{L}^{(L-)}_{\mathrm{E},(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta} = \mathcal{L}^{(L-)}_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}. \quad (124)$$

The diagrammatic representations of the integral equations (121)–(124) are given in Figs. 8(a) and 8(b).

Self-Energy Ring Diagrams

We refer to the ring diagrams in $\mathcal{L}_{\mathrm{C},\alpha}$ as *self-energy ring diagrams*, because these diagrams, characterized by only one incoming external line and one outgoing external line, are closely associated with the momentum-space ordering which may occur at very low temperatures in a many-body system. (This momentum-space ordering is formally achieved by the Λ transformation of II, which takes one from a particle description of the many-body system to a quasiparticle description.)

One must be careful when attempting to write down a general expression for $\mathcal{L}_{\mathrm{C},\alpha}$, for the correct symmetry numbers are not duplicated by simply connecting the (external) β lines of $\mathcal{L}^{(S)}_{\mathrm{C}}|_{\tau=\beta}$. This latter expression gives many of the terms of $\mathcal{L}_{\mathrm{C},\alpha}$ more than once and it also overlooks the fact that a "double bond" *may* occur when the β lines are connected. In order to account for the last possibility, we first define a function L_{db} as follows:

$$L_{\mathrm{db}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix}t_1s_1 \\ t_0s_0\end{matrix}_{\alpha\beta}$$

$$\equiv (1-\tfrac{1}{2}\delta_{\alpha\beta})\epsilon_\alpha\epsilon_\beta\sum_{\mathbf{l}_1\mathbf{l}_2}\Big\langle\begin{matrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{l}_2\mathbf{k}_4\end{matrix}\Big\rangle^{t_1t_0}_{s_0}\Big\langle\begin{matrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{l}_1\end{matrix}\Big\rangle^{s_0s_1}_{t_0}. \quad (125)$$

We next define a function $L_{\mathrm{C},\alpha}$ by the equation

$$L_{\mathrm{C},\alpha}(t_1, t_0, \mathbf{k}_1) \equiv \sum_{\beta}\sum_{\mathbf{k}_2}\int_0^\beta ds_0 L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_1\mathbf{k}_3\end{pmatrix}\begin{matrix}t_1s_0 \\ t_0s_0\end{matrix}_{\alpha\beta} + L'_{\mathrm{C},\alpha}(t_1, t_0, \mathbf{k}_1), \quad (126)$$

where

$$L'_{\mathrm{C},\alpha}(t_1, t_0, \mathbf{k}_1)$$

$$\equiv \sum_{\beta}\sum_{\mathbf{k}_2}\int_0^\beta ds_0\Bigg\{L^{(2)}_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_1\mathbf{k}_3\end{pmatrix}\begin{matrix}t_1s_0 \\ t_0s_0\end{matrix}_{\alpha\beta} - L_{\mathrm{db}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_1\mathbf{k}_3\end{pmatrix}\begin{matrix}t_1s_0 \\ t_0s_0\end{matrix}_{\alpha\beta}$$

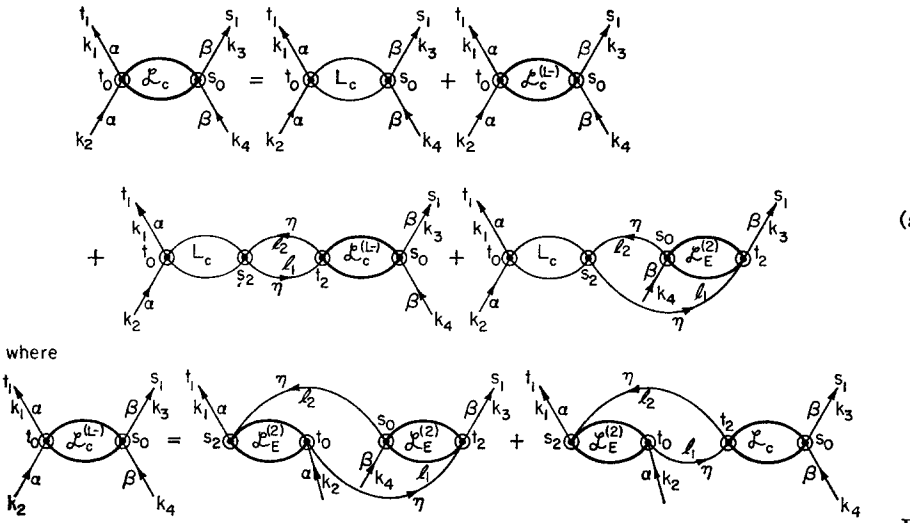
$$+ \epsilon_\alpha\epsilon_\beta\sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta ds_2\,dt_2\Bigg[L^{(2)}_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_3\mathbf{l}_2\end{pmatrix}\begin{matrix}t_1t_2 \\ s_2s_0\end{matrix}_{\alpha\beta}\mathcal{L}^{(2)}_{\mathrm{C}}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_1\end{pmatrix}\begin{matrix}s_0s_2 \\ t_2t_0\end{matrix}_{\beta\alpha}$$

$$+ L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_3\mathbf{l}_2\end{pmatrix}\begin{matrix}t_1t_2 \\ s_0s_2\end{matrix}_{\alpha\beta}\mathcal{L}^{(L-)}_{\mathrm{C}}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_1\end{pmatrix}\begin{matrix}s_2s_0 \\ t_2t_0\end{matrix}_{\beta\alpha}\Bigg]\Bigg\}$$

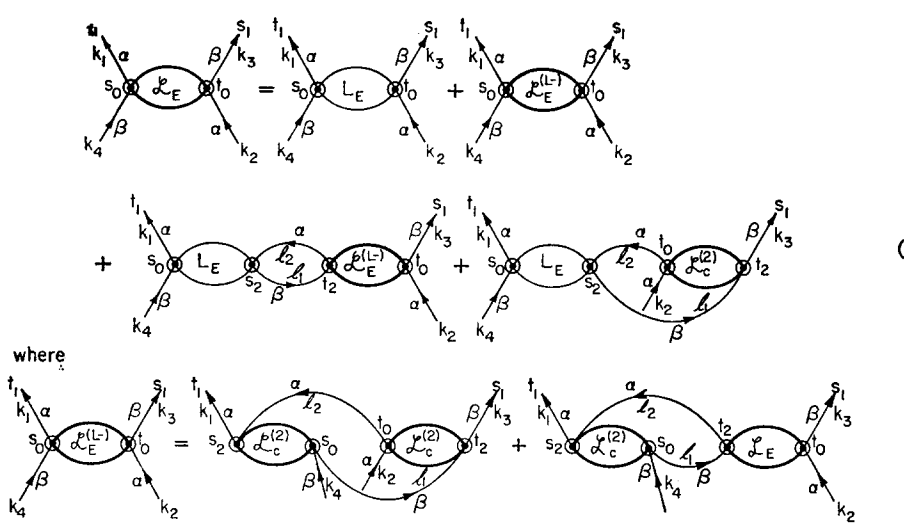
$$+ \sum_{\beta\neq\alpha}\sum_{\mathbf{k}_2}\int_0^\beta ds_0\,ds_2\,dt_2\epsilon_\alpha\epsilon_\beta$$

$$\times\sum_{\mathbf{l}_1\mathbf{l}_2}\Bigg[L^{(2)}_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{l}_2\mathbf{k}_3\end{pmatrix}\begin{matrix}t_1t_2 \\ s_0s_2\end{matrix}_{\alpha\beta}\mathcal{L}^{(2)}_{\mathrm{E}}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_1\mathbf{l}_1\end{pmatrix}\begin{matrix}s_0s_2 \\ t_0t_2\end{matrix}_{\alpha\beta}$$

$$+ L_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{l}_2\mathbf{k}_3\end{pmatrix}\begin{matrix}t_1t_2 \\ s_2s_0\end{matrix}_{\alpha\beta}\mathcal{L}^{(L-)}_{\mathrm{E}}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_1\mathbf{l}_1\end{pmatrix}\begin{matrix}s_0s_2 \\ t_0t_2\end{matrix}_{\alpha\beta}\Bigg]. \quad (127)$$



(a)



(b)

FIG. 8. (a) The diagrammatic representations of Eqs. (121) and (123). (b) The diagrammatic representations of Eqs. (122) and (124).

Then the complete expression for $\mathfrak{L}_{C,\alpha}$ is

$$\mathfrak{L}_{C,\alpha}(t_1, t_0, \mathbf{k}_1) = L_{C,\alpha}(t_1, t_0, \mathbf{k}_1) + \sum_{\beta}\sum_{\mathbf{l}_1}\int_0^{\beta} ds_2\, dt_2 \epsilon_\beta \Big\{ \mathfrak{L}_C^{(R-)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_1\mathbf{l}_1\end{pmatrix}\begin{matrix} t_1t_2 \\ t_0s_2\end{matrix}\Big)_{\alpha\beta} \times \sum_{\eta}\sum_{\mathbf{k}_3}\int_0^{\beta} ds_0 L_C\begin{pmatrix}\mathbf{l}_1\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_3\end{pmatrix}\begin{matrix} s_2s_0 \\ t_2s_0\end{matrix}\Big)_{\beta\eta} + \mathfrak{L}_E^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_1\mathbf{l}_1\end{pmatrix}\begin{matrix} t_1t_2 \\ t_0s_2\end{matrix}\Big)_{\alpha\beta} \times L_{C,\beta}(s_2, t_2, \mathbf{l}_1) + \mathfrak{L}_C\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_1\mathbf{l}_1\end{pmatrix}\begin{matrix} t_1t_2 \\ t_0s_2\end{matrix}\Big)_{\alpha\beta} L'_{C,\beta}(s_2, t_2, \mathbf{l}_1)\Big\}. \tag{128}$$

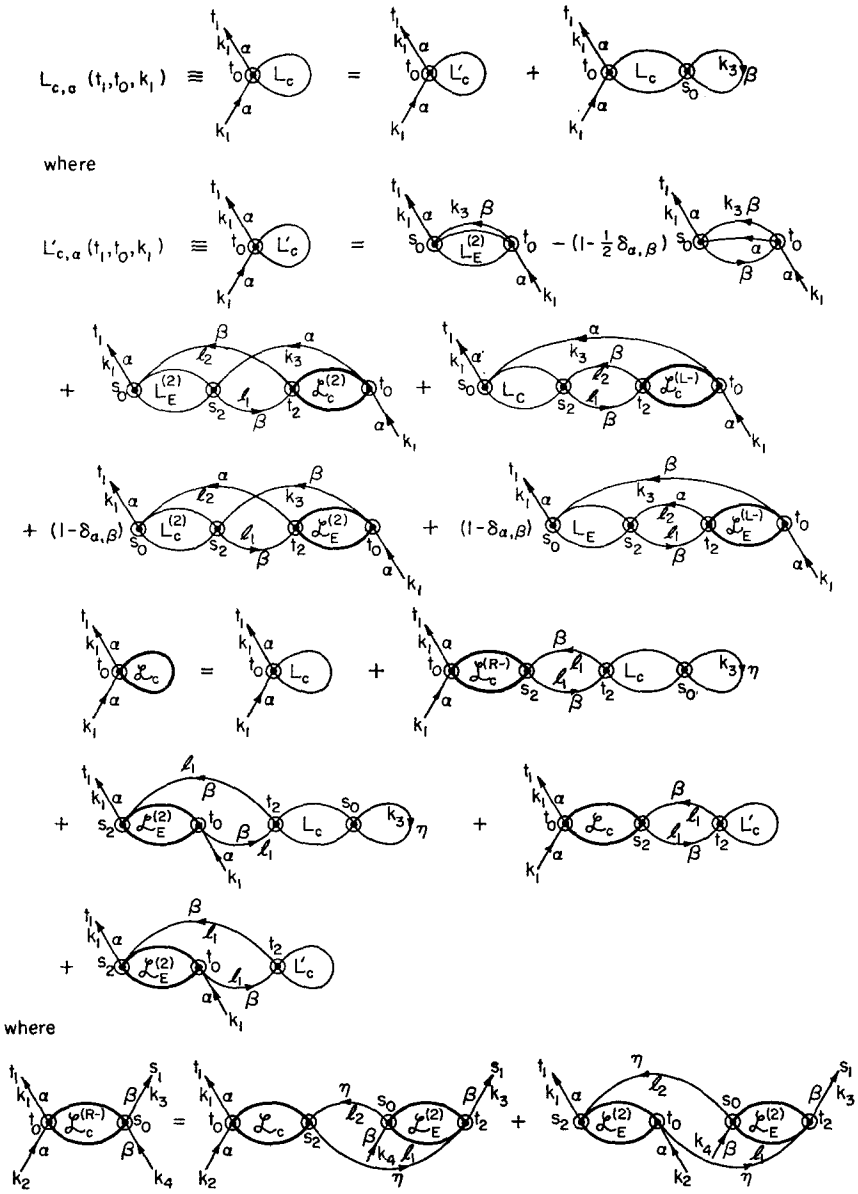
It should be clear that

$$\mathfrak{L}_{C,\alpha}(t_1, t_0, \mathbf{k}_1) \to L'_{C,\alpha}(t_1, t_0, \mathbf{k}_1) + \sum_{\beta}\sum_{\mathbf{k}_3} {}^{t_1t_0}\Big\langle \begin{matrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_1\mathbf{k}_3\end{matrix}\Big\rangle_{t_0}^{\alpha\beta} \tag{128a}$$

in the master-graph formulation, because the remaining part of (128) is composed of reducible graphs. The function $\mathfrak{L}_C^{(R-)}$ is given by

$$\mathfrak{L}_C^{(R-)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}\begin{matrix} t_1s_1 \\ t_0s_0\end{matrix}\Big)_{\alpha\beta} = \sum_{\eta}\epsilon_\eta \sum_{\mathbf{l}_1,\mathbf{l}_2}\int_0^{\beta} ds_2 \int_0^{\beta} dt_2 \times \mathfrak{L}_C^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{pmatrix}\begin{matrix} t_1t_2 \\ t_0s_2\end{matrix}\Big)_{\alpha\eta} \mathfrak{L}_E^{(2)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}\begin{matrix} s_2s_1 \\ t_2s_0\end{matrix}\Big)_{\eta\beta}. \tag{129}$$

The diagrammatic representations of Eqs. (126)–(129) are given in Figs. 9(a) and 9(b). Note that the incoming external lines of the functions (126)–(128)



(a)

(b)

FIG. 9. (a) The diagrammatic representations of Eqs. (126) and (127). (b) The diagrammatic representations of Eqs. (128) and (129).

all attach at t_0-vertices, as they should [see above Eq. (92)].

Closed Ring Diagrams

We refer to the ring diagrams in $\mathfrak{L}_C$, Eq. (117), as *closed ring diagrams*. In order to write down the complete expression for $\mathfrak{L}_C$, we need the following three functions:

$$\mathfrak{L}^{(--)}_{C,(\tau)}\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\,\middle|\,\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)_{\alpha\beta}$$

$$\equiv \sum_{\eta}\epsilon_\eta \sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta ds_2\int_0^\tau dt_2\Bigg[\mathfrak{L}^{(L-)}_{C,(\tau)}\left(\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{k}_2\mathbf{l}_2\end{matrix}\,\middle|\,\begin{matrix}t_1t_2\\ t_0s_2\end{matrix}\right)_{\alpha\eta}$$

$$+\mathfrak{L}^{(2)}_{E,(\tau)}\left(\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{k}_2\mathbf{l}_2\end{matrix}\,\middle|\,\begin{matrix}t_1t_2\\ t_0s_2\end{matrix}\right)_{\alpha\eta}\Bigg]\mathfrak{L}^{(2)}_{E,(\tau)}\left(\begin{matrix}\mathbf{l}_2\mathbf{k}_3\\ \mathbf{l}_1\mathbf{k}_4\end{matrix}\,\middle|\,\begin{matrix}s_2s_1\\ t_2s_0\end{matrix}\right)_{\eta\beta}$$

$$\underset{\tau\to\beta}{\longrightarrow}\mathfrak{L}^{(--)}_{C,(\beta)}\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\,\middle|\,\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)_{\alpha\beta}\equiv\mathfrak{L}^{(--)}_{C}\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\,\middle|\,\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)_{\alpha\beta}, \tag{130}$$

$$\mathfrak{L}^{(--)}_{E,(\tau)}\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\,\middle|\,\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)_{\alpha\beta}$$

$$\equiv \epsilon_\alpha\epsilon_\beta\sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\beta dt_2\int_0^\tau ds_2\Bigg[\mathfrak{L}^{(2)}_{C,(\tau)}\left(\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{l}_2\mathbf{k}_4\end{matrix}\,\middle|\,\begin{matrix}t_1t_2\\ s_2s_0\end{matrix}\right)_{\alpha\beta}$$

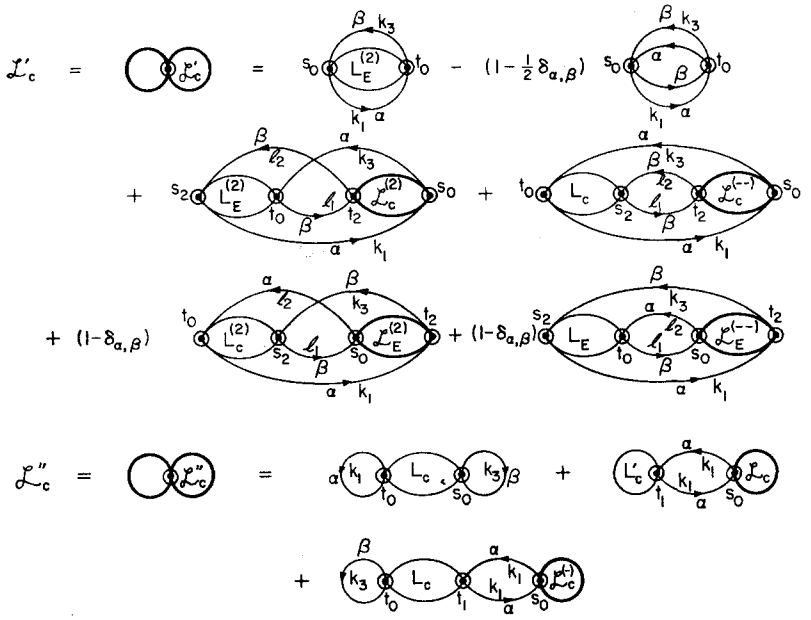


FIG. 10. The diagrammatic representations of Eqs. (133) and (134).

$$+\mathfrak{L}_{\mathrm{E},(\tau)}^{(L-)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & t_1t_2\\ \mathbf{l}_2\mathbf{k}_4 & s_2s_0\end{pmatrix}_{\alpha\beta}\Big]\mathfrak{L}_{\mathrm{C},(\tau)}^{(2)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 & s_2s_1\\ \mathbf{k}_2\mathbf{l}_1 & t_0t_2\end{pmatrix}_{\alpha\beta}, \tag{131}$$

$$\mathfrak{L}_{\mathrm{C},\alpha}^{(-)}(t_1,\,t_0,\,\mathbf{k}_1)$$
$$\equiv L'_{\mathrm{C},\alpha}(t_1,\,t_0,\,\mathbf{k}_1)+\sum_{\beta}\sum_{\mathbf{l}_1}\int_0^{\beta}ds_2\,dt_2\epsilon_\beta$$
$$\times\Big\{\mathfrak{L}_{\mathrm{C}}^{(--)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & t_1t_2\\ \mathbf{k}_1\mathbf{l}_1 & t_0s_2\end{pmatrix}_{\alpha\beta}\sum_{\eta}\sum_{\mathbf{k}_2}\int_0^{\beta}ds_0L_{\mathrm{C}}\begin{pmatrix}\mathbf{l}_1\mathbf{k}_3 & s_2s_0\\ \mathbf{l}_1\mathbf{k}_3 & t_2s_0\end{pmatrix}_{\beta\eta}$$
$$+\mathfrak{L}_{\mathrm{E}}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & t_1t_2\\ \mathbf{k}_1\mathbf{l}_1 & t_0s_2\end{pmatrix}_{\alpha\beta}L_{\mathrm{C},\beta}(s_2,\,t_2,\,\mathbf{l}_1)$$
$$+\mathfrak{L}_{\mathrm{C}}^{(L-)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & t_1t_2\\ \mathbf{k}_1\mathbf{l}_1 & t_0s_2\end{pmatrix}_{\alpha\beta}L'_{\mathrm{C},\beta}(s_2,\,t_2,\,\mathbf{l}_1)\Big\}, \tag{132}$$

where $\mathfrak{L}_{\mathrm{C}}^{(L-)}$ and $\mathfrak{L}_{\mathrm{E}}^{(L-)}$ are defined by Eqs. (123) and (124), respectively.

We next define two quantities $\mathfrak{L}'_{\mathrm{C}}$ and $\mathfrak{L}''_{\mathrm{C}}$:

$$\mathfrak{L}'_{\mathrm{C}}\equiv\frac{1}{2}\sum_{\alpha,\beta}\sum_{\mathbf{k}_1\mathbf{k}_3}\int_0^{\beta}dt_0\int_0^{t_0}ds_0\Big[L_{\mathrm{E},(t_0)}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 & t_0s_0\\ \mathbf{k}_1\mathbf{k}_3 & t_0s_0\end{pmatrix}_{\alpha\beta}$$
$$-L_{\mathrm{db}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 & t_0s_0\\ \mathbf{k}_1\mathbf{k}_3 & t_0s_0\end{pmatrix}_{\alpha\beta}\Big]+\frac{1}{2}\sum_{\alpha,\beta}\sum_{\mathbf{k}_1\mathbf{k}_3}\sum_{\mathbf{l}_1\mathbf{l}_3}\int_0^{\beta}dt_0\,ds_2\,ds_0$$
$$\times\int_0^{t_0}dt_2\,\epsilon_\alpha\epsilon_\beta\Big[L_{\mathrm{E}}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & s_0t_2\\ \mathbf{k}_3\mathbf{l}_2 & t_0s_2\end{pmatrix}_{\alpha\beta}\mathfrak{L}_{\mathrm{C},(t_0)}^{(2)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 & s_2t_0\\ \mathbf{l}_1\mathbf{k}_1 & t_2s_0\end{pmatrix}_{\beta\alpha}$$
$$+L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & s_0t_2\\ \mathbf{k}_3\mathbf{l}_2 & t_0s_2\end{pmatrix}_{\alpha\beta}\mathfrak{L}_{\mathrm{C},(t_0)}^{(--)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 & s_2t_0\\ \mathbf{l}_1\mathbf{k}_1 & t_2s_0\end{pmatrix}_{\beta\alpha}\Big]$$
$$+\frac{1}{2}\sum_{\substack{\alpha\\ \beta\neq\alpha}}\sum_{\mathbf{k}_1\mathbf{k}_3}\sum_{\mathbf{l}_1\mathbf{l}_3}\int_0^{\beta}dt_0\,ds_2\,ds_0\int_0^{t_0}dt_2\,\epsilon_\alpha\epsilon_\beta$$
$$\times\Big[L_{\mathrm{C}}^{(2)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & t_2s_0\\ \mathbf{l}_2\mathbf{k}_3 & t_0s_2\end{pmatrix}_{\alpha\beta}\mathfrak{L}_{\mathrm{E},(t_0)}^{(2)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 & t_0s_2\\ \mathbf{k}_1\mathbf{l}_1 & t_2s_0\end{pmatrix}_{\alpha\beta}$$
$$+L_{\mathrm{E}}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 & t_2s_0\\ \mathbf{l}_2\mathbf{k}_3 & t_0s_2\end{pmatrix}_{\alpha\beta}\mathfrak{L}_{\mathrm{E},(t_0)}^{(--)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 & t_0s_2\\ \mathbf{k}_1\mathbf{l}_1 & t_2s_0\end{pmatrix}_{\alpha\beta}\Big], \tag{133}$$

$$\mathfrak{L}''_{\mathrm{C}}\equiv\frac{1}{2}\sum_{\alpha,\beta}\sum_{\mathbf{k}_1\mathbf{k}_3}\int_0^{\beta}dt_0\,ds_0\,L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 & t_0s_0\\ \mathbf{k}_1\mathbf{k}_3 & t_0s_0\end{pmatrix}_{\alpha\beta}$$
$$+\frac{1}{2}\sum_{\alpha}\epsilon_\alpha\sum_{\mathbf{k}_1}\int_0^{\beta}dt_1\,ds_0\Big\{L'_{\mathrm{C},\alpha}(s_0,\,t_1,\mathbf{k}_1)\mathfrak{L}_{\mathrm{C},\alpha}(t_1,s_0,\mathbf{k}_1)$$
$$+\Big[\sum_{\beta}\sum_{\mathbf{k}_3}\int_0^{\beta}dt_0L_{\mathrm{C}}\begin{pmatrix}\mathbf{k}_3\mathbf{k}_1 & t_0s_0\\ \mathbf{k}_3\mathbf{k}_1 & t_0t_1\end{pmatrix}_{\beta\alpha}\Big]\mathfrak{L}_{\mathrm{C},\alpha}^{(-)}(t_1,\,s_0,\,\mathbf{k}_1)\Big\}. \tag{134}$$

The complete explicit expression for $\mathfrak{L}_{\mathrm{C}}$ is

$$\mathfrak{L}_{\mathrm{C}}=\mathfrak{L}'_{\mathrm{C}}+\mathfrak{L}''_{\mathrm{C}}, \tag{135}$$

where in the master-graph formulation of quantum statistics

$$\mathfrak{L}_{\mathrm{C}}\to\mathfrak{L}'_{\mathrm{C}}+\frac{1}{2}\sum_{\alpha,\beta}\sum_{\mathbf{k}_1\mathbf{k}_3}\int_0^{\beta}dt_0\,{}^{t_0t_0}\Big\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_1\mathbf{k}_3\end{matrix}\Big\rangle_{t_0}^{\alpha\beta}, \tag{135a}$$

because the remaining part of $\mathfrak{L}''_{\mathrm{C}}$ is composed of reducible graphs.

The diagrammatic representations of Eqs. (133) and (134) are given in Fig. 10. It should be observed

that in Eq. (133) we have set τ of Eqs. (110)–(131) equal to t_0. By referring to Figs. 8 and 10, we can see that it is always possible to specify which temperature variables should be integrated only from 0 to t_0. These are the temperature variables at the left end of an L_C or an $\mathfrak{L}_C$ and the right end of an L_E or an $\mathfrak{L}_E$.

In order to demonstrate that Eqs. (133)–(135) give the correct expression for $\mathfrak{L}_C$, including the correct symmetry numbers, one must make use of the following identity: If $f(t_1, t_2, \cdots, t_m)$ is a cyclic function in the m temperature variables, then

$$\frac{1}{m}\int_0^\beta dt_m \int_0^\beta dt_{m-1} \cdots \int_0^\beta dt_1 f(t_1, t_2, \cdots, t_m) = \int_0^\beta dt_m \int_0^{t_m} dt_{m-1} \int_0^{t_m} dt_{m-2} \cdots \int_0^{t_m} dt_1 \times f(t_1, t_2, \cdots, t_m). \quad (136)$$

We observe that none of the L_C or L_E functions in the second two terms of (133), or in Eqs. (121), carries a subscript $\tau = t_0$, a fact which should be clear from symmetry considerations.

IX. STUDY OF THE FUNCTIONS L_C AND L_E

In the preceding section, we have set down a formalism for the systematic analysis of the effect of Coulomb interactions in a many-body system with charged particles. We have shown that the three principle functions of Fig. 7, i.e., $\mathfrak{L}_C^{(S)}$, $\mathfrak{L}_{C,\alpha}$, and $\mathfrak{L}_C$, can each be calculated entirely in terms of the functions L_C and L_E defined by Eqs. (110) and (111). In this section, we examine these latter two functions in detail.

Each vertex in a ring, Fig. 5, which corresponds to two identical particles, is associated with both a *direct* and an *exchange* interaction matrix element. If the particles are not identical, the vertex is associated with only one or the other of these matrix elements. Thus, the vertices in L_E, Eq. (111), are all associated with exchange matrix elements (see Fig. 6).

One observes that in a typical ring chain in L_C identical particles will occasionally interact at vertices along the chain. The product of matrix elements corresponding to such a chain may look like

$$(D_{\alpha\beta})(D_{\beta\eta})(D_{\eta\eta} + E_{\eta\eta})(D_{\eta\eta} + E_{\eta\eta}) \times (D_{\eta\xi})(D_{\eta\eta})(D_{\xi\xi} + E_{\xi\xi}) \cdots,$$

where $D_{\alpha\alpha}$ and $E_{\alpha\alpha}$ are, respectively, direct and exchange matrix elements for α particles. Therefore, each chain in L_C can essentially be written as a sum of identical ring chains, but with different matrix elements at some of the vertices. We see that it is possible to have chains of all direct matrix elements, chains of all exchange matrix elements, and chains of all possible combinations of the two.

We begin this section by separating the contributions from the direct and exchange matrix elements in L_C, Eq. (110). To this end we first define the function L_D by an integral equation involving only direct matrix elements [indicated by a superscript (d)]

$$L_{D,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} \equiv {}^{t_1s_1}\left\langle \begin{matrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\right\rangle_{\alpha\beta}^{(d)}{}_{t_0} \delta(t_0 - s_0) + \sum_\eta \epsilon_\eta \sum_{l_1 l_2} \int_0^\tau dt_2 \, {}^{t_1t_2}\left\langle \begin{matrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{matrix}\right\rangle_{\alpha\eta}^{(d)}{}_{t_0} L_{D,(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}_{\eta\beta}\begin{vmatrix} t_0s_1 \\ t_2s_0\end{vmatrix}$$

$$\underset{\tau\to\beta}{\longrightarrow} L_{D,(\beta)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} \equiv L_D\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix}. \quad (137)$$

We next define two functions G_{DE} and G_{ED} by integral equations,

$$G_{DE,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} \equiv L_{DE,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} + \sum_\eta \epsilon_\eta \sum_{l_1 l_2} \int_0^\tau dt_2 \, ds_2 \, L_{DE,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{pmatrix}_{\alpha\eta}\begin{vmatrix} t_1t_2 \\ t_0s_2\end{vmatrix} \times G_{DE,(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}_{\eta\beta}\begin{vmatrix} s_2s_1 \\ t_2s_0\end{vmatrix}, \quad (138)$$

$$G_{ED,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} \equiv L_{ED,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} + \sum_\eta \epsilon_\eta \sum_{l_1 l_2} \int_0^\tau dt_2 \, ds_2 \, L_{ED,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{pmatrix}_{\alpha\eta}\begin{vmatrix} t_1t_2 \\ t_0s_2\end{vmatrix} \times G_{ED,(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{l}_1\mathbf{k}_4\end{pmatrix}_{\eta\beta}\begin{vmatrix} s_2s_1 \\ t_2s_0\end{vmatrix}, \quad (139)$$

where

$$L_{DE,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_3 \\ \mathbf{k}_2\mathbf{k}_4\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1s_1 \\ t_0s_0\end{vmatrix} \equiv \sum_{l_1 l_2} \int_0^\tau dt_2 \, ds_2 \, L_{D,(\tau)}\begin{pmatrix}\mathbf{k}_1\mathbf{l}_1 \\ \mathbf{k}_2\mathbf{l}_2\end{pmatrix}_{\alpha\beta}\begin{vmatrix} t_1t_2 \\ t_0s_2\end{vmatrix} \times L_{E,(\tau)}\begin{pmatrix}\mathbf{l}_2\mathbf{k}_3 \\ \mathbf{k}_4\mathbf{l}_1\end{pmatrix}_{\beta\beta}\begin{vmatrix} s_2s_1 \\ s_0t_2\end{vmatrix}, \quad (140)$$

$$L_{\mathrm{ED},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} \equiv \sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\tau dt_2\,ds_2\,L_{\mathrm{E},(\tau)}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{l}_2\mathbf{k}_2\end{matrix}\middle|\begin{matrix}t_1t_2\\ s_2t_0\end{matrix}\right)} \times L_{\mathrm{D},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{l}_2\mathbf{k}_3\\ \mathbf{l}_1\mathbf{k}_4\end{matrix}\middle|\begin{matrix}s_2s_1\\ t_2s_0\end{matrix}\right)}. \tag{141}$$

We note that one must use only direct matrix elements in the expressions for L_{E} to be used in Eqs. (140) and (141), because exchange has already been explicitly included by the notation of Eq. (111).

It is now possible to write down a detailed equation for L_{C} in terms of L_{D} and L_{E},

$$L_{\mathrm{C},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} = L_{\mathrm{D},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} + \epsilon_\alpha\delta_{\alpha\beta}L_{\mathrm{E},(\tau)}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_4\mathbf{k}_2\end{matrix}\middle|\begin{matrix}t_1s_1\\ s_0t_0\end{matrix}\right)} + G_{\mathrm{C},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)}, \tag{142}$$

where

$$G_{\mathrm{C},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} \equiv G_{\mathrm{DE},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} + G_{\mathrm{ED},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} + \sum_\eta\epsilon_\eta\sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\tau dt_2\,ds_2 \times L_{\mathrm{D},(\tau)}\underset{\alpha\eta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{k}_2\mathbf{l}_2\end{matrix}\middle|\begin{matrix}t_1t_2\\ t_0s_2\end{matrix}\right)}G_{\mathrm{ED},(\tau)}\underset{\eta\beta}{\left(\begin{matrix}\mathbf{l}_2\mathbf{k}_3\\ \mathbf{l}_1\mathbf{k}_4\end{matrix}\middle|\begin{matrix}s_2s_1\\ t_2s_0\end{matrix}\right)} + \sum_{\mathbf{l}_1\mathbf{l}_2}\int_0^\tau dt_2\,ds_2\,L_{\mathrm{E},(\tau)}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{l}_1\\ \mathbf{l}_2\mathbf{k}_2\end{matrix}\middle|\begin{matrix}t_1t_2\\ s_2t_0\end{matrix}\right)}G_{\mathrm{DE},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{l}_2\mathbf{k}_3\\ \mathbf{l}_1\mathbf{k}_4\end{matrix}\middle|\begin{matrix}s_2s_1\\ t_2s_0\end{matrix}\right)}. \tag{143}$$

Equation (142) for L_{C} can easily be verified by observing that it includes all possible ways of alternating direct and exchange matrix elements.

We have now shown that the principle vertex functions $\mathfrak{L}_{\mathrm{C}}^{(\mathrm{S})}$, $\mathfrak{L}_{\mathrm{C},\alpha}$, and $\mathfrak{L}_{\mathrm{C}}$ can each be calculated entirely in terms of the functions L_{D} and L_{E}, defined by Eqs. (137) and (111), respectively. We show below that it is the function L_{D} which includes the extremely singular terms discussed below Eq. (109). Moreover, the leading contributions (in powers of e) to the principle vertex functions arise from the L_{D} terms in L_{C} and $L_{\mathrm{E}}^{(2)}$. We therefore next write the first approximations to these functions. From Eqs. (119)–(122), we have for $\mathfrak{L}_{\mathrm{C}}^{(\mathrm{S})}$

$$\mathfrak{L}_{\mathrm{C}}^{(\mathrm{S})}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} \cong L_{\mathrm{D}}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} + \epsilon_\alpha\delta_{\alpha\beta}L_{\mathrm{D}}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_4\mathbf{k}_2\end{matrix}\middle|\begin{matrix}t_1s_1\\ s_0t_0\end{matrix}\right)}. \tag{144}$$

From Eqs. (126)–(128) and (113), we have for $\mathfrak{L}_{\mathrm{C},\alpha}$

$$\mathfrak{L}_{\mathrm{C},\alpha}(t_1,\,t_0,\,\mathbf{k}_1) \cong \sum_\beta\sum_{\mathbf{k}_3}\int_0^\beta ds_0\Bigg[L_{\mathrm{D}}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_1\mathbf{k}_3\end{matrix}\middle|\begin{matrix}t_1s_0\\ t_0s_0\end{matrix}\right)} + \epsilon_\alpha\delta_{\alpha\beta}L_{\mathrm{D}}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_3\mathbf{k}_1\end{matrix}\middle|\begin{matrix}t_1s_0\\ s_0t_0\end{matrix}\right)}\Bigg], \tag{145}$$

where in the master-graph formulation this approximation becomes

$$\mathfrak{L}_{\mathrm{C},\alpha}(t_1,\,t_0,\,\mathbf{k}_1) \cong \sum_\beta\sum_{\mathbf{k}_3}\Bigg[{}^{t_1t_0}\underset{\alpha\beta}{\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_1\mathbf{k}_3\end{matrix}\right\rangle}^{(\mathrm{D})}_{t_0} + \epsilon_\alpha\delta_{\alpha\beta}\int_0^\beta ds_0\,L_{\mathrm{D}}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_3\mathbf{k}_1\end{matrix}\middle|\begin{matrix}t_1s_0\\ s_0t_0\end{matrix}\right)}\Bigg]. \tag{145a}$$

Finally, Eqs. (133)–(135) give for the first approximation to $\mathfrak{L}_{\mathrm{C}}$

$$\mathfrak{L}_{\mathrm{C}} \cong \frac{1}{2}\sum_{\alpha,\beta}\sum_{\mathbf{k}_1\mathbf{k}_3}\int_0^\beta dt_0\Bigg[\int_0^\beta ds_0\,L_{\mathrm{D}}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_1\mathbf{k}_3\end{matrix}\middle|\begin{matrix}t_0s_0\\ t_0s_0\end{matrix}\right)} + \epsilon_\alpha\delta_{\alpha\beta}\int_0^{t_0} ds_0\,L_{\mathrm{D},(t_0)}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_3\mathbf{k}_1\end{matrix}\middle|\begin{matrix}t_0s_0\\ s_0t_0\end{matrix}\right)}\Bigg], \tag{146}$$

which becomes in the master-graph formulation

$$\mathfrak{L}_{\mathrm{C}} \cong \frac{1}{2}\sum_{\alpha,\beta}\sum_{\mathbf{k}_1\mathbf{k}_3}\int_0^\beta dt_0\Bigg[{}^{t_0t_0}\underset{\alpha\beta}{\left\langle\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_1\mathbf{k}_3\end{matrix}\right\rangle}^{(\mathrm{d})}_{t_0} + \epsilon_\alpha\delta_{\alpha\beta}\int_0^{t_0} ds_0\,L_{\mathrm{D},(t_0)}\underset{\alpha\alpha}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_3\mathbf{k}_1\end{matrix}\middle|\begin{matrix}t_0s_0\\ s_0t_0\end{matrix}\right)}\Bigg]. \tag{146a}$$

We next investigate the three functions L_{D}, L_{E}, and L_{db} [Eq. (125)] in greater detail by using the explicit expression (108) for the Coulomb-interaction matrix element. From Eqs. (137), (98), (91), and (38), we have for L_{D}

$$L_{\mathrm{D},(\tau)}\underset{\alpha\beta}{\left(\begin{matrix}\mathbf{k}_1\mathbf{k}_3\\ \mathbf{k}_2\mathbf{k}_4\end{matrix}\middle|\begin{matrix}t_1s_1\\ t_0s_0\end{matrix}\right)} = -(2\pi)^6\Omega^{-2}\delta^{(3)}(\mathbf{k}_1+\mathbf{k}_3-\mathbf{k}_2-\mathbf{k}_4)\delta_{m_1m_2}\delta_{m_3m_4} \times \frac{Z_\alpha Z_\beta e^2}{2\pi^2q^2}\epsilon_\alpha\epsilon_\beta\int_0^\beta dt_1'\,ds_1'\,\mathcal{G}_\alpha(t_1,\,t_1',\,\mathbf{k}_1)\,\mathcal{G}_\beta(s_1,\,s_1',\,\mathbf{k}_3)$$

$$\times \theta(t_1' - t_0)\theta(s_1' - s_0) \exp t_0[\omega_\alpha(k_1) - \omega_\alpha(k_2)]$$
$$\times L_{\mathrm{D},(\tau)}(q \mid t_0 s_0) \exp s_0[\omega_\beta(k_3) - \omega_\beta(k_4)], \quad (147)$$

where

$$L_{\mathrm{D},(\tau)}(q \mid t_0 s_0) = \delta(t_0 - s_0) - \tfrac{1}{2} \sum_\eta \epsilon_\eta (2S_\eta + 1)$$
$$\times \left(\frac{Z_\eta e}{\pi q}\right)^2 \int d^3 l_2 \int_0^\tau dt_2 \int_0^\beta dt_1'' \, ds_1''$$
$$\times \mathcal{G}_\eta(t_2, t_1'', \mathbf{l}_2 - \mathbf{q}) \mathcal{G}_\eta(t_0, s_1'', \mathbf{l}_2) \theta(t_1'' - t_0)\theta(s_1'' - t_2)$$
$$\times \{\exp (t_0 - t_2)[\omega_\eta(\mathbf{l}_2 - \mathbf{q}) - \omega_\eta(l_2)]\} L_{\mathrm{D},(\tau)}(q \mid t_2 s_0). \quad (148)$$

Similarly, Eq. (111) for L_{E} can be written as

$$L_{\mathrm{E},(\tau)}\begin{pmatrix} \mathbf{k}_1 \mathbf{k}_3 \\ \mathbf{k}_2 \mathbf{k}_4 \end{pmatrix} \begin{vmatrix} t_1 s_1 \\ t_0 s_0 \end{pmatrix}_{\alpha\beta}$$
$$= -(2\pi)^6 \Omega^{-2} \delta^{(3)}(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_2 - \mathbf{k}_4) \delta_{m_1 m_2} \delta_{m_3 m_4}$$
$$\times \frac{Z_\alpha Z_\beta e^2}{2\pi^2 q^2} \epsilon_\alpha \epsilon_\beta \int_0^\beta dt_1' \, ds_1' \mathcal{G}_\alpha(t_1, t_1', \mathbf{k}_1) \mathcal{G}_\beta(s_1, s_1', \mathbf{k}_3)$$
$$\times \theta(t_1' - s_0)\theta(s_1' - t_0) \exp s_0[\omega_\alpha(k_1) - \omega_\beta(k_4)]$$
$$\times L_{\mathrm{E},(\tau)}(\mathbf{k}_1, \mathbf{q}, \mathbf{K} \mid t_0 s_0)_{\alpha\beta} \exp t_0[\omega_\beta(k_3) - \omega_\alpha(k_2)], \quad (149)$$

where $\mathbf{K} = \mathbf{k}_1 - \mathbf{k}_4$, and

$$L_{\mathrm{E},(\tau)}(\mathbf{k}_1, \mathbf{q}, \mathbf{K} \mid t_0 s_0)_{\alpha\beta} = \delta(t_0 - s_0)$$
$$- \tfrac{1}{2}(Z_\alpha Z_\beta e^2/\pi^2) \int d^3 l_2 \int_0^\tau ds_2 \int_0^\beta dt_1'' \, ds_1''$$
$$\times \mathcal{G}_\beta(s_2, t_1'', \mathbf{l}_2 - \mathbf{K}) \mathcal{G}_\alpha(s_0, s_1'', \mathbf{l}_2)$$
$$\times \theta(t_1'' - s_0)\theta(s_1'' - s_2)(\mathbf{l}_2 - \mathbf{k}_1)^{-2}(\mathbf{l}_2 - \mathbf{k}_1 + \mathbf{q})^{-2} q^2$$
$$\times \exp (s_0 - s_2)[\omega_\beta(\mathbf{l}_2 - \mathbf{K}) - \omega_\alpha(l_2)]$$
$$\times L_{\mathrm{E},(\tau)}(\mathbf{l}_2, \mathbf{l}_2 + \mathbf{q} - \mathbf{k}_1, \mathbf{K} \mid t_0 s_2)_{\alpha\beta}. \quad (150)$$

Finally, we may write for L_{db}, Eq. (125),

$$L_{\mathrm{db}}\begin{pmatrix} \mathbf{k}_1 \mathbf{k}_3 \\ \mathbf{k}_2 \mathbf{k}_4 \end{pmatrix} \begin{vmatrix} t_1 s_1 \\ t_0 s_0 \end{pmatrix}_{\alpha\beta}$$
$$= (1 - \tfrac{1}{2}\delta_{\alpha\beta})(2\pi)^6 \Omega^{-2} \delta^{(3)}(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_2 - \mathbf{k}_4) \epsilon_\alpha \epsilon_\beta$$
$$\times \left(\frac{Z_\alpha Z_\beta e^2}{2\pi^2}\right)^2 \int d^3 l_2 \int_0^\beta dt_1' \, ds_1' \, dt_1'' \, ds_1'' \mathcal{G}_\alpha(t_1, t_1', \mathbf{k}_1)$$
$$\times \theta(t_1' - s_0) \mathcal{G}_\beta(s_1, s_1', \mathbf{k}_3) \theta(s_1' - t_0)$$
$$\times \mathcal{G}_\beta(t_0, t_1'', \mathbf{l}_2 - \mathbf{K}) \theta(t_1'' - s_0)$$
$$\times \mathcal{G}_\alpha(s_0, s_1'', \mathbf{l}_2) \theta(s_1'' - t_0)$$
$$\times \exp s_0[\omega_\alpha(k_1) - \omega_\beta(k_4)]$$
$$\times \exp (s_0 - t_0)[\omega_\beta(\mathbf{l}_2 - \mathbf{K}) - \omega_\alpha(l_2)]$$
$$\times \exp t_0[\omega_\beta(k_3) - \omega_\alpha(k_2)]$$
$$\times \{\delta_{m_1 m_2} \delta_{m_3 m_4} (\mathbf{l}_2 - \mathbf{k}_1)^{-2}(\mathbf{l}_2 - \mathbf{k}_1 + \mathbf{q})^{-2}$$
$$+ \delta_{\alpha\beta} \delta_{m_1 m_4} \delta_{m_2 m_3} K^{-2}[(2S_\alpha + 1)K^{-2}$$
$$+ \epsilon_\alpha (\mathbf{l}_2 - \mathbf{k}_1)^{-2} + \epsilon_\alpha (\mathbf{l}_2 - \mathbf{k}_1 + \mathbf{q})^{-2}]\}. \quad (151)$$

In the application of the above explicit expressions, one must observe that $\mathbf{q} = 0$ in the integrands of $\mathfrak{L}_{\mathrm{C},\alpha}$ and $\mathfrak{L}_{\mathrm{C}}$. As we shall see, however, L_{D} is well defined at $\mathbf{q} = 0$. Moreover, the leading term of L_{E} has already been included in the second terms of (144)–(146). Thus, one is led to examine q^{-2} times the second term in the iteration of (150). One sees that at $\mathbf{q} = 0$, there is a singularity in the integrand at $\mathbf{l}_2 = \mathbf{k}_1$. One then finds that this singularity is precisely cancelled by corresponding singularities in L_{db} when these terms are substituted into Eqs. (127) or (133). Singularities at $\mathbf{q} = 0$ in the higher-order terms of L_{E} have not yet been examined.

Applications; High-Temperature, Low-Density Limit

The value of any theory, of course, is in the new results to which it can lead. Detailed application of the above equations to any real system in a particular temperature-density range is fairly lengthy, but it is in order to briefly mention some of the problems to which the foregoing theory can readily be applied. In the general ionized gas one must consider as constituents electrons, ions (in different stages of ionization), neutral atoms, and photons. [As we have seen, if other types of nonconserved particles are important in a system they are easily included in the above formalism, and external fields have formally been included in Eq. (23).[18]] The major difficulties arising from the Coulomb interactions among ions and electrons have been treated above, and the lowest-order contribution from the nonring interaction of charged particles is probably of order e^6. Nonring diagrams are contained in the function $F(\beta, N_\alpha, \Omega)$ of Eq. (107).

In the consideration of a partially ionized gas one must examine the contribution to the thermodynamic quantities from the internal states of ions and atoms. As noted previously, sums over internal states are included implicitly in the formalism, but several subtle questions relating to the calculation of these bound-state contributions remain to be answered. There is reason to believe that some of these questions are intimately related to the calculation of nonring diagrams, so that this "bound-state problem" is one of those under present investigation. One result of subsequent studies via our formalism will be corrections to the Saha equation.

In Sec. IV we have paved the way for including radiative corrections to all diagrams involving charged particles, which is a necessary step toward including all possible effects due to photon interactions in the ionized gas. One should observe, also, that other photon–charged particle interactions are included in Eqs. (71) and (106), besides those of Sec. IV. The systematic study of these terms, along with a study of the photon momentum distribution, is an important investigation which should be undertaken as soon as possible. Completion of such a study should, for example, lend insight into higher-order corrections to Planck's law.

Finally, there are two limiting cases which are of immediate interest. The low-temperature, high-density electron gas has been studied previously, resulting in the expression of Gell-Mann and Brueckner.[34] The present formalism can be used along the lines of II to study this limit further, and an extension in this direction would be very desirable. In the opposite limit of high temperature and low density, one encounters the case of fully ionized gases. Others have previously calculated the lowest-order contributions to the grand potential in this limit, but we calculate it again both to illustrate the use of the preceding equations and to demonstrate the reduction of our expressions to a known result. In this limit we not only restrict contributions to those from ring diagrams, but also we approximate the sum over all ring diagrams by Eq. (146). This implies that we ignore complications such as internal states and photons.

One may approximately solve the integral equation (148) for L_D in the high-temperature, low-density limit. The criteria which we adopt for this limit is that

$$\lambda_\alpha \ll l_\alpha \ll \lambda_{(D)}, \tag{152}$$

where λ_α is the thermal wave length, Eq. (16), for α particles, l_α is related to the density ρ_α of α particles by $\rho_\alpha = l_\alpha^{-3}$, and $\lambda_{(D)}$ is the *Debye length* defined by

$$\lambda_{(D)} = (4\pi e^2\beta \sum_\alpha \rho_\alpha Z_\alpha^2)^{-\frac{1}{2}}. \tag{153}$$

We use the linked-pair formulation (Sec. V) of quantum statistics, rather than the master-graph formulation, in this limit. This is equivalent to writing the functions $\mathcal{G}_\alpha$ in Eq. (148) as

$$\mathcal{G}_\alpha(t_2, t_1, \mathbf{k}) = \delta(t_2 - t_1) + \epsilon_\alpha \nu_\alpha(\mathbf{k})\delta(\beta - t_1). \tag{154}$$

We may then approximate $\mathcal{G}_\alpha$ in the region (152) by

$$\mathcal{G}_\alpha(t_2, t_1, \mathbf{k}) \cong \delta(t_2 - t_1) + \epsilon_\alpha \vartheta_\alpha \delta(\beta - t_1) \times \exp[-\beta\omega_\alpha(k)], \tag{154a}$$

because in this limit.

$$\vartheta_\alpha \equiv \exp(\beta g_\alpha) \cong (2S_\alpha + 1)^{-1}\rho_\alpha\lambda_\alpha^3 \times \{1 - \tfrac{1}{2}\beta(Z_\alpha e)^2\lambda_{(D)}^{-1}\} \ll 1, \tag{155}$$

as we show below.

With the aid of the approximations (152) and (154a), one can show that Eq. (148) can be written as

$$L_{D,(\tau)}(q \mid t_0 s_0) \cong \delta(t_0 - s_0) - \pi \sum_\eta (2S_\eta + 1)\vartheta_\eta\lambda_\eta^{-3}(2Z_\eta e/q)^2 \times \int_0^\tau dt_2\, L_{D,(\tau)}(q \mid t_2 s_0). \tag{156}$$

In deriving Eq. (156), we have used the fact that $[L_D - \delta(t_0 - s_0)]$ is appreciable only when $q \lesssim \lambda_{(D)}^{-1}$, a result which follows from the solution to (156),

$$L_{D,(\tau)}(q \mid t_0 s_0) = \delta(t_0 - s_0) - \beta^{-1}\theta'(\tau - s_0)[(\tau/\beta) + (q\lambda'_{(D)})^2], \tag{157}$$

where $\theta'(t - s)$ differs from the step functions introduced in Sec. IV by requiring that it be unity when $t = s$, and

$$\lambda'_{(D)} = [4\pi e^2\beta \sum_\alpha (2S_\alpha + 1)\vartheta_\alpha Z_\alpha^2\lambda_\alpha^{-3}]^{-\frac{1}{2}} \cong \lambda_{(D)}. \tag{158}$$

With Eq. (157), we have demonstrated that in the region (152) L_D is not divergent at $\mathbf{q} = 0$. Moreover, the Debye length $\lambda_{(D)}$ can be identified as the screening length for the Coulomb interaction in any charged particle many-body system characterized by (152), [see discussion following (109)]. This latter statement becomes clearer when one substitutes Eqs. (147) and (157) into Eq. (145) for $\mathcal{L}_{C,\alpha}$. The result is

$$\begin{aligned}\mathcal{L}_{C,\alpha}(t_1, t_0, \mathbf{k}_1) \cong\ & -\epsilon_\alpha Z_\alpha\{\theta(t_1 - t_0) + \epsilon_\alpha\vartheta_\alpha \exp[-\beta\omega_\alpha(k_1)]\} \\ & \times \sum_\beta (2S_\beta + 1)\frac{Z_\beta e^2}{2\pi^2}\vartheta_\beta \int d^3\mathbf{k}_3 \exp[-\beta\omega_\beta(k_3)] \\ & \times \int_0^\beta ds_0[q^{-2}L_D(q \mid t_0 s_0)]_{q=0} - \epsilon_\alpha \frac{Z_\alpha^2 e^2}{2\pi^2}\int_0^\beta ds_0 \\ & \times \{\theta(t_1 - s_0) + \epsilon_\alpha\vartheta_\alpha \exp[-\beta\omega_\alpha(k_1)]\} \\ & \times \int d^3\mathbf{k}_3 \exp(s_0 - t_0)[\omega_\alpha(k_1) - \omega_\alpha(k_3)]\{\theta(s_0 - t_0) \\ & + \epsilon_\alpha\vartheta_\alpha \exp[-\beta\omega_\alpha(k_3)]\}K^{-2}L_D(K \mid s_0 t_0)\end{aligned}$$

[34] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

$$\cong -4\pi\epsilon_\alpha Z_\alpha e^2\lambda_{(D)}^2 \sum_\beta \rho_\beta Z_\beta[1 - \tfrac{1}{2}\beta(Z_\beta e)^2\lambda_{(D)}^{-1}]$$

$$+ 2(\pi\beta)^{-1}\epsilon_\alpha(Z_\alpha e)^2 \int_{t_0}^{t_1} ds_0 \int_0^\infty dK[1 + (K\lambda_{(D)})^2]^{-1}$$

$$\times \exp[-(s_0 - t_0)\omega_\alpha(K)] - 2\vartheta_\alpha(Z_\alpha e)^2\lambda_\alpha^{-1}\theta(t_1 - t_0)$$

$$\cong 2\pi\beta\lambda_{(D)}\epsilon_\alpha Z_\alpha e^4\theta(t_1 - t_0) \sum_\beta \rho_\beta Z_\beta^3$$

$$+ \epsilon_\alpha(Z_\alpha e)^2\lambda_{(D)}^{-1}\theta(t_1 - t_0)(t - t_0)/\beta, \qquad (159)$$

where we have used Eq. (155) in the second set of terms, and the fact that $\Sigma_\alpha \rho_\alpha Z_\alpha = 0$ for a neutral system. According to Fig. 7, one may interpret $\mathcal{L}_{C,\alpha}$ as an "effective" single-particle potential energy, and therefore, the above result shows that this effective energy is $\sim e^2/\lambda_{(D)}$ in the region (152).

One may finally evaluate Eq. (146) in the high-temperature, low-density limit. The result is

$$\Omega^{-1}\mathcal{L}_C \cong [12\pi(\lambda'_{(D)})^3]^{-1}, \qquad (160)$$

where $\lambda'_{(D)}$ is defined by Eq. (158). According to Eqs. (71) and (77), an approximate expression for the grand potential in the region (152) is then

$$f \cong \sum_\alpha (2S_\alpha + 1)\vartheta_\alpha\lambda_\alpha^{-3} + \Omega^{-1}\mathcal{L}_C. \qquad (161)$$

Equation (155) can now be verified by substituting (161) into Eq. (7). Finally, we may use Eq. (6) to derive for the pressure of an ionized gas

$$\mathcal{P} \cong \beta^{-1}\rho[1 - (24\pi\rho\lambda_{(D)}^3)^{-1}], \qquad (162)$$

which is the well-known result of Debye and Hückel.[35]

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Quantum Mechanics of a Many-Boson System and the Representation of Canonical Variables*

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We present a method of treating the assembly of interacting bosons under Bose–Einstein condensation. Without applying the Bogoliubov approximation in which the creation and the annihilation operators of zero-momentum particles are replaced by a c number, we keep the quantum nature of these operators—thus the title, "Quantum Mechanics." The method is a quantum mechanical adaptation of the theory of small oscillation. The oscillation means the fluctuation of the number of condensed particles. The interaction between particles determines the stability of this oscillation. When it is stable and its amplitude is not macroscopic, the Bogoliubov approximation is valid. In this way, our method provides a validity criterion for the Bogoliubov approximation as well as an estimation of the errors thereby committed. We have to note that the excitations associated with the fluctuation of condensed particles can never be obtained within that approximation. Our method is applied to the Huang model, the assembly of bosons interacting through a hard core plus weak attractive potential. Having found that, within the physically accessible range of the particle density, the above-mentioned oscillation is stable, we can conclude that Huang's treatment is well founded. We have discussed the mathematical background of our approximation by invoking the representation theory of canonical variables of an infinitely large system.

I. INTRODUCTION

WHEN we consider the many-body problem of bosons, the standard procedure is to apply the Bogoliubov method of approximation,[1,2,3] in which, taking advantage of the macroscopic occupation of the lowest single-particle level, we replace the corresponding creation and annihilation operators, $a_0^\dagger$ and a_0, by a c number $N_0^{\frac{1}{2}}$, the square root of the occupation number of the level.

It is very long since the approximation was invented and the method has been applied to various problems yielding physically reasonable results.[4,5]

However, as Yang and Huang noticed in their paper,[3,4] the approximation has been justified merely by the consistency of the procedure and the consistency does not necessarily mean the correctness. In particular, there has not been known any method for estimating the errors committed. Recently, Foldy and Bassichis[6] have examined a soluble model of one-dimensional Bose gas to show that, under some circumstances, the macroscopic occupation of the lowest single-particle level is destroyed by the interaction between particles thus invalidating the Bogoliubov approximation. It is now urgent to establish some validity criterions for the approximation.

In the work of Bogoliubov and also in those of the others, the c-number replacement of the creation and annihilation operators was motivated by a physical intuition. In this paper, however, we are going to pave the way to the Bogoliubov approximation by the orthodox machineries of quantum mechanics throughout. The operators, $a_0^\dagger$ and a_0, will not be replaced by a c number but by $N_0^{\frac{1}{2}} + a_0^{\mathrm{F}\dagger}$ and $N_0^{\frac{1}{2}} + a_0^{\mathrm{F}}$, respectively, which are in fact operators obeying the canonical commutation relations; we require, say, $[a_0^{\mathrm{F}}, a_0^{\mathrm{F}\dagger}] = 1$ so that $[N_0^{\frac{1}{2}} + a_0^{\mathrm{F}}, N_0^{\frac{1}{2}} + a_0^{\mathrm{F}\dagger}] = 1$. Needless to say, these replacements do not involve any approximation at all.

Then, our method of approximation is to construct a quantum analog of the method of small oscillation in the classical mechanics. In the above replacements, $N_0^{\frac{1}{2}}$ stands for the equilibrium position around which the many-body system undergoes the small fluctuation to be described by $a_0^{\mathrm{F}\dagger}$ and a_0^{F}. The approximation consists in expanding the Hamiltonian in powers of $a_0^{\mathrm{F}\dagger}$ and a_0^{F}. The mode of the fluctuation is determined by the interaction between particles. Sometimes, the fluctuation turns out to be of a harmonic-oscillator type with amplitude much smaller than $N_0^{\frac{1}{2}}$, when the Bogoliubov approxima-

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[4] K. Huang, Phys. Rev. **115**, 765 (1959). As for the discussion on the validity of the approximation, see Sec. V of this paper.

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tion is valid. But, depending upon the interaction, the fluctuation can be unstable so that the amplitude grows larger and larger to compensate the background occupation N_0. In this case, the assumption of the macroscopic occupation is not valid and the Bogoliubov approximation fails. In this way, we obtain the validity criterion for the approximation in terms of the interaction between particles. The errors induced by the approximation can also be estimated.

Two interesting features appear when we consider the limit of infinitely large system. First, some of the terms in the expanded Hamiltonian become exactly negligible under the condition that the fluctuation be not macroscopic. Second, we come across the theory of inequivalent representations of the canonical commutation relations[7] to see the above replacement is imperative if we want to deal with an irreducible representation. In fact, when the occupation number N_0 is finite, the above replacement, $a_0 \to N_0^{\frac{1}{2}} + a_0^{\mathrm{F}}$, etc., can be effected by an unitary transformation. But, in the limit $N_0 \to \infty$, such a transformation does not exist at all and we have to construct a new representation suitable for the infinite system. At least in the case of free bosons, the requirement is met when we use the well-known Fock representation for $a_0^{\mathrm{F}\dagger}$ and a_0^{F} *after* the replacement. We shall see that some interesting questions arise concerning the conservation of particle number as well as the states with sharp particle number.

Now, in Sec. 2, the basic ideas will be explained. There, the model used for the illustration is the assembly of free bosons. In the sections thereafter, we shall take up the example of Huang model[4] in which the particles interact through a long-range attractive force with a hard core. For the sake of easy reference, we shall recapitulate the definition of the model in Sec. 3. Then, in Sec. 4 the "Hamiltonian" (the Hamiltonian with the chemical potential times the number operator subtracted) will be expanded according to the method of the small oscillation and the orders of magnitudes of each component will be estimated. In Sec. 5, the diagonalization of the "Hamiltonian" is carried out in the lowest-order approximation, in which we have to deal only with the particles of momenta larger than some critical value k_0 ($1/k_0$ is the range of the attractive potential). These sections, 3, 4, and 5, constitute a preparatory step for the further developments. In these sections, we claim nothing new except for the use of the chemical potential which is absolutely necessary for the adaptation of the method of small oscillation. But, it would be interesting to see how the chemical potential works and how our method compares with Huang's.

In Sec. 6, we reach the position to treat the fluctuation described by the operators $a_0^{\mathrm{F}\dagger}$ and a_0^{F}. The stability condition will be written down in terms of the parameters of the interparticle potential. This condition is called the $\mathbf{k} = 0$-stability condition. We find that the fluctuation cannot be stable if the attractive force is too strong. In the same spirit we treat the particles of momenta $\mathbf{k}$, $0 < |\mathbf{k}| < k_0$, in Sec. 7. Here, we obtain another stability condition which we call the $\mathfrak{R}_{\mathrm{I}}$ 0-stability condition. This condition is found to be equivalent to the statement that the sound velocity of the system be real.

On the basis of these calculations, we discuss the properties of the Huang system in Sec. 8. As stressed by Huang, the system possesses the equilibrium density ρ_{L} at which the energy is minimum. As far as the system is at temperature zero, the system cannot be brought into the state of density $\rho < \rho_{\mathrm{L}}$: If we try to expand the container, we shall see the system lump like a liquid drop (the neglect of the surface energy will be justified for a sufficiently large system). One of the most interesting conclusions of this paper is that both the $\mathbf{k} = 0$- and the $\mathfrak{R}_{\mathrm{I}}$-stability conditions are satisfied by the Huang system with the physically accessible density $\rho \geq \rho_{\mathrm{L}}$: In this sense, the use of the Bogoliubov approximation is completely justified for the Huang system at absolute-zero temperature.

What happens in the higher temperature is an open question. We believe that the same approximation scheme can be used without any difficulty to investigate the lower excited states. The stability conditions will be the most interesting subjects. From the point of view of the representation theory of the canonical commutation relations, however, the occurrence of many series of energy spectrum will be the most remarkable, because each series is found to belong to one of the many mutually inequivalent representations[8] of canonical commutation relations. The inequivalence accounts for the orthogonality between the states belonging to different series of the energy spectrum. Since we have invoked the chemical potential and its value can be different depending on which state is concerned, the orthogonality is not guaranteed in such an ordinary

[7] L. Gårding and A. S. Wightman, Proc. Natl. Acad. Sci. U. S. 40, 622 (1954); A. S. Wightman and S. S. Schweber, Phys. Rev. 98, 812 (1955).

[8] Each of them is labeled by the density N_0/V of the particles in the Bose–Einstein condensation.

way that the eigenvectors of one and the same Hermitian operator are orthogonal.

In Section 9, we discuss the mathematical background of our approximation scheme by generalizing the arguments given by Araki and Woods[9] for the case of the free Bose gas. We want to show that the replacement $a_0 \to N_0^{\frac{1}{2}} + a_0^{\mathrm{F}}$ is an inevitable consequence of our presumption of the Bose–Einstein condensation *if the system is infinitely large*. In order to prove this statement in its most general form, we have to compute the Wightman functional without any assumption but for the condensation. But, for the sake of a clear presentation, we shall be satisfied with treating some oversimplified models. We still believe that these models will be sufficient to indicate the realistic situation and then to show the necessity of the replacement. The point we emphasize here is the c-number addition as represented by $N_0^{\frac{1}{2}}$ in the above. The more elaborate discussion will be given elsewhere.

The concluding remarks are given in Sec. 10.

In Appendix I, we collect some useful formulas of the Bogoliubov transformation. In Appendix II, we compute the fluctuation of the particle number in the condensed state, on the basis of which the mathematical models in Sec. 9 will be constructed. Appendix III gives a derivation of the mathematical formula used in Sec. 9 together with its generalization.

II. BASIC IDEAS

Throughout this paper, we consider an assembly of Bose particles in a state of Bose–Einstein condensation. The Hamiltonian $\mathcal{H}$ of the system can be represented in terms of the creation and the annihilation operators, $a_{\mathbf{k}}^{\dagger}$ and $a_{\mathbf{k}}$ for the bosons of momentum $\mathbf{k}$:

$$\mathbf{k} = (2\pi/V^{\frac{1}{3}})(n_x, n_y, n_z), \qquad n_x = 0, \pm 1, \cdots, \text{etc.}, \tag{2.1}$$

where V is the volume of a cubic box containing the system.

In treating such a system, the nowadays standard procedure is to apply the approximation method developed by Bogoliubov,[1] Lee, Huang, and Yang[2]: By taking advantage of the fact that the individual particle level with zero momentum (hereafter, we call it the $\mathbf{k} = 0$-level) is occupied by a macroscopic number of particles we replace the corresponding operators, $a_0^{\dagger}$ and a_0, by a c number,

$$a_0^{\dagger}, a_0 \to N_0^{\frac{1}{2}}, \tag{2.2}$$

where N_0 is the occupation number of the $\mathbf{k} = 0$-level in the unperturbed state and "macroscopic" means that N_0 is proportional to the size V of the system, $N_0 = \rho_0 V$. In fact the matrix elements of operators are such that $(N_0 \pm 1)^{\frac{1}{2}} = N_0^{\frac{1}{2}} + O(1/N_0^{\frac{1}{2}})$ and the approximation has been quite successful.[4,5]

However, it is unsatisfactory that the fluctuation in number of the $\mathbf{k} = 0$-particles is neglected when the replacement (2.2) is done. The fluctuation is not necessarily of quantum origin but can be caused by the interaction between the $\mathbf{k} = 0$- and $\mathbf{k} \neq 0$-particles.[10]

Such a fluctuation due to interaction can partly be taken into account by adopting an additional prescription for the operators quadratic in $a_0^{\dagger}$ and/or a_0:

$$a_0^{\dagger}a_0^{\dagger},\ a_0^{\dagger}a_0,\ a_0a_0 \to N_0 - \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}, \tag{2.3}$$

as has been done by Lee, Huang and Yang.[2] Since, as will be shown later, the fluctuation effect caused by the interaction linear in $a_0^{\dagger}$ or a_0, say

$$V^{-1} \sum_{\substack{\mathbf{p}\neq 0 \\ \mathbf{p}+\mathbf{k}\neq 0}} v_{\mathbf{k}} a_{\mathbf{p}+\mathbf{k}}^{\dagger} a_{+\mathbf{k}}^{\dagger} a_{\mathbf{p}} a_0 + \text{Herm. conj.} \tag{2.4}$$

in a well-known notation, is negligible under certain circumstances, the above procedure may seem fairly reasonable.

The question we want to ask concerns the *stability* of the assumed Bose–Einstein condensation, which cannot be examined within the approximation (2.2). It is true that this approximation scheme leads us to a consistent theory,[4] but we cannot still exclude the possibility that the interaction would violate the condensation to smear out the particle distribution in momentum space in contradiction to the starting assumption.

Method of Small Oscillation

In order to discuss the stability, we can use the method of small oscillation around an equilibrium position. Instead of the replacement (2.2), we make a change of variables[11]:

$$a_0 = N_0^{\frac{1}{2}} + a_0^{\mathrm{F}}, \tag{2.5}$$

where a_0^{F} is a new annihilation operator intended for the description of the small oscillation. By requiring a_0^{F} and its adjoint $a_0^{\mathrm{F}\dagger}$ to satisfy the canonical commutation relations,

$$[a_0^{\mathrm{F}}, a_0^{\mathrm{F}\dagger}] = 1, \qquad [a_0^{\mathrm{F}}, a_0^{\mathrm{F}}] = [a_0^{\mathrm{F}\dagger}, a_0^{\mathrm{F}\dagger}] = 0, \tag{2.6}$$

[9] H. Araki and E. J. Woods, J. Math. Phys. **4**, 637 (1963).

[10] By $\mathbf{k} = 0$-particles we mean the particles with $\mathbf{k} = 0$ and by $\mathbf{k} \neq 0$-particles those with $\mathbf{k} \neq 0$.

[11] In the elementary particle physics, this kind of transformation was first introduced by S. Kamefuchi and H. Umezawa, Nuovo Cimento **31**, 429 (1964).

we make a_0 and $a_0^\dagger$ also a canonical pair of operators, thus achieving an improvement over the replacement (2.2). The more important point is that, while the shift of equilibrium point $N_0^{\frac{1}{2}}$ is macroscopic, we expect the matrix elements of a_0^{F} not to be proportional to the size of the system V. In other words, we develop an approximation scheme under the assumption that the amplitude of the small oscillation be remaining finite and small even when the system becomes infinitely large, $V \to \infty$.

Then, according to the usual method of small oscillation, we can expand the Hamiltonian in powers of a_0^{F} and neglect the terms of higher powers than the second to compute the eigenfrequency of the a_0^{F} oscillation. To be emphasized is that, as will be seen later, some terms in the expansion are exactly negligible in the limit $V \to \infty$. The stability of the oscillation and therefore of the Bose–Einstein condensation can be judged in the following way: If the frequency of the a_0^{F} oscillation comes out to be real, then the condensation is stable against the disturbance caused by the interaction with the $\mathbf{k} \neq 0$-particles. If the frequency becomes imaginary, then it is unstable and the matrix elements of a_0^{F} will not remain finite to prove the replacements, Eqs. (2.2) and (2.5), inadequate for that system.

In the case of stable condensation, the total density of particles will be computed as a function of the density of $\mathbf{k} = 0$-particles, $\rho_0 = N_0/V$. When the total density is given by an experimental setting, the inversion of this relation determines the equilibrium point $N_0^{\frac{1}{2}}$.

Chemical Potential

If one would hesitate to adopt the change of variables (2.5), it might be because the change violates the conservation of particle number $\mathfrak{N} = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ which is inherent in the many-body Hamiltonian. In order to take care of the conservation, we have to invoke the chemical potential μ.

What happens will be most clearly seen when we take up an example of the Hamiltonian of relativistic free Bose gas, $\mathfrak{H} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ with $\omega_{\mathbf{k}} = (k^2 + m^2)^{\frac{1}{2}}$. Instead of the Hamiltonian itself, we have to deal with the operator $\mathfrak{K} = \mathfrak{H} - \mu\mathfrak{N}$ in the new representation where a_0 and $a_0^\dagger$ are replaced according to Eq. (2.5). The operator to be diagonalized is then

$$\mathfrak{K} = (m - \mu)[a_0^{\mathrm{F}\dagger} a_0^{\mathrm{F}} + N_0^{\frac{1}{2}}(a_0^{\mathrm{F}\dagger} + a_0^{\mathrm{F}}) + N_0] + \sum_{\mathbf{k}\neq 0} (\omega_{\mathbf{k}} - \mu) a_{\mathbf{k}}^\dagger a_{\mathbf{k}}. \tag{2.7}$$

The only question is how to eliminate the terms linear in a_0^{F} and $a_0^{\mathrm{F}\dagger}$. If one tries to do this by such a displacement of origin as $a_0^{\mathrm{F}} \to a_0^{\mathrm{F}} + A$ with some c-number A, then the result is to come back to the original operator a_0. Therefore one must choose the chemical potential to be

$$\mu = m, \tag{2.8}$$

and the remaining operator becomes obviously diagonal in the usual occupation-number representation. When the total number of particles is given by a c-number N, the energy of the system $\mathfrak{K} + \mu N$ turns out to be

$$E = \sum_{\mathbf{k}\neq 0} (\omega_{\mathbf{k}} - m) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + mN. \tag{2.9}$$

This result is easy to understand, because the second term represents the excitation energy. Since for the ground-state energy $E_0 = mN$ we have

$$\partial E_0/\partial N = \mu, \tag{2.10}$$

we know that our way of determining the chemical potential is equivalent to the usual one. This will be seen to hold also for the interacting bosons.

In the later discussion of interacting bosons, also, we shall invoke the chemical potential to eliminate the unwanted terms linear in a_0^{F} and $a_0^{\mathrm{F}\dagger}$.

The State with Sharp Particle Number

We are now prepared for applying our approximation scheme to any many-boson system in which Bose–Einstein condensation takes place. The stability of the condensation serves as the validity criterion for our approximation. Yet, one may wonder if the above procedure of diagonalizing $\mathfrak{K} - \mu\mathfrak{N} = \mathfrak{K}$ is in fact equivalent to the diagonalization of $\mathfrak{H}$ itself with the particle-number conservation explicitly taken into account. To answer this question we shall show a way to construct the simultaneous eigenvector of $\mathfrak{H}$ and $\mathfrak{N}$. This method has once been presented for fermion case[12] by the present author.

For the purpose of illustrating this method, the model of free bosons is not so suitable because the operator $\mathfrak{K}$ with μ put equal to m contains no a_0^{F} nor $a_0^{\mathrm{F}\dagger}$ thus having no preference for any state of "a_0^{F}-quasiparticles"; the eigenvector of $\mathfrak{K}$ is indeterminate to this extent. Here, remembering the assumption of small oscillation, we assume the vacuum $|\Omega\rangle$ of a_0^{F} and $a_{\mathbf{k}}$ ($\mathbf{k} \neq 0$) to be the "eigenvector" of $\mathfrak{K}$, (the true vacuum): $\langle\Omega \mid \Omega\rangle = 1$ and

$$\mathfrak{K}\,|\Omega\rangle = 0;\ a_0^{\mathrm{F}}\,|\Omega\rangle = 0,\ a_{\mathbf{k}}\,|\Omega\rangle = 0\ (\mathbf{k} \neq 0). \tag{2.11}$$

We know that the number of physical particles should be counted by $\mathfrak{N} = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$, the vacuum of

[12] H. Ezawa, J. Math. Phys. 5, 1078 (1964).

which shall be denoted by $|0\rangle$:

$$a_0 |0\rangle = 0, \qquad \langle 0 \mid 0\rangle = 1. \tag{2.12}$$

Now, the first step is initiated by an important observation: The conservation of particle number implies the invariance of the Hamiltonian under the phase transformation, $a_k \to a_k e^{i\alpha}$ and $a_k^\dagger \to a_k^\dagger e^{-i\alpha}$. Then, imagine we have employed the transformed operators from the beginning. The Hamiltonian and also the operator $\mathcal{K}$ takes the same forms as before. But, the change of variables we make will be

$$a_0 e^{i\alpha} = N_0^{\frac{1}{2}} + a_0^{\mathrm{F}} e^{i\alpha}. \tag{2.13}$$

If the old replacement (2.5) provides us with an useful approximation scheme, the new one (2.13) must work as well yielding the same value for the approximate eigenvalue of $\mathcal{K}$. In fact, in the case of the free bosons, we can see immediately that this is true. As will be seen in the following sections, it is true also for interacting bosons: After the change of variables [(2.5) or (2.13)] has been done, the apparent forms of $\mathcal{K}$'s, the old and the new, may be different from each other (as it is actually the case for interacting bosons), but their eigenvalues will be found to coincide. The operator $\mathcal{K}$ written in terms of the new variable $a_k^{\mathrm{F}} e^{i\alpha}$ will be denoted by $\mathcal{K}_\alpha$.

The second step is to notice that the change of variables (2.13) can be looked upon as an unitary transformation within the representation space of a_0 and $a_0^\dagger$. In fact,

$$a_0^{\mathrm{F}} e^{i\alpha} = \mathfrak{U}_\alpha a_0 e^{i\alpha} \mathfrak{U}_\alpha^\dagger, \tag{2.14}$$

where

$$\mathfrak{U}_\alpha \equiv \exp\left[-N_0^{\frac{1}{2}}(a_0 e^{i\alpha} - a_0^\dagger e^{-i\alpha})\right]. \tag{2.15}$$

Then, the true vacuum of $\mathcal{K}_\alpha$ is related to the vacuum of a_0 as

$$|\Omega_\alpha\rangle = \mathfrak{U}_\alpha |0\rangle, \tag{2.16}$$

the suffix α being supplied to the vector $|\Omega\rangle$ in Eq. (2.9). As has been anticipated, the true vacuum $|\Omega_\alpha\rangle$ is a superposition of the states with different occupation numbers.

In the actual case of the interacting bosons, the construction of the true vacuum is not so simple as in the above example. After the change of variables, the operator $\mathcal{K}_\alpha$ will depend on a_0^{F} and $a_0^{\mathrm{F}\dagger}$ so that some further transformation will be necessary to diagonalize it. Anyhow, the true vacuum can be related to the free vacuum $|0\rangle$ by the operator, $a_k e^{i\alpha}$ and $a_k^\dagger e^{-i\alpha}$ [see, for example Eq. (5.8)].

We are now in the position to construct the simultaneous eigenvectors of $\mathfrak{K}$ and $\mathfrak{N}$. The key is to make the following observations: Since the vectors, $|\Omega_\alpha\rangle$'s $(0 \leq \alpha \leq 2\pi)$, are the respective eigenvectors of $\mathcal{K}_\alpha$'s with one and the same eigenvalue and the operators $\mathcal{K}_\alpha$ are expected to approximate $\mathfrak{K} - \mu\mathfrak{N}$ equally well under the condition of the Bose–Einstein condensation, any superposition of $|\Omega_\alpha\rangle$'s must be as good approximation to the eigenvector of $\mathfrak{K} - \mu\mathfrak{N}$ as each $|\Omega_\alpha\rangle$ is.[13] Then, we construct a special superposition,

$$|\Omega_\alpha\rangle = [\langle \Omega_N \mid \Omega_N\rangle]^{-\frac{1}{2}} \cdot \int_0^{2\pi} e^{iN\alpha} |\Omega_\alpha\rangle \, d\alpha, \tag{2.17}$$

which is by nature an eigenvector of the number operator $\mathfrak{N}$, and therefore the simultaneous eigenvector of $\mathfrak{K}$ and $\mathfrak{N}$. This concludes our approximation scheme.

In the case of the free bosons, the vector $|\Omega_N\rangle$ is simply given by

$$|\Omega_N\rangle = (N!)^{-\frac{1}{2}} (a_0^\dagger)^N |0\rangle. \tag{2.18}$$

If one suspects that we might have made an unnecessary detour, he should remember the whole procedure of our approximation: The point is that the change of variables (2.13) provides us with a tractable method of approximation if the Bose–Einstein condensation is assumed. It is well-known method of small oscillation. Once such a change of variables is adopted, we are forced to abandon the conservation of particle number. The use of a chemical potential is a partial remedy, and, at the last stage, we have to return to the original variables (by the transformation $\mathfrak{U}_\alpha$) to construct the state with sharp particle number.

In the following application to the case of the interacting bosons, we shall not try to construct the state with sharp particle number. The full discussion of the state vector will be given elsewhere.

Infinite Volume Limit

Hitherto the change of variables (2.13) has been looked upon as an useful means of developing an approximation scheme. Now, we want to explain that it becomes imperative when we consider the limit of infinitely large system ($N_0 \to \infty$ or $V \to \infty$ with $\rho_0 = N_0/V$ kept constant). The argument here is of heuristic nature and the detailed one will be given in Sec. 9.

We use the model of free bosons, again. Before entering into the main subject, it will be instructive to examine the limit $V \to \infty$ of our true vacuum

[13] Here, we are speaking in terms of the original representation: The operators $\mathfrak{K}$ and $\mathfrak{N}$ are written in terms of $a_k e^{i\alpha}$ and $a_k^\dagger e^{-i\alpha}$ and the state is created by the suitable applications of $a_k^\dagger e^{-i\alpha}$ on $|0\rangle$.

(2.16): The true vacuum has the form of direct product of vectors representing the particles with various momenta $\mathbf{k}$. Let us avoid the complication due to the scale transformation needed to relate the representations in boxes of different sizes V by concentrating our attention to the $\mathbf{k} = 0$-component of the state vector, for which the scale transformation is unity. The infinite volume limit is easily seen not to exist. In fact, if that component of the true vacuum is denoted by $|\Omega_\alpha(V)\rangle_0$ and the norm of a vector by $||\ \ ||$, then

$$
\begin{aligned}
&{}_0\langle\Omega_\alpha(V) \mid \Omega_{\alpha'}(V')\rangle_0 \\
&= \exp\left[-\tfrac{1}{2}\rho_0\{V + V' - 2V^{\frac{1}{2}}V'^{\frac{1}{2}}e^{i(\alpha'-\alpha)}\}\right], \qquad (2.19)
\end{aligned}
$$

and therefore

$$
\begin{aligned}
&|| \ |\Omega_\alpha(V)\rangle_0 - |\Omega_\alpha(V')\rangle_0 \ || \\
&\qquad = 2\{1 - \exp\left[-\tfrac{1}{2}\rho_0(V^{\frac{1}{2}} - V'^{\frac{1}{2}})^2\right]\}, \qquad (2.20)
\end{aligned}
$$

so that the Cauchy condition for the (strong) convergence,

$$
|| \ |\Omega_\alpha(V)\rangle_0 - |\Omega_\alpha(V')\rangle_0 \ || \to 0 \text{ as } V, V' \to \infty \qquad (2.21)
$$

is obviously violated.

In the same way, we can conclude the nonexistence of the limit, $\lim_{V\to\infty} |\Omega_N\rangle$ with $\rho_0 = N_0/V$ kept constant. Precisely speaking, we have to say that the limit does not exist in the Fock space for a_0 and $a_0^\dagger$. This is quite understandable because the Fock space is defined as the closure of the space spanned by the eigenvectors of the number operator with finite eigenvalues.[7] Any vector with an infinite occupation number cannot have a finite length.

The nonexistence of the limit means that the infinite system cannot be dealt with unless we construct a new Hilbert space suitable for representing it. In order to accomplish this, we have to invoke the Gelfand construction.[14]

In the Gelfand construction, we restrict ourselves to the smeared-out field operators, i.e.,

$$
\phi(f) = \sum_{\mathbf{k}} (2V)^{-\frac{1}{2}}[\tilde{f}^*(\mathbf{k})a_{\mathbf{k}}^\dagger + \tilde{f}(\mathbf{k})a_{\mathbf{k}}] \qquad (2.22)
$$

and its canonical conjugate

$$
\pi(g) = \sum_{\mathbf{k}} i(2V)^{-\frac{1}{2}}[\tilde{g}^*(\mathbf{k})a_{\mathbf{k}}^\dagger - \tilde{g}(\mathbf{k})a_{\mathbf{k}}], \qquad (2.23)
$$

where the functions, f and g, are assumed to be normalizable,

$$
\int |f(\mathbf{k})|^2 \, d\mathbf{k} < \infty, \quad \text{etc.}
$$

The construction of the space is achieved when we obtain all the vacuum expectation values of the products of these operators, (the Wightman functionals).[15] The vacuum expectation values in the infinite volume representation (which we want to construct) will be obtained as the limit of those expectation values computed with $|\Omega_\alpha(V)\rangle$ or $|\Omega_N\rangle$ employed as the vacuum vector.

Let us now consider what will happen if we take the vacuum to be the state with sharp particle number. The reason why we take it is that the ground state of the interacting bosons will be of this nature and that the ground state is required to be contained in the Hilbert space [conventionally denoted by $\mathfrak{H}_N(V \to \infty)$]. In order to obtain all the vacuum expectation values, it is convenient to compute

$$
E_N(f, g) = \langle\Omega_N| \, e^{i\varphi(f)}e^{i\pi(g)} \, |\Omega_N\rangle, \qquad (2.24)
$$

and to take the limit $V = N/\rho \to \infty$ with ρ fixed.

According to Eq. (2.15), we have

$$
\begin{aligned}
E_N(f, g) = [\langle\Omega_N \mid \Omega_N\rangle]^{-1} &\int_0^{2\pi} d\beta \int_0^{2\pi} d\alpha \\
&\times e^{iN(\alpha-\beta)} \, \langle\Omega_\beta| \, e^{i\varphi(f)}e^{i\pi(g)} \, |\Omega_\alpha\rangle. \qquad (2.25)
\end{aligned}
$$

Since we are interested in the limit of infinite system ($N \to \infty$), the method of steepest descent is the most suitable for the computation. The same sort of computation has been carried out for the case of fermions in the BCS model.[12] Without repeating it, we write down the result:

$$
\begin{aligned}
E_N(f, g) \sim [\langle\Omega_N \mid \Omega_N\rangle]^{-1} &\\
\times \int_{-\infty}^{\infty} d\beta \int_0^{2\pi} d\alpha \, &\exp\left[-\tfrac{1}{2}\rho V(\alpha - \beta)^2\right] \\
\times \exp\left[i(2\rho)^{\frac{1}{2}}\{\tilde{f}(0)\cos\alpha + \tilde{g}(0)\sin\alpha\}\right] \qquad &(2.26)
\end{aligned}
$$

where we have put $\tilde{f}(\mathbf{k}) = \tilde{g}(\mathbf{k}) = 0$ for $\mathbf{k} \neq 0$ because these are immaterial for the present discussion. What we have to emphasize here is that, in the limit $V \to \infty$, the contribution to the integral comes only from the neighborhood of $\alpha = \beta$, and the Gaussian integral cancels the normalization factor that can be computed in a similar way. The concentration of the integrand around $\alpha = \beta$ means that

$$
\begin{aligned}
\lim_{V\to\infty} [\langle\Omega_N \mid \Omega_N\rangle]^{-1}e^{iN(\alpha-\beta)} \, &\langle\Omega_\beta| \, e^{i\varphi(f)}e^{i\pi(g)} \, |\Omega_\alpha\rangle \qquad (2.27) \\
&\propto \delta(\alpha - \beta).
\end{aligned}
$$

As is seen from Eq. (2.19), the vectors, $|\Omega_\alpha(V)\rangle$ and

[14] A. S. Wightman, Phys. Rev. **101**, 860 (1956). R. Haag, *Lectures in Theoretical Physics* (Interscience Publishers, Inc., New York, 1961), Vol. III. M. A. Naimark, *Normed Rings* (P. Nordhoff Ltd., Groningen, The Netherlands, 1959), Chap. IV.

[15] This is because the Hilbert space is so constructed as to be spanned by the vectors generated by the repeated application of field operators on the vacuum (the cyclic representation). The collection of the vacuum expectation values can then be regarded as giving all the matrix elements of the field operator.

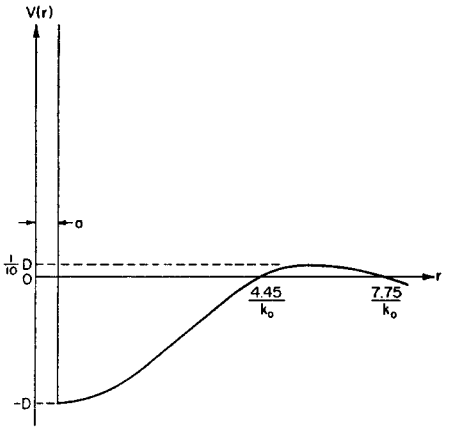

FIG. 1. The two-body potential in the present model.

$|\Omega_\beta(V)\rangle (\alpha \neq \beta)$, are orthogonal in the limit $V \to \infty$. In addition, we have just found that these two vectors cannot be connected with any powers of the smeared-out field operators. Then, we have to conclude that the representation of the field operators with the sharp-particle-number ground state is reducible: The Hilbert space $\mathfrak{H}_N(V \to \infty)$ is decomposable into the direct sum of those $\mathfrak{H}_\alpha(V \to \infty)$'s which are constructed by a repeated application of the field operators upon $|\Omega_\alpha(V)\rangle$ together with the limiting procedure $V \to \infty$ applied to the Wightman functions.

Now, it is not difficult to see that the representation with $|\Omega_\alpha\rangle$ employed as the vacuum is irreducible, or in other words, all the vectors in $\mathfrak{H}_\alpha(V \to \infty)$ can be connected each other by the application of the smeared-out field operators, since the representation is provided by the Fock representation for $a_{\mathbf{k}}^\dagger$ introduced in Eq. (2.13), (for $\mathbf{k} \neq 0$, $a_{\mathbf{k}}^F = a_{\mathbf{k}}$).[16] This completes our argument.

The conclusion is the following: When the system is infinitely large and is in the state of Bose–Einstein condensation, the change of variables (2.13) is imperative if one wants to use an irreducible representation of the creation and annihilation operators.[17]

The corresponding arguments for the interacting boson system is given in Sec. 9, where the present discussion of free Bose gas will be useful as a reference.

III. DEFINITION OF THE MODEL

The model we discuss is the same as that treated by Huang[4] in 1959. But, for the sake of convenient reference, we briefly resume the characteristic features of the model. We take units so that $\hbar = 1$ and $2m = 1$, m being the mass of the particle.

Two-Body Potential

We consider a dilute assembly of Bose particles interacting through a two-body central potential which, as is shown in Fig. 1, consists of a hard core of radius a and a weak attractive part $w(r)$ extending outside. (r: interparticle distance).

To simplify computations we choose the attractive part $w(r)$ such that its Fourier transform is a step function:

$$w_{\mathbf{k}} \equiv \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} w(r) = \begin{cases} -8\pi(a+b) & \text{for } |\mathbf{k}| < k_0 \\ 0 & \text{for } |\mathbf{k}| > k_0. \end{cases} \quad (3.1)$$

In the coordinate space, it amounts to

$$w(r) = -3D\, j_1(k_0 r)/(k_0 r), \quad (3.2)$$

where $j_1(x)$ is a spherical Bessel function and D is the depth of the potential:

$$D = |w(0)| = (32\pi^2/3)(a+b)k_0^3. \quad (3.3)$$

As is seen in Fig. 1, the range may be represented by

$$r_0 = 4.5/k_0. \quad (3.4)$$

Now, in order to discuss the many-body problem it will be sufficient to take the binary collision only because we assume the gas to be of low density. In addition we require

$$D^{\frac{1}{2}}a \ll 1, \quad (3.5)$$

so that the hard-sphere part of the interaction will affect the S wave only at least for the low-energy particles ($D^{\frac{1}{2}}$ gives the wavenumber of zero-energy particles in the potential) which would form the major part of the gas near the Bose–Einstein condensation. Thus the interaction can be substituted for by

$$v(r) = 8\pi a \delta(\mathbf{r})(\partial/\partial r)r + w(r), \quad (3.6)$$

the first term being the pseudopotential[18,19] that is to represent the hardsphere part. We have to note that the pseudopotential is not Hermitian.

The Hamiltonian; the Subtraction Prescription

In the second-quantized form, the Hamiltonian is given by

$$\mathfrak{H} = \sum_{\mathbf{k}} k^2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k}}{}' v_{\mathbf{k}} \sum_{\mathbf{p},\mathbf{q}} a_{\mathbf{p}+\mathbf{k}}^\dagger a_{\mathbf{q}-\mathbf{k}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}}, \quad (3.7)$$

[16] The detailed discussion is given in Sec. 9.

[17] Precisely speaking we have to say "if one wants to use an irreducible representation of the smeared-out fields." When we restrict the field operators to the smeared ones, we are presuming that every quantity of physical interest can be expressed in terms of them only. See Refs. 9 and 12.

[18] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

[19] E. Fermi, Ricerca Sci. **7**, 13 (1936). J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), p. 74.

where

$$v_{\mathbf{k}} \equiv \int d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}[8\pi a\delta(\mathbf{r}) + w(r)] = \begin{cases} 8\pi a & \text{for } \mathbf{k} \in \mathfrak{R}_{II}, \\ -8\pi b & \text{for } \mathbf{k} \in \{0, \mathfrak{R}_I\}, \end{cases} \tag{3.8}$$

with the sets of momenta defined as follows:

$$\mathfrak{R}_I = \{\mathbf{k}; 0 < |\mathbf{k}| < k_0\}, \quad \mathfrak{R}_{II} = \{\mathbf{k}; k_0 < |\mathbf{k}|\}. \tag{3.9}$$

One may notice that b gives the total scattering length at zero energy.

The differential operator $(\partial/\partial r)r$ in the pseudopotential has been taken care of by the subtraction procedure indicated by the prime in the summation over $\mathbf{k}$ in (3.7). Suppose that a matrix element $f(\mathbf{k})$ arising from (3.7) behaves like

$$f(\mathbf{k}) \sim Ak^{-2} + O(k^{-3}) \quad \text{at} \quad k \to \infty, \tag{3.10}$$

then the subtraction is defined as

$$\sum_{\mathbf{k}}{}' f(\mathbf{k}) = \sum_{\mathbf{k}} [f(\mathbf{k}) - Ak^{-2}]. \tag{3.11}$$

The detailed account has been given in the Ref. 18.

Orders of Magnitude

The parameters of our model, ρ, a, b, and k_0, are characterized by the smallness of the following dimensionless quantities:

$$(\rho a^3)^{\frac{1}{2}} \sim b/a \sim k_0 a \sim \epsilon, \tag{3.12}$$

all of which are assumed to be of the same order of magnitude[20] as designated by ϵ.

While $(\rho a^3)^{\frac{1}{2}} \sim \epsilon$ says that the space occupied by the gas molecule (hard sphere) is small compared with the volume of the gas, the number of the molecules within the range of the attractive potential

$$(1/k_0^3)\rho \sim 1/\epsilon \tag{3.13}$$

is not small at all. However, the hard core suppresses the total scattering length at zero energy and therefore the number of molecules within the sphere of radius b is small:

$$b^3\rho \sim \epsilon^5. \tag{3.14}$$

In the following we find it most convenient to take $8\pi\rho a$ as the unit of energy.

IV. ANATOMY OF THE "HAMILTONIAN"

We start on our job to determine the energy eigenstates of the gas. Since, as explained in Sec. 2, we have to make a transformation that violates the conservation of the particle number anticipated from the very structure of our Hamiltonian (3.7), what we have to diagonalize is not the Hamiltonian itself but

$$\mathfrak{K} = \mathfrak{H} - \mu\mathfrak{N}, \tag{4.1}$$

where μ is the chemical potential and $\mathfrak{N}$ is the number operator, $\mathfrak{N} = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$. The energy eigenvalue of the gas is given by the eigenvalue of $\mathfrak{K}$ plus μN_{tot}, where N_{tot} is the total number of gas molecules.[21] We shall call the operator $\mathfrak{K}$ "Hamiltonian".

Based on the idea presented in Sec. 2, we make the replacement

$$a_0 \to a_0 + N^{\frac{1}{2}}e^{-i\alpha}, \tag{4.2}$$

where a_0 on the right-hand side stands for the annihilation operator in a new representation[22] and N is the average number, both belonging to the unperturbed eigenstate of zero momentum $\mathbf{k} = 0$. α is the phase angle ($0 \leq \alpha \leq 2\pi$) characterizing, together with N, the irreducible representation of the Bose commutation relation.

Remark: It is not *ab initio* obvious if the replacement (4.2) allows the use of Fock representation in the limit $N \to \infty$. Anyhow, the smallness of the matrix element of a_0 on the right-hand side should be checked at the end of the calculation.

After the replacement (4.2) is done, it is convenient to anatomize the Hamiltonian to obtain the following components. In this analysis we ignore the phase factor $e^{i\alpha}$ in Eq. (4.2) to avoid the unnecessary complication. It is true that the phase factor can be removed from the "Hamiltonian" by carrying out a phase transformation.

$$a_{\mathbf{k}} \to a_{\mathbf{k}}e^{i\alpha}, \tag{4.3}$$

but, as shown in Sec. 2, this transformation cannot be effected by any unitary transformation. Nevertheless, we can easily check that the phase factor does not affect the eigenvalue of the "Hamiltonian" at all.

Now, the anatomy. After the replacement (4.2), we divide the "Hamiltonian" into several components: in addition to the one that contains the operators a_0 and $a_0^\dagger$ only (the $\mathbf{k} = 0$-component), we have $\mathfrak{R}_I$-, $\mathfrak{R}_{II}$-component and the components that describe the interactions among $\mathbf{k} = 0$-, $\mathfrak{R}_I$-, and

[20] Because of the discontinuity of the occupation number distribution, we cannot come to the case of pure hard core by taking limit $k_0 \to 0$.

[21] In Sec. 2, the total number was denoted by N and the number of the $\mathbf{k} = 0$-particles by N_0.

[22] For the sake of simple notation, we omit the superscript F that have hitherto been attached to the operator a_0 on the right-hand side.

TABLE I. The components of the "Hamiltonian": their orders of magnitude in unit of $8\pi a\rho$.

	$\mathcal{K}_0$	$\mathcal{K}_0^{(1)}$	$\mathcal{K}_0^{(2)}$	$\mathcal{K}_{II}$	$\mathcal{K}_{0II}$	$\mathcal{K}_{0II}^{(1)}$	$\mathcal{K}_{0II}^{(2)}$	$\mathcal{K}_{0II}^{(3)}$
$8\pi a\rho\times$	ϵ	$\frac{\epsilon}{N^{\frac{1}{2}}}$	$\frac{\epsilon}{N}$	ϵN	$\epsilon N^{\frac{1}{2}}$	$\epsilon^2 N^{\frac{1}{2}}$	ϵ	ϵ^2

	$\mathcal{K}_I$	$\mathcal{K}_{0I}$	$\mathcal{K}_{0I}^{(1)}$	$\mathcal{K}_{0I}^{(2)}$	$\mathcal{K}_{0I}^{(3)}$	$\tilde{\mathcal{K}}_{III}$
$8\pi a\rho\times$	$\epsilon^2 N$	$\epsilon^2 N^{\frac{1}{2}}$	$\epsilon^2 N^{\frac{1}{2}}$	ϵ^2	ϵ^2	—

$\mathfrak{R}_{II}$-particles. There comes the $\mathbf{k}=0$-component first:

$$\mathcal{K}_0=\left(\frac{N^2}{2V}v_0-N\mu\right)+\left(\frac{N^{\frac{1}{2}}}{V}v_0-N^{\frac{1}{2}}\mu\right)(a_0^\dagger+a_0)+\frac{N}{2V}v_0(a_0^\dagger a_0^\dagger+a_0a_0)+\left(\frac{N}{V}v_0-\mu\right)a_0^\dagger a_0, \quad (4.4)$$

$$\mathcal{K}_0^{(1)}=\frac{N^{\frac{1}{2}}}{V}v_0(a_0^\dagger a_0^\dagger a_0+a_0^\dagger a_0a_0), \quad (4.5)$$

$$\mathcal{K}_0^{(2)}=\frac{1}{2V}v_0a_0^\dagger a_0^\dagger a_0a_0.$$

Then, there follows the component for the $\mathfrak{R}_{II}$-particles (the particles with momentum $\mathbf{k}\in\mathfrak{R}_{II}$), which will constitute the heart of the matter in the present analysis:

$$\mathcal{K}_{II}=\sum_{II}k^2a_\mathbf{k}^\dagger a_\mathbf{k}+\frac{N}{2V}\sum_{II}{}'v_\mathbf{k}(a_\mathbf{k}^\dagger a_{-\mathbf{k}}^\dagger+2a_\mathbf{k}^\dagger a_\mathbf{k}+a_\mathbf{k}a_{-\mathbf{k}})+\left(\frac{N}{V}v_0-\mu\right)\sum_{II}a_\mathbf{k}^\dagger a_\mathbf{k}, \quad (4.6)$$

where the summation $\sum_{II}$ extends over $\mathfrak{R}_{II}$ and the prime thereon indicates the subtraction. One may notice that the structure of $\mathcal{K}_{II}$ is slightly different from the structure of $\mathcal{K}_0$.

The interaction between the $\mathbf{k}=0$-particle and the $\mathfrak{R}_{II}$-particle consists of four parts,: $\mathcal{K}_{0II}+\mathcal{K}_{0II}^{(1)}+\mathcal{K}_{0II}^{(2)}+\mathcal{K}_{0II}^{(3)}$. The most important one is given by

$$\left.\begin{aligned}&\mathcal{K}_{0II}=\mathcal{V}_{II}+\mathcal{V}_{II}^\dagger,\\ &\mathcal{V}_{II}\equiv\frac{N^{\frac{1}{2}}}{V}a_0\sum_{II}{}'v_\mathbf{k}(a_\mathbf{k}^\dagger a_{-\mathbf{k}}^\dagger+a_\mathbf{k}^\dagger a_\mathbf{k})\end{aligned}\right\}. \quad (4.7)$$

where

The other three are:

$$\mathcal{K}_{0II}^{(1)}=\mathcal{V}_{II}^{(1)}+\mathcal{V}_{II}^{(1)\dagger},\quad \text{etc.},$$

where

$$\mathcal{V}_{II}^{(1)}\equiv\frac{N^{\frac{1}{2}}}{V}v_0\sum_{II}a_\mathbf{k}^\dagger a_\mathbf{k}a_0,$$

$$\mathcal{V}_{II}^{(2)}\equiv\frac{1}{2V}\sum_{II}{}'v_\mathbf{k}(a_\mathbf{k}^\dagger a_{-\mathbf{k}}^\dagger a_0a_0+a_\mathbf{k}^\dagger a_\mathbf{k}a_0^\dagger a_0), \quad (4.8)$$

$$\mathcal{V}_{II}^{(3)}\equiv\frac{1}{V}v_0\sum_{II}{}'a_\mathbf{k}^\dagger a_\mathbf{k}a_0^\dagger a_0.$$

The term

$$\mathcal{K}_{0II}^{(4)}=V^{-1}\sum_{\substack{\mathbf{p}\neq0\\ \mathbf{p}+\mathbf{k}\neq0}}v_\mathbf{k}a_{\mathbf{p}+\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_\mathbf{p}a_0+\text{Herm. conj.},$$

though existent too, will be shown to be negligible. (See Refs. 28 and 29, pp. 390 and 391, resp.) The outstanding role of the $\mathfrak{R}_{II}$-particles can be understood by referring to the order of magnitude assumption $b/a\ll1$ in Eq. (3.12). The interest in the $\mathbf{k}=0$-particles comes from the stability question of the macroscopic occupation of $\mathbf{k}=0$ level (Bose–Einstein condensation).

The component for the $\mathfrak{R}_I$-particles,[23]

$$\mathcal{K}_I+\mathcal{K}_{0I}+\mathcal{K}_{0I}^{(1)}+\mathcal{K}_{0I}^{(2)}+\mathcal{K}_{0I}^{(3)}, \quad (4.9)$$

can be obtained from the above [Eqs. (4.7) and (4.8)] by replacing the summation $\sum_{II}$ by $\sum_I$. The remark that the structure of $\mathcal{K}_{II}$ is slightly different from that of $\mathcal{K}_0$ applies also to $\mathcal{K}_I$. This difference will be important when we deal with the phonon spectrum of $\mathfrak{R}_I$-particles and the stability of the macroscopic $\mathbf{k}=0$-occupation, the former in Sec. 7 and the latter in Sec. 6.

Finally, we have the interaction between $\mathfrak{R}_I$- and $\mathfrak{R}_{II}$-particles,

$$\tilde{\mathcal{K}}_{I\,II}=\frac{1}{2V}\sum_{I,II}v_\mathbf{k}a_{\mathbf{p}+\mathbf{k}}^\dagger a_{\mathbf{q}-\mathbf{k}}^\dagger a_\mathbf{p}a_\mathbf{q}, \quad (4.10)$$

which will be analyzed in detail in Section 7. The tilde above $\mathcal{K}_{I\,II}$ is just for the sake of later convenience.

Now, in order to see the relative importance of the above components, their "orders of magnitude" (in the unit of $8\pi a\rho$)[24] are presented in Table I. The estimation is based on the following anticipation: (1) The "order of magnitude" of the operator a_0 will be 1. (2) The summation over the momenta $(1/V)\sum_{II}$ will result in $k_0^3\sim\rho\epsilon$ and also $(1/V)\sum_I\cdots\sim\rho\epsilon$. It should be noted that the "orders of magnitudes" of operators are not necessarily multiplicative. For example, the diagonal element of the operator $(\mathcal{K}_{0II})^2$ is of the order of $(8\pi a\rho)^2\epsilon$ but not of $(8\pi a\rho)^2\epsilon^2N$ because the momentum conservation restricts the phase volume.

If the above assumption (1) is accepted, we may neglect $\mathcal{K}_0^{(1)}$ and $\mathcal{K}_0^{(2)}$ exactly in the limit $N\to\infty$ because the intermediate "phase space" consists of

[23] Since the fifth part $\mathcal{K}_{0I}^{(4)}$ is again negligible, we don't write it down here.

[24] By order of magnitude of an operator we mean the orders of magnitude of its representative matrix element.

a single level, $\mathbf{k} = 0$, only. But, a reservation should be made to this statement since the operator a_0 is unbounded and the state in question can be an infinite superposition of the states with different occupation number in the $\mathbf{k} = 0$-level.

We see from Table I that the most important component is $\mathcal{K}_{II}$, which will be diagonalized first in the next section to form the backbone of our analysis.

V. DIAGONALIZATION; THE LOWEST ORDER

Before entering into the diagonalization of $\mathcal{K}_{II}$, we have to determine the value of the chemical potential μ. This can be done by the requirement that the "Hamiltonian" should not contain the term linear in a_0 or $a_0^\dagger$ (see Sec. 2). In the lowest order, we see from Eq. (4.4) that

$$\mu^{(0)} = \rho v_0 = -8\pi\rho b. \tag{5.1}$$

Then, the last term in Eq. (4.6) vanishes and the operator $\mathcal{K}_{II}$ turns out to be

$$\mathcal{K}_{II} = \sum\nolimits'_{II}\{P_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + 2Q_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + P_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}\},$$

where (5.2)

$$P_{\mathbf{k}} = \tfrac{1}{2}\rho v_{\mathbf{k}} = 4\pi a\rho, \qquad Q_{\mathbf{k}} = \tfrac{1}{2}k^2 + 4\pi a\rho.$$

According to the formulas in Appendix I, this operator is diagonalized by the following Bogoliubov transformation,

$$a_{\mathbf{k}} = b_{\mathbf{k}} \cosh\theta_{\mathbf{k}} - b_{-\mathbf{k}}^\dagger \sinh\theta_{\mathbf{k}}. \tag{5.3}$$

For the sake of the convenient reference, we list two equations that define the angle $\theta_{\mathbf{k}}$ for $\mathbf{k} \in \mathfrak{R}_{II}$:

$$\sinh^2\theta_{\mathbf{k}} = \frac{k^2 + 8\pi a\rho}{2k(k^2 + 16\pi a\rho)^{\frac{1}{2}}} - \frac{1}{2} \sim \frac{(8\pi a\rho)^2}{4k^4},$$

$$\cosh\theta_{\mathbf{k}} \sinh\theta_{\mathbf{k}} \tag{5.4}$$

$$= \frac{8\pi a\rho}{2k(k^2 + 16\pi a\rho)^{\frac{1}{2}}} \sim \frac{4\pi a\rho}{k^2} - \frac{(8\pi a\rho)^2}{2k^4},$$

where $\sim$ indicates the asymptotic behavior at $k \to \infty$. The diagonalized operator is given by

$$\mathcal{K}_{II} = \sum_{II} k(k^2 + 16\pi a\rho)^{\frac{1}{2}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + C_{II}, \tag{5.5}$$

where

$$C_{II} = \sum_{II}{}' [\tfrac{1}{2}k(k^2 + 16\pi a\rho)^{\frac{1}{2}} - \tfrac{1}{2}(k^2 + 8\pi a\rho)] \tag{5.6}$$

$$= 8\pi a\rho N \tfrac{64}{15}\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}} F_1(\nu)$$

with[25]

$$\nu \equiv k_0/(16\pi a\rho)^{\frac{1}{2}},$$

$$F_1(\nu) \equiv \tfrac{15}{2}[\tfrac{1}{3}(1+\nu^2)^{\frac{3}{2}} - \tfrac{1}{5}(1+\nu^2)^{5/2} - \tfrac{1}{8}\nu + \tfrac{1}{6}\nu^3 + \tfrac{1}{5}\nu^5].$$

The zero-point energy C_{II} is computed by applying the subtraction procedure indicated in Eq. (3.11). Since the summand behaves like $-(4\pi a\rho)^2/k^2$ as $k \to \infty$, the summation goes as follows:

$$C_{II} = \frac{V}{(2\pi)^3}\int_{k_0}^{\infty}\left[\frac{k}{2}(k^2 + 16\pi a\rho)^{\frac{1}{2}} - \frac{1}{2}(k^2 + 8\pi a\rho) + \frac{(4\pi a\rho)^2}{k^2}\right]4\pi k^2\, dk.$$

The excitation described by Eq. (5.5) is exactly of phonon type.

The transformation (5.3) is effected by

as
$$\mathfrak{U}(\theta_{\mathbf{k}}) = \exp[\theta_{\mathbf{k}}(a_{\mathbf{k}}a_{-\mathbf{k}} - a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger)] \tag{5.7}$$
$$b_{\mathbf{k}} = \mathfrak{U}(\theta_{\mathbf{k}}) a_{\mathbf{k}} \mathfrak{U}^\dagger(\theta_{\mathbf{k}}).$$

Then, the vacuum $|\Omega_{II}\rangle$ of $b_{\mathbf{k}}$ (or of $\mathcal{K}_{II}$) is related to the vacuum $|0\rangle$ of $a_{\mathbf{k}}$:

$$|\Omega_{II}\rangle = \Pi_{II}\mathfrak{U}(\theta_{\mathbf{k}})\ |0\rangle. \tag{5.8}$$

One may notice that the right-hand side is an infinite product and the convergence should be examined. It turns out that the infinite product does not converge when the system is infinitely large and therefore that we have to construct a new representation. But, we want to defer the detailed discussion to the succeeding paper on the mathematical structure of the Huang model.

Remark: In this approximation, we get the equation corresponding to Eq. (2.14) if $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ are replaced by $a_{\mathbf{k}}e^{i\alpha}$ and $a_{\mathbf{k}}^\dagger e^{-i\alpha}$, respectively, and if we apply the additional transformation $\mathfrak{U}_\alpha$ in Eq. (2.13) to take care of the change of variables. Here, we don't want to calculate the state vector with sharp particle number.

VI. THE FLUCTUATION OF THE CONDENSED STATE

In the last section, we have diagonalized the $\mathfrak{R}_{II}$-part of the "Hamiltonian." Now, we are in the position to depart from Huang's theory; we are going to diagonalize the $\mathbf{k} = 0$-part. Under the condition (5.1), however, Eq. (4.4) results in the instability of the Bose–Einstein condensation.[26] In fact,

$$\mathcal{K}_0 = \tfrac{1}{2}\rho v_0(a_0^\dagger a_0^\dagger + a_0 a_0 - N), \tag{6.1}$$

can be regarded as the Hamiltonian of a harmonic oscillator with an imaginary frequency, $\mathcal{K}_0 =$

[25] In Huang's formula for $F_1(\nu)$, the term $-\frac{1}{8}\nu$ is missing. If the subtraction prescription is followed, $F_1(\nu)$ should vanish when $\nu \to \infty$ because it is given by a convergent integral over the range (ν, ∞). Thus the term $-\frac{1}{8}\nu$ is indispensable.

[26] Huang has notice in his paper[4] that a similar instability arises for the $\mathfrak{R}_I$-particle when its interaction with the $\mathfrak{R}_{II}$-particle is neglected.

$\frac{1}{2}\rho v_0(p^2 - x^2 - N)$, because the creation and the annihilation operator can be represented by a canonical pair of the momentum p and the coordinate x:

$$a_0 = 2^{-\frac{1}{2}}(p - ix), \qquad a_0^\dagger = 2^{-\frac{1}{2}}(p + ix), \qquad [p, x] = -i. \tag{6.2}$$

There would not exist even the normalizable ground state.

This paradox will be solved quite naturally if we take into account the interaction between the $\mathbf{k} = 0$-particles and the $\mathfrak{N}_{II}$-particles. While the most important interaction of this type is $\mathcal{K}_{0II}$ given by Eq. (4.7), we shall see later that $\mathcal{K}_{0II}^{(2)}$ should be taken into account as well.

In order to take care of these interactions, let us first diagonalize $\mathcal{K}_{II} + \mathcal{K}_{0II} + \mathcal{K}_{0II}^{(2)}$ with respect to the $\mathfrak{N}_{II}$-degrees of freedom. Then, $\mathcal{K}_0 + (\mathcal{K}_{II} + \mathcal{K}_{0II} + \mathcal{K}_{0II}^{(2)})$ can be regarded as consisting of the diagonal array (labeled by the states of $\mathfrak{N}_{II}$) of submatrices which are labeled by the quantum numbers of the $\mathbf{k}=0$-particles. We shall carry out the diagonalization of $\mathcal{K}_{II} + \mathcal{K}_{0II} + \mathcal{K}_{0II}^{(2)}$ by using the perturbation theory. In this section,[27] the unperturbed state of $\mathcal{K}_{II}$ is taken to be $|\Omega_{II}\rangle$ of Eq. (5.8).

If we start from the first-order perturbation theory, what we meet first is a small correction to the phonon spectrum, Eq. (5.5). The eigenmode of the condensed $\mathbf{k} = 0$-particles will come into question later.

Correction to the Phonon Spectrum

In the first-order perturbation theory, $\mathcal{K}_{0II}$ yields the terms linear in a_0 or $a_0^\dagger$:

$$\langle\Omega_{II}|\ \mathcal{K}_{0II}\ |\Omega_{II}\rangle = N^{\frac{1}{2}}a_0 \frac{1}{V}\sum_{II}{}' v_{\mathbf{k}}\ \langle\Omega_{II}|\ \{a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\}\ |\Omega_{II}\rangle + \text{Herm. conj.} \tag{6.3a}$$

The expectation value can be computed, for example, as

$$\begin{aligned}\langle\Omega_{II}|\ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\ |\Omega_{II}\rangle &= \langle 0|\ \mathfrak{U}^\dagger(\theta_{\mathbf{k}})a_{\mathbf{k}}^\dagger\mathfrak{U}(\theta_{\mathbf{k}})\mathfrak{U}^\dagger(\theta_{\mathbf{k}})a_{-\mathbf{k}}^\dagger\mathfrak{U}(\theta_{\mathbf{k}})\ |0\rangle \\ &= \langle 0|\ (a_{\mathbf{k}}^\dagger \cosh\theta_{\mathbf{k}} - a_{-\mathbf{k}}\sinh\theta_{\mathbf{k}}) \\ &\qquad \times (a_{-\mathbf{k}}^\dagger \cosh\theta_{\mathbf{k}} - a_{\mathbf{k}}\sinh\theta_{\mathbf{k}})\ |0\rangle \\ &= -\sinh\theta_{\mathbf{k}}\cosh\theta_{\mathbf{k}},\end{aligned} \tag{6.3b}$$

where use has been made of Eqs. (5.3), (5.7), and (5.8). In addition to the contribution from $\mathcal{K}_{0II}$, [Eq. (6.3)], the linear terms may come from $\mathcal{K}_{0II}^{(1)}$, too [cf. Eq. (4.8)]. But the latter contribution is smaller than the former by $b/a \sim \epsilon$ and is neglected.[28]

The term linear in a_0 or $a_0^\dagger$ must be canceled by changing the chemical potential from the value of (5.1) to $\mu = \mu^{(0)} + \mu^{(1)}$, where $\mu^{(1)}$ is given by the coefficient of a_0 on the right-hand side of Eq. (6.3): Carrying the integration over $\mathbf{k}$ with the subtraction prescription in mind, we get

$$\mu^{(1)} = 8\pi\rho a\cdot 8(\rho a^3/\pi)^{\frac{1}{2}}[G_1(\nu) + G_2(\nu)] \tag{6.4a}$$

with $\nu \equiv k_0/(16\pi a\rho)^{\frac{1}{2}}$ and

$$G_1(\nu) \equiv (1+\nu^2)^{\frac{1}{2}} - \nu, \qquad G_2(\nu) \equiv (1+\nu^2)^{\frac{1}{2}} - \tfrac{2}{3}(1+\nu^2)^{\frac{3}{2}} + \tfrac{2}{3}\nu^3. \tag{6.4b}$$

It is remarkable that $\mu^{(1)}$ is of the same order as $\mu^{(0)}$. For the sake of convenient reference, we list the origin of these functions:

$$\begin{aligned}8\pi a\frac{1}{(2\pi)^3}\int_{II}{}'\langle\Omega_{II}|\ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\ |\Omega_{II}\rangle\, d\mathbf{k} &= 8\pi\rho a\cdot 8(\rho a^3/\pi)^{\frac{1}{2}}G_1(\nu), \\ 8\pi a\frac{1}{(2\pi)^3}\int_{II}{}'\langle\Omega_{II}|\ a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\ |\Omega_{II}\rangle\, d\mathbf{k} &= 8\pi\rho a\cdot 8(\rho a^3/\pi)^{\frac{1}{2}}G_2(\nu),\end{aligned} \tag{6.4c}$$

where the subtraction is indicated by prime.

Now, the change in the chemical potential causes the last term of Eq. (4.6) to revive thus affecting the coefficient $Q_{\mathbf{k}}$ in Eq. (5.2); its new value is

$$Q_{\mathbf{k}} = \tfrac{1}{2}k^2 + 4\pi a\rho + \Delta Q_{\mathbf{k}}, \quad \Delta Q_{\mathbf{k}} = -\tfrac{1}{2}\mu^{(1)}. \tag{6.5}$$

If, however, one wants to know the effect on the phonon spectrum in Eq. (5.5) now, it is to hasty because we are now asking the perturbation only on the ground state $|\Omega_{II}\rangle$ of $\mathfrak{N}_{II}$-particles. What we can conclude at this stage is the change of the zero-point energy C_{II} in Eq. (5.5), the corrected value of which is found in the spirit of the perturbation theory as

$$C_{II}' = C_{II} + \Delta C_{II}, \tag{6.6a}$$

with

$$\Delta C_{II} \equiv \sum_{II}{}' 2\Delta Q_{\mathbf{k}}\ \langle\Omega_{II}|\ a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\ |\Omega_{II}\rangle = -8\pi a\rho N\frac{512}{3}\frac{\rho a^3}{\pi}F_2(\nu), \tag{6.6b}$$

where

$$F_2(\nu) \equiv 3(1+\nu^2)^{\frac{1}{2}} - 2(1+\nu^2)^{\frac{3}{2}} + 2\nu^3. \tag{6.6c}$$

[27] In a separate paper, we shall discuss the behavior of the system related to the excited states of the $\mathfrak{N}_{II}$-particles.

[28] The first-order contribution from $\mathcal{K}_{0II}{}^{(4)}$ is zero because the state consists of pairs of particles with opposite momenta. See Eq. (I.8) in Appendix I.

It might be interesting to note here that this correction can be obtained also by modifying Eq. (5.6) in the following way as suggested by Eqs. (5.2) and (6.5):

$$C'_{II} = \sum_{II}{}' \{\tfrac{1}{2}[(k^2 - \mu^{(1)})(k^2 + 16\pi a\rho - \mu^{(1)})]^{\frac{1}{2}} - \tfrac{1}{2}(k^2 + 8\pi a\rho - \mu^{(1)})\}. \quad (6.7)$$

The Stability of the Condensed State

Having settled the question of terms linear in a_0 and $a_0^\dagger$, we now proceed to the quadratic terms. In addition to $\mathcal{K}_0$, Eq. (4.4), we have some correction terms induced by the interaction between the $\mathbf{k} = 0$-particles and the $\mathfrak{R}_{II}$-particles. Thus, the determination of the coefficients of "perturbed Hamiltonian,"

$$\mathcal{K}'_0 = 8\pi a\rho \frac{1}{2}\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}[Pa_0^\dagger a_0^\dagger + 2Qa_0^\dagger a_0 + Pa_0 a_0] + C_0, \quad (6.8)$$

will be the main task of this section. In this equation, C_0 stands for the zero-point "energy" of the $\mathbf{k} = 0$-mode.

Hitherto, our arguments have been based on the assumption of the Bose–Einstein condensation introduced in Secs. 2 and 4. Namely, we have assumed that, after the change of variable $a_0 \sim a_0 + N^{\frac{1}{2}}$ with some macroscopic number N, the matrix elements of a_0 should be of order 1. Now, if we fix the coefficients in Eq. (6.8), we can ask the condition that guarantees this assumption. It will be called the stability condition for the condensed state, or the $\mathbf{k} = 0$-stability condition. According to Appendix I, the eigenfrequency of $\mathcal{K}'_0$ would be imaginary suggesting the decay of the condensed state, unless $(Q - P)(Q + P) \geq 0$. Here, we have to exclude the equality, because, as is seen also in Appendix I, it makes the spectrum of $\mathcal{K}'_0$ continuous in contradiction to the normalizability postulate of the ground state. Finally, we have to require $Q > 0$ so that the spectrum be bounded below, otherwise the $\mathbf{k} = 0$-mode of oscillation would grow up wildly thus violating the finiteness assumption of the matrix elements of a_0 and $a_0^\dagger$. Summarizing, we find that

$$(Q - P)(Q + P) > 0 \quad \text{and} \quad Q > 0 \quad (6.9)$$

constitute the necessary condition for the Bose–Einstein condensation. In the last part of this section we shall examine the "orders of magnitude" of a_0 and $a_0^\dagger$ to know that, in the present case, the condition (6.9) is also sufficient for the condensation.

Now, we are in the position to determine the coefficients in Eq. (6.8) by computing the perturbation effects due to the $\mathfrak{R}_{II}$ particles, which, as we shall find, amounts to the same order of magnitude as the unperturbed part $\mathcal{K}_0$. The effect of $\mathfrak{R}_I$-particles is negligible because of the assumption $b/a \ll 1$.

Within the first-order perturbation theory, important is the interaction $\mathcal{K}^{(2)}_{0II}$ in Eq. (4.8) that induces

$$\langle \Omega_{II}|\ \mathcal{K}^{(2)}_{0II}\ |\Omega_{II}\rangle = 8\pi a\rho \cdot 4\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}[G_1(\nu)a_0^\dagger a_0^\dagger + 2G_2(\nu)a_0^\dagger a_0 + G_1(\nu)a_0 a_0], \quad (6.10)$$

where G_1 and G_2 have been given in Eq. (6.4). The effect of $\mathcal{K}^{(3)}_{0II}$ can be neglected.

In the second order, the interaction $\mathcal{K}_{0II}$ in Eq. (4.8) can induce the quadratic correction of the same order of magnitude as $\mathcal{K}^{(2)}_{0II}$ did in the first order:

$$\sum_{\frac{1}{2}II}{}' \frac{\langle \Omega_{II}|\ \mathcal{K}_{0II}\ |\mathbf{k}, -\mathbf{k}\rangle\langle \mathbf{k}, -\mathbf{k}|\ \mathcal{K}_{0II}\ |\Omega_{II}\rangle}{-2k(k^2 + 16\pi a\rho)^{\frac{1}{2}}}$$

$$= 8\pi a\rho \cdot 8\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}[G_3(\nu)a_0^\dagger a_0^\dagger + 2\{G_1(\nu) + G_3(\nu)\}a_0^\dagger a_0 + G_3(\nu)a_0 a_0 + G_4(\nu)], \quad (6.11a)$$

where

$$G_3(\nu) \equiv \tfrac{1}{2}(1 + \nu^2)^{-\frac{1}{2}},$$

$$G_4(\nu) \equiv \tfrac{1}{2}[(1 + \nu^2)^{\frac{1}{2}} - \nu - \tfrac{1}{2}(1 + \nu^2)^{-\frac{1}{2}} + \tfrac{1}{2}\pi - \tan^{-1}\nu], \quad (6.11b)$$

and the intermediate states are defined as

$$|\mathbf{k}, -\mathbf{k}\rangle = [\Pi_{II}\mathfrak{U}(\theta_{\mathbf{k}})]a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\ |0\rangle. \quad (6.12)$$

It would be instructive to add the following remarks: First, one should not overlook the factor 2, for example, in

$$\langle \Omega_{II}|\ \mathcal{V}_{II}\ |\mathbf{k}, -\mathbf{k}\rangle = \frac{N^{\frac{1}{2}}}{V} a_0 \sum_{\mathbf{p}\in II}{}' v_{\mathbf{p}}\ \langle \Omega_{II}|\ a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger\ |\mathbf{k}, -\mathbf{k}\rangle = 2 \times \frac{N^{\frac{1}{2}}}{V} a_0 v_{\mathbf{k}} \sinh^2\theta_{\mathbf{k}}, \quad (6.13)$$

that accounts for the two possibilities of the intermediate state, $\mathbf{p} = \pm\mathbf{k}$. Second, as warned by II/2 of $\sum'_{II/2}$ in Eq. (6.11a), the summation over the intermediate states should not be duplicated by taking $|-\mathbf{k}, \mathbf{k}\rangle$ in addition to $|\mathbf{k}, -\mathbf{k}\rangle$.

The above two exhaust[29] the induced parts of $\mathcal{K}'_0$ that are of the same order of magnitude as the unperturbed part $\mathcal{K}_0$. Summing up Eq. (4.4), (6.10), and (6.11), we get the coefficients in Eq. (6.8),

[29] The second-order effect of $\mathcal{K}_{0II}{}^{(4)}$ vanishes again because of the structure of $|\Omega_{II}\rangle$ mentioned in the previous footnote.

$$P = X - \frac{b}{a}\left(\frac{\pi}{\rho a^3}\right)^{\frac{1}{2}},$$
$$Q = X, \tag{6.14}$$

where[30]

$$X \equiv 8[(1+\nu^2)^{\frac{1}{2}} - \nu + (1+\nu^2)^{-\frac{1}{2}}],$$

and the value of the chemical potential [(5.1) and (6.4)], has been used to compute Q. The zero-point "energy" is found to be

$$C_0 = [\tfrac{1}{2}\rho v_0 - (\mu^{(0)} + \mu^{(1)})]N + 8\pi a\rho \cdot \frac{1}{2}\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}} \cdot [(Q^2 - P^2)^{\frac{1}{2}} - Q + 16G_4(\nu)]. \tag{6.15a}$$

and the excitation spectrum to be multiples of ω_0, where

$$\omega_0 = 8\pi a\rho\left(\frac{b}{a}\right)^{\frac{1}{2}}\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{4}}\left[2X - \frac{b}{a}\left(\frac{\pi}{\rho a^3}\right)^{\frac{1}{2}}\right]^{\frac{1}{4}}. \tag{6.15b}$$

From Eq. (6.14), we see immediately that $Q > 0$ and $Q - P > 0$ so that the condition (6.9) can be written as $Q + P > 0$. Namely,

$$\frac{b}{a}\left(\frac{\pi}{\rho a^3}\right)^{\frac{1}{2}} < 2X. \tag{6.16}$$

We call this the $\mathbf{k} = 0$-stability condition to differentiate it from the stability condition for $\mathfrak{R}_{\mathrm{I}}$-particles which will be discussed in the next section.

It is interesting to remark here that we would get the same condition as Eq. (6.16) even if we did not take the unit $\hbar = 1$, $2m = 1$. This is because we can restore m and $\hbar$ if we multiply every term of $\mathcal{K}$ by a common factor $\hbar^2/(2m)$. Thus, the condensation condition is independent of the mass when it is written in terms of the scattering lengths. Suppose we take the hard-core radius a as the unit of length, then the right-hand side of Eq. (6.16) is a function of the range $1/k_0$ of the attractive potential (see Fig. 1). It is reasonable that the more likely the condensation is the larger the density ρ we take; qualitatively, this tendency is shared by the free Bose gas.[31] The limit on b means that the total scattering length or the strength of the attractive potential should not be too large. However, it seems to be hard to understand that the limit on b decreases as the range $1/k_0$ becomes smaller. The further discussion of this condition is given in Sec. 8.

Now, in order to find the ground state $|\Omega_0\rangle$ of $\mathcal{K}_0'$ we can use the formulas in Appendix I:

$$|\Omega_0\rangle = \mathfrak{U}(\theta_0)\,|0\rangle. \tag{6.17}$$

Since P and Q in Eq. (6.14) is of order 1, we see that the matrix elements of a_0 and $a_0^\dagger$ are also of the order of magnitude 1, thus confirming our starting assumption of the "small oscillation." In conclusion, the condition (6.16) is necessary and sufficient for the condensation assumption to be valid, when the order of magnitude relation (3.12) is presumed.

VII. THE $\mathfrak{R}_{\mathrm{I}}$-PART

Now, we want to conclude the diagonalization of the "Hamiltonian" by determining the $\mathfrak{R}_{\mathrm{I}}$-part of the energy spectrum. If one is familiar with Huang's work,[4] it will be interesting to discuss the relation between his method and ours of managing the conservation of particle number: while Huang took it into account somewhat explicitly, we have taken an implicit way by invoking the chemical potential. The approximation we make is the same as Huang's.

Diagonalization

The first task is to determine the effective interaction among $\mathfrak{R}_{\mathrm{I}}$-particles induced by their interaction $\tilde{\mathcal{K}}_{\mathrm{I\,II}}$, Eq. (4.10), with the $\mathfrak{R}_{\mathrm{II}}$-particles. According to Huang, the interaction $\tilde{\mathcal{K}}_{\mathrm{I\,II}}$ can be approximated by the sum of the following two:

$$\mathcal{K}_{\mathrm{I\,II}} = \mathcal{V}_{\mathrm{I\,II}} + \mathcal{V}_{\mathrm{I\,II}}^\dagger \quad \text{and} \quad \mathcal{K}_{\mathrm{I\,II}}^{(2)} = \mathcal{V}_{\mathrm{I\,II}}^{(2)} + \mathcal{V}_{\mathrm{I\,II}}^{(2)\dagger},$$

where

$$\mathcal{V}_{\mathrm{I\,II}} = 8\pi a\frac{N^{\frac{1}{2}}}{V}\sum_{\mathbf{K}}\sum_{\lambda,\mathbf{P}}\delta(\mathbf{P}+\mathbf{K}-\lambda) \times (a_{\mathbf{P}}^\dagger a_{\mathbf{K}}^\dagger + a_{\mathbf{P}}^\dagger a_{-\mathbf{K}})a_\lambda$$
$$\mathcal{V}_{\mathrm{I\,II}}^{(2)} = 8\pi a\frac{1}{2V}\sum_{\mathbf{K}}{}'\sum_{\lambda}(a_{\mathbf{K}}^\dagger a_{-\mathbf{K}}^\dagger a_\lambda a_{-\lambda} + a_{\mathbf{K}}^\dagger a_{\mathbf{K}} a_\lambda^\dagger a_\lambda); \tag{7.1}$$

the Roman capitals and the Greek denote the momenta in $\mathfrak{R}_{\mathrm{II}}$ and $\mathfrak{R}_{\mathrm{I}}$, respectively,

$$\mathbf{K}, \mathbf{P} \in \mathfrak{R}_{\mathrm{II}} \quad \text{and} \quad \lambda \in \mathfrak{R}_{\mathrm{I}}.$$

Since these two, $\mathcal{K}_{\mathrm{I\,II}}$ and $\mathcal{K}_{\mathrm{I\,II}}^{(2)}$, are quite similar to $\mathcal{K}_{0\mathrm{II}}$ and $\mathcal{K}_{0\mathrm{II}}^{(2)}$, respectively, we can determine the influence of the $\mathfrak{R}_{\mathrm{II}}$-particles on the $\mathfrak{R}_{\mathrm{I}}$ just in the same way as we have determined that of the $\mathfrak{R}_{\mathrm{II}}$ on the $\mathbf{k} = 0$-particles. In fact, it can be obtained from the results in the last section by a simple substitution, $a_0 \to a_\lambda$ (we take advantage of the fact $|\lambda| \ll |\mathbf{p}|$).

As for the unperturbed part of the "Hamiltonian,"

[30] Apart from the normalization, this function is different from Huang's by the term $-\nu$, which is due to the subtraction.

[31] L. D. Landau and E. M. Lifschitz, *Statistical Physics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1958).

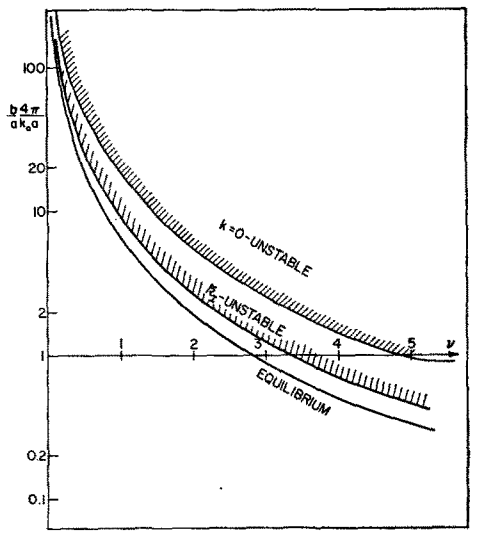

FIG. 2. The relations between the parameters of the potential and the particle density. They represent the relation in the lowest energy state, Eq. (8.11), the $\mathbf{k} = 0$-stability condition, [Eq. (6.16) or (8.12)] and the $\mathfrak{R}_I$-stability condition [Eq. (7.7b) or (8.12)].

our attention should be called, however, to the slight difference in structure between $\mathcal{K}_0$ and $\mathcal{K}_I$ as remarked below Eq. (4.9): in addition to the terms that have counterparts in $\mathcal{K}_0$, we have $-8\pi b(N/V)\cdot\sum_I a_k^\dagger a_k$ in $\mathcal{K}_I$ which together with the kinetic energy term makes the Q_λ, Eq. (7.3), different from the corresponding quantity Q for $\mathbf{k} = 0$-particles, Eq. (6.14).

Thus, by applying the necessary modifications to Eqs. (6.8), (6.14), and (6.15), we obtain the perturbed "Hamiltonian" for $\mathfrak{R}_I$-particle:

$$\mathcal{K}_I' = \sum_I [P_\lambda a_\lambda^\dagger a_{-\lambda}^\dagger + 2Q_\lambda a_\lambda^\dagger a_\lambda + P_\lambda a_\lambda a_\lambda] + C_I, \quad (7.2)$$

with

$$P_\lambda \equiv 8\pi a\rho\cdot\frac{1}{2}\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}\left[X - \frac{b}{a}\left(\frac{\pi}{\rho a^3}\right)^{\frac{1}{2}}\right], \quad (7.3)$$

$$Q_\lambda \equiv \tfrac{1}{2}\lambda^2 + P_\lambda$$

and

$$C_I \equiv 8\pi a\rho\cdot 4\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}\sum_\lambda{}' O(1). \quad (7.4)$$

The spectrum of $\mathcal{K}_I'$ is readily obtained by the use of the Bogoliubov transformation to be

$$\mathcal{K}_I' = \sum_\lambda \lambda(\lambda^2 + 16\pi a'\rho)^{\frac{1}{2}} + C_I$$

with

$$a'/a = (\rho a^3/\pi)^{\frac{1}{2}}X - (b/a), \quad (7.5)$$

where X is given in Eq. (6.14). We have to note here that the stability condition

$$\lambda^2 + 16\pi a'\rho > 0 \quad (7.6)$$

is satisfied by all $\lambda \in \mathfrak{R}_I$ when and only when

$$a' > 0, \quad (7.7a)$$

or written out explicitly,

$$\frac{b}{a}\left(\frac{\pi}{\rho a^3}\right)^{\frac{1}{2}} < X. \quad (7.7b)$$

This condition differs from the stability condition for the $\mathbf{k} = 0$-particles [Eq. (6.16)] only by a factor 2 on the right-hand side of the latter. Even if the latter condition is satisfied, a' can be negative so that the condition (7.6) can be violated by some λ's. We call this kind of instability $\mathfrak{R}_I$-instability. The relation (7.7b) is shown in Fig. 2. In the same way as explained for $\mathbf{k} = 0$-instability, we can see that the $\mathfrak{R}_I$-instability results in large matrix elements of $a_\lambda^\dagger a_\lambda$ etc., thus violating our starting assumption (see Sec. 4). We see in Sec. 8 that Eq. (7.7) is nothing but the condition for the sound velocity to be real.

Method of the Chemical Potential

Now, let us proceed to compare the method of Huang and ours to manage the conservation of particle number.

In order to secure the conservation Huang made a substitution (2.3) as seen in Eq. (34) of his paper, while we are relying upon the chemical potential. Obviously, there is no one-to-one correspondence between the terms of Huang's $\mathcal{H}$ and our $\mathcal{K}$. Nevertheless, the energy spectra resulting from these two theories are quite similar to each other, the only difference consisting in what is meant by the particle density ρ: while our ρ means the average density of the $\mathbf{k} = 0$-particles,[32] Huang's ρ means the total density. Remembering the applicability limit of the pseudopotential, however, we know that this difference is not so substantial.

For the sake of indicating that there is still some sort of correspondence among the terms of Huang's $\mathcal{H}$ and our $\mathcal{K}$, we compare Huang's $\mathcal{H}_I$ in his Eq. (68) with our $\mathcal{K}_I + \mathcal{K}_{I\,II} + \mathcal{K}_I^{(2)}{}_{II}$, both being intended for the Hamiltonian of the $\mathfrak{R}_I$-particles in interaction with the $\mathfrak{R}_{II}$-particles. One of the remarkable differences consists in that the term

$$-4\pi a V^{-1}\sum_K (a_K^\dagger a_{-K}^\dagger + a_K a_{-K})a_\lambda^\dagger a_\lambda \quad (7.8)$$

[32] Thus, the so-called depletion effect is automatically taken into account.

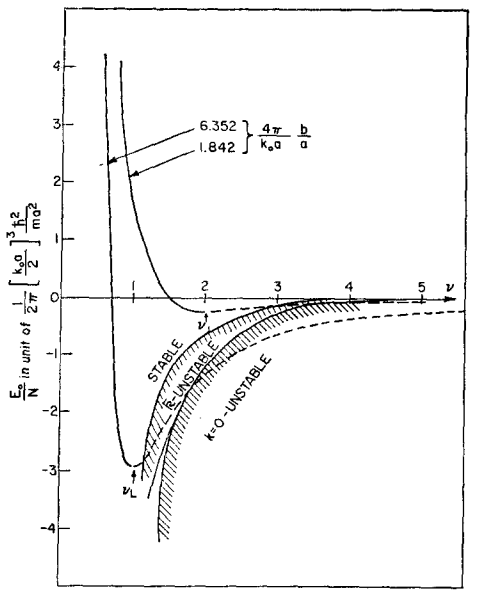

FIG. 3. The energy per particle is shown as a function of the particle density. The parameters of the potential are fixed. The regions of stability are also shown.

in Huang's Eq. (68) is missing in our $\mathcal{K}_{\rm I}+\mathcal{K}_{\rm I\,II}+\mathcal{K}^{(2)}_{\rm I\,II}$. This term is generated by his substitution (2.3). At the same time, we observe that the terms

$$8\pi a V^{-1}\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}a_{\lambda}^{\dagger}a_{\lambda}-\mu^{(1)}a_{\lambda}^{\dagger}a_{\lambda} \tag{7.9}$$

in our "Hamiltonian" do not find their counterpart in Huang's, in which the second term does not exist by its very nature and the first one is amalgamated into his V_0', thus being neglected [see Eq. (29) and Sec. 4 of his paper]. These constitute the only difference that may affect the first-order perturbation effects by the $\mathfrak{N}_{\rm II}$-particles. Now, by taking the matrix elements with the ground state of $\mathfrak{N}_{\rm II}$-particles we see in fact that Eq. (7.8) and Eq. (7.9) result in one and the same effective interaction among the $\mathfrak{N}_{\rm I}$-particles! This completes the comparison between Huang's method and ours.

VIII. PROPERTIES OF THE SYSTEM

Having completed the diagonalization of the "Hamiltonian," we can draw various conclusions concerning the properties of the Huang model, among which we want to concentrate our attention to the properties of the ground state.

Ground-State Energy vs Density

Now, assuming that the system is in the ground state with no phonon excited, we collect the zero-point "energies" in Eqs. (5.6), (6.6a), (6.15a), and (7.4), to which we add $(\mu^{(0)}+\mu^{(1)})N_{\rm tot}$ to obtain the ground state energy E_0 in its true sense of words. We know, however, that the second term of C_0, Eq. (6.15a), is not macroscopic and $\Delta C_{\rm II}$ and $C_{\rm I}$, Eqs. (6.6b) and (7.4), are smaller by ϵ than the other contributions so that they are neglected. Thus,

$$\frac{E_0}{N}=-4\pi\rho b+8\pi\rho a\cdot\frac{64}{15}\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}F_1(\nu). \tag{8.1}$$

In our approximation, N can be regarded as the *total* number of particles since, as seen from Eq. (6.4c), even the average number of particles in $\mathfrak{N}_{\rm II}$ is given by

$$\frac{V}{(2\pi)^3}\int_{\rm II}'\langle\Omega_{\rm II}|\,a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\,|\Omega_{\rm II}\rangle\,d\mathbf{k}$$
$$=N\cdot 8\left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}}G_2(\nu)\sim\epsilon N. \tag{8.2}$$

It is quite satisfactory that the energy of the system is thus proved to be an extensive quantity.

By the way, it was from this result, Eq. (8.2), that Huang and others concluded the consistency of their approximation procedure.[2,4] As we have seen, however, the condensation can be unstable even when the theory yields Eq. (8.2).

In Fig. 3, we plot the energy per particle as a function of $\nu=k_0/(16\pi a\rho)^{\frac{1}{2}}$; written down explicitly, Eq. (8.1) is cast into the following form,

$$\frac{E_0}{N}=\frac{4\pi^2}{a^2}\left(\frac{k_0a}{4\pi}\right)^3\frac{1}{\nu^2}\left[-\frac{4\pi}{k_0a}\frac{b}{a}+2\cdot\frac{64}{15}\frac{1}{\nu}F_1(\nu)\right]. \tag{8.3}$$

When the parameters of the potential are fixed, the variable ν can be regarded as representing the particle density ρ. The unit of energy can be taken as $(4\pi^2/a^2)(k_0a/4\pi)^2$, which turns out to be

$$\frac{1}{2\pi}\left(\frac{k_0a}{2}\right)^3\frac{\hbar^2}{2ma^2}$$

if we call back the mass of the particle m (that has been set equal to $\frac{1}{2}$) and the Planck constant $\hbar$.

Finally, we notice that Eq. (2.10) holds in this case, too. In fact we see from Eqs. (8.1), (5.1), and (6.4) that

$$(\partial/\partial\rho)(E_0/V)=\mu^{(0)}+\mu^{(1)}.$$

Sound Velocity

Since the excitation of the Huang system is of phonon type, it is interesting to compute the sound velocity c from the energy-density relation, Eq. (8.1), and to confirm that the excitation with low momentum $\mathbf{p}$ actually has the energy quantum

$$\omega(\mathbf{p})\cong cp \tag{8.4}$$

as suggested by Landau.[31,33] Although the computa-

[33] L. D. Landau, J. Phys. (USSR) 5, 71 (1940).

tion of c was done by Huang, we have to renew it because our functions involved, $F_1(\nu)$ and X, are slightly different from Huang's (see Footnotes 25 and 30).

The sound velocity is related to the compressibility of the system,

$$c^2 = -2\,\partial P/\partial\rho, \tag{8.5}$$

where

$$P = \rho^2\,(\partial/\partial\rho)(E_0/N) \tag{8.6}$$

is the pressure at absolute zero and we have taken into account that the mass of the particle has been put equal to $\frac{1}{2}$. Combining the above two, we have

$$\frac{c^2}{4\rho} = \left(\frac{\partial}{\partial\rho} + \frac{1}{2}\,\rho\,\frac{\partial}{\partial\rho^2}\right)\frac{E_0}{N}. \tag{8.7}$$

The derivatives will be conveniently computed in terms of ν:

$$\rho = (A/\nu)^2, \quad \partial/\partial\rho = -\tfrac{1}{2}A^{-2}\nu^3\,(\partial/\partial\nu) \qquad A \equiv k_0/(16\pi a)^{\frac{1}{2}}. \tag{8.8}$$

Then, from Eq. (8.1) we obtain

$$c^2 = 16\pi a'\rho,$$

where a' is related to the excitation spectrum [Eq. (7.5)] to show the correctness of our anticipation (8.4). We see also that the condition for the $\mathfrak{N}_1$-stability, Eq. (7.7), is equivalent to the condition for the sound velocity to be real.

Liquid State

From Eq. (8.3), we see that the energy per particle behaves in the following way:

$$\frac{E_0}{N} \sim \begin{cases} 8\pi a\rho\cdot\frac{64}{15}(\rho a^3/\pi)^{\frac{1}{2}} (\nu \sim 0), \\ -4\pi b\rho \qquad\qquad (\nu \to \infty). \end{cases} \tag{8.9}$$

Thus, a minimum is reached at some $\nu = \nu_L$ where

$$\frac{\partial}{\partial\rho}\left(\frac{E_0}{N}\right) = 0 \quad \text{and} \quad \frac{\partial^2}{\partial\rho^2}\left(\frac{E_0}{N}\right) > 0. \tag{8.10}$$

If one wants to know the relation between ν_L and the force parameters, it is convenient to rewrite the first condition in Eq. (8.10) as

$$\frac{b}{a}\frac{4\pi}{k_0 a} = 32\,\frac{1}{\nu}\left[(1+\nu^2)^{\frac{1}{2}} - (1+\nu^2)^{\frac{3}{2}} + \frac{2}{5}(1+\nu^2)^{5/2} - \frac{1}{4}\nu - \frac{2}{5}\nu^5\right] \quad (\nu = \nu_L). \tag{8.11}$$

We call the density ρ_L corresponding to ν_L the equilibrium density. The behavior of E_0/N is illustrated in Fig. 3 and the relation (8.11) in Fig. 2.

Now, taking Eq. (8.10) into account, we know from Eq. (8.7) that, at the equilibrium density, the Huang system satisfies the $\mathfrak{N}_1$-stability condition and therefore the $\mathbf{k} = 0$-stability condition as well. We can conclude that the consistency of our approximation scheme is thus guaranteed at least for the purpose of investigating the states in the neighborhood of the lowest energy.

Since we are considering the Huang system at the temperature absolute zero, it is quite natural that the system has an equilibrium density: In fact, it means the liquid state. If the volume containing it is fixed at such a value that $N/V > \rho_L$, the system would first tend to expand when V is increased from this value. This is the state of compressed liquid. However, when V is made to increase further until the equilibrium density is reached, $N/V = \rho_L$, the presence of the box becomes immaterial. Any further increase of V beyond this point leaves the energy and the density of the system unaffected; rather, we shall see the system lump in some part of the container. This is the characteristic feature of a liquid. We have to conclude that the part of the energy-density curve for $\nu > \nu_L$ cannot be reached unless the system is heated.

Stability Conditions

In the above argument we have seen that the stability conditions are satisfied at the equilibrium point. Now, we want to show that the conditions are also satisfied by any state physically accessible at absolute zero. In other words, the conditions are always satisfied by the system with density

$$\rho \geq \rho_L.$$

Then, the consistency of our approximation scheme will be confirmed also for the compressed state of the Huang liquid with the obvious reservation that the liquid should remain at low density, $(\rho a^3)^{\frac{1}{2}} \ll 1$. For this purpose, it is sufficient to rewrite the stability conditions as

$$\frac{b}{a}\frac{4\pi}{k_0 a} < \begin{Bmatrix} 16 \\ 8 \end{Bmatrix}\frac{1}{\nu}\left[(1+\nu^2)^{\frac{1}{2}} - \nu + (1+\nu^2)^{-\frac{1}{2}}\right], \tag{8.12}$$

where the factor 16 in the curly bracket stands for the $\mathbf{k} = 0$-stability and 8 for $\mathfrak{N}_1$-stability. Since we know that the above inequalities hold for $\nu = \nu_L$, we can conclude the stability for $\rho > \rho_L$ from the fact that the right-hand side of Eq. (8.12) is a decreasing function of ν. Now, let $\nu_c^{(i)}$ $(i = 1, 2)$ represent the critical densities which correspond to the $\mathfrak{N}$- and $\mathbf{k} = 0$-instability respectively; namely for $\nu > \nu_c^{(i)}$ the corresponding instability occurs. In

Fig. 3, we present the boundaries of instabilities which are described by the points $(\nu_0^{(i)}, E_0/N)$ when the force parameters are varied. The conditions (8.12) are shown in Fig. 2 together with the equilibrium condition (8.11).

IX. MATHEMATICAL BACKGROUND

In the previous sections, we have seen that the replacement (4.2) can provide a consistent approximation scheme for the eigenvalue problem of the Huang model when the Bose–Einstein condensation is presumed. But, is the replacement (4.2) a necessary consequence of the condensation presumption? Since we have been trying to find the lowest eigenstate and its neighbors, it seems physically reasonable to presume the condensation. However, it is not *a priori* obvious that there exists no other approximation scheme that would yield the lower eigenstates than the ones we obtained in our scheme.

In this section, we want to present a mathematical background that would make the following statement plausible, though not firmly established: The Bose–Einstein condensation necessitates the replacement (4.2) when the system is infinitely large ($N \to \infty$). Here, the Bose–Einstein condensation in the interacting system is defined by the requirements (1) that the fluctuation[34] of the occupation number n_0 of $\mathbf{k} = 0$-level is at most of the order of $\langle n_0 \rangle_{\rm av}^{\frac{1}{2}}$ and (2) that $\langle n_0 \rangle_{\rm av}$ is the finite fraction of $N_{\rm tot}$, the total number of particles, when $N_{\rm tot} \to \infty$. For the more specific definition, see Eq. (9.19) below. We have also to add that the above statement is the consequence of the irreducibility requirement for the representation of canonical commutation relations, which constitute our first subject.

Representation of Canonical Variables

The many-body system under consideration can be described by a Bose field,

$$\phi(\mathbf{x}) = \sum_{\mathbf{k}} (2V)^{-\frac{1}{2}}[a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\mathbf{x}} + a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{x}}], \tag{9.1}$$

and its canonical conjugate

$$\pi(\mathbf{x}) = \sum_{\mathbf{k}} i(2V)^{-\frac{1}{2}}[a_{\mathbf{k}}^{\dagger} e^{-i\mathbf{k}\mathbf{x}} - a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{x}}], \tag{9.2}$$

where $\mathbf{k} = (2\pi/V^{\frac{1}{3}})\cdot\mathbf{n}$ and $\mathbf{n} = (n_x, n_y, n_z)$, $n_x = 0, \pm 1, \pm 2, \cdots$, etc. They are self-adjoint and satisfy the canonical commutation relations

$$[\phi(f), \pi(g)] = i(f, g), \tag{9.3}$$

$$[\phi(f), \phi(g)] = [\pi(f), \pi(g)] = 0, \tag{9.4}$$

where

$$\phi(f) = \int d\mathbf{x}\, f(\mathbf{x})\phi(\mathbf{x}), \quad \pi(g) = \int d\mathbf{x}\, g(\mathbf{x})\pi(\mathbf{x}),$$
$$(f, g) = \int d\mathbf{x}\, f(\mathbf{x})g(\mathbf{x}), \tag{9.5}$$

and the test functions, $f(\mathbf{x})$ and $g(\mathbf{x})$, are assumed to be real and $\in L_2$, the first assumption being necessary for $\phi(f)$ and $\pi(g)$ to be self-adjoint and the second for (f, g), or more especially for $||f|| = (f, f)^{\frac{1}{2}}$ to exist. Later, we see the need to assume further $f, g \in L_1$.

The representation is realized when we construct an appropriate Hilbert space $\mathfrak{H}$ and define the action of $\phi(f)$ and $\pi(g)$ therein. A well-known example is the Fock representation in which the Hilbert space is spanned by the eigenstates of $a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$ belonging to the rational class of Gårding–Wightman,[7] so that $a_{\mathbf{k}}^{\dagger}$ and $a_{\mathbf{k}}$ serve as creation and annihilation operators, respectively.

In order to explain the other way of constructing the representation, which is called the Gelfand construction,[14] we introduce the Wightman functional,

$$E(f, g) = \langle \Psi, U(f)V(g)\Psi \rangle, \tag{9.6}$$

where Ψ is a cyclic vector[35] and

$$U(f) = \exp[i\phi(f)], \qquad V(g) = \exp[i\pi(g)]. \tag{9.7}$$

These operators are unitary and satisfy the following version of the commutation relations [(9.3) and (9.4)]:

$$U(f)V(g) = V(g)U(f) \exp[-i(f, g)], \tag{9.8}$$

$$U(f)U(g) = U(f + g), \quad V(f)V(g) = V(f + g). \tag{9.9}$$

In terms of the Wightman functional, the commutation relation (9.8) takes the form

$$E^*(f, g) = E(-f, -g) \exp[-i(f, g)], \tag{9.10a}$$

and the others [Eq. (9.9)] are implicit in the definition of the functional. In addition to the obvious condition,

$$E(0, 0) = 1; \tag{9.10b}$$

it should satisfy the positivity condition

$$\sum_{i,j} \lambda_i \lambda_j^* E(f_i - f_j, g_i - g_j) \times \exp[-i(f_i - f_j, g_i)] \geq 0, \tag{9.10c}$$

which says that any vector of the form

$$|u\rangle = \sum_i \lambda_i U(f_i)V(g_i)\,|\Psi\rangle$$

should have a nonnegative norm.

[34] The fluctuation of n_0 in the Huang model is computed in Appendix II. It is in fact proportional to $\langle n_0 \rangle_{\rm av}^{1/2}$.

[35] We confine ourselves to a representation with cyclic vector. See Footnote 15.

Conversely, if a functional $E(f, g)$ satisfies the conditions (9.10a–c) it can be shown to define a representation of canonical commutation relations up to unitary equivalence. This is accomplished by the Gelfand construction.

In the Fock representation, the Wightman functional is given by[9]

$$E_{\mathrm{F}}(f, g) = \langle 0|\, U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |0\rangle = \exp\left[-\tfrac{1}{4}\,||f||^2 - \tfrac{1}{4}\,||g||^2 - \tfrac{1}{2}i(f, g)\right], \quad (9.11)$$

when we take the cyclic vector to be the vacuum $|0\rangle$. The field operators in this representation are denoted by $\phi_{\mathrm{F}}(\mathbf{x})$ and $\pi_{\mathrm{F}}(\mathbf{x})$.

The Case of Free Bose Gas

Araki and Woods have constructed a representation suitable for describing the *infinite* free Bose gas under Bose–Einstein condensation. The necessity of constructing a representation other than Fock's has already been shown in Sec. 2 of this paper.

They have begun with considering a free Bose gas of density ρ confirmed in a cubic volume $V < \infty$. When we require the representation space to contain the ground state, it is natural to identify the cyclic vector Ψ with the ground state itself. Thus, assuming the gas to be of temperature zero, they take the normalized state vector in which all the particles are found condensed in the $\mathbf{k} = 0$-level,

$$|\Psi(V)\rangle = |N\rangle \equiv |n_0 = N, n_{\mathbf{k}} = 0 \text{ for } \mathbf{k} \neq 0\rangle, \quad (9.12)$$

to compute the Wightman functional

$$E_V(f, g) = \langle N|\, U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |N\rangle \quad (N = \rho V). \quad (9.13)$$

The point here is that, as far as $N < \infty$, we can use the Fock operators $U_{\mathrm{F}}(f)$ and $V_{\mathrm{F}}(g)$ to represent the Bose field.

Now, in order to obtain a Wightman functional that provides a representation of the infinite system, they take the limit $V \to \infty$ keeping $\rho = N/V$ constant, to find[36]

$$\lim_{V\to\infty} E_V(f, g) = \int_0^{2\pi} E_\alpha(f, g)\,\frac{d\alpha}{2\pi}. \quad (9.14)$$

This expression corresponds to Eq. (2.26) in Sec. 2 with Eq. (2.27) taken into account. As has been explained there, the integral expression (9.14) means that the representation reached through the limiting procedure is reducible to a direct sum of representations labeled by α, $0 \leq \alpha \leq 2\pi$. In addition, Araki and Woods have shown that the new representations defined by the integrand Wightman functionals $E_\alpha(f, g)$ can readily be related to the Fock representation. In terms of the Wightman functionals, it means that we have the following expression for the integrand of Eq. (9.14):

$$E_\alpha(f, g) = \langle 0|\, U_\alpha(f)V_\alpha(g)\, |0\rangle, \quad (9.15)$$

where U_α and V_α are obtained from those in Eq. (9.7) by replacements,

$$\begin{aligned} \phi(\mathbf{x}) &\to \phi_\alpha(\mathbf{x}) \equiv \phi_{\mathrm{F}}(\mathbf{x}) + (2\rho)^{\frac{1}{2}} \cos\alpha, \\ \pi(\mathbf{x}) &\to \pi_\alpha(\mathbf{x}) \equiv \pi_{\mathrm{F}}(\mathbf{x}) + (2\rho)^{\frac{1}{2}} \sin\alpha. \end{aligned} \quad (9.16)$$

Since the representation is fixed by the Wightman functional, we can conclude that the component representations in Eq. (9.14) is realized by using the operators, $\phi_\alpha(\mathbf{x})$ and $\pi_\alpha(\mathbf{x})$, together with the cyclic vector $|0\rangle$. We have also to note that the irreducibility of these component representations follows from the irreducibility of the Fock representation.

Referring to the expansions of field operators [Eqs. (9.1) and (9.2)], one may notice that the relation (9.15) can, roughly speaking, be written as

$$a_{\mathbf{k}} \to a_{\mathbf{k}}^{\mathrm{F}} + (\rho V)^{\frac{1}{2}} e^{i\alpha}\delta_{\mathbf{k},0}, \quad (9.17)$$

which is the replacement we have adopted in the previous discussions [see Eqs. (2.5) and (4.2)]. More precisely, we are to make the substitution (9.17) already in the case of finite system $V < \infty$, where this procedure can be regarded as an unitary transformation, and it does not matter which operator, the left- ($a_{\mathbf{k}}$ means the Fock operator here) or right-hand side of Eq. (9.17), to use. When we go to the limit $V \to \infty$, the original Fock representation [left-hand side of Eq. (9.17)] becomes decomposable. If, however, we start with using the representation on the right-hand side of Eq. (9.17), we can keep the irreducibility of the representation at $V \to \infty$. Moreover, the matrix elements of a_0^{F} do not grow up with $V \to \infty$. This last property can be conveniently used to construct an approximation scheme for the many-boson problems.

The convergence of the "Hamiltonian" in this limiting procedure can be discussed in the same way as in the fermion case treated before.[12]

In conclusion, we have to go through the following process if we want to take an irreducible representation to describe an infinite free Bose gas: Make the replacement (9.17) first and then let $V \to \infty$ after computing the quantities of physical interest!

The Case of Interacting Bosons

We now proceed to the consideration of the case of interacting bosons. The point is to replace the

[36] The explicit form of the integrand is given in Eq. (III.10) in Appendix III.

free-particle ground state (9.12) by a superposition of states in which some of the particles are brought into the excited states by the interparticle interaction. Though the model employed here is a little too simple to simulate the realistic model of Huang, it would serve to indicate what could happen in the limit of infinite system.

We compute the Wightman functional by taking a normalized cyclic vector of the form

$$|\Psi(V)\rangle = \sum_{\nu} |N-\nu\rangle\, |\Psi^{(\nu)}(V)\rangle, \qquad (9.18)$$

where $N-\nu$ is the number of the $\mathbf{k}=0$-particles [see Eq. (9.12) above], $|\Psi^{(\nu)}\rangle$ represents the state of ν particles which are excited to the $\mathbf{k}\neq 0$ levels by the interaction, and $\sum_{\nu} ||\Psi^{(\nu)}(V)||^2 = 1$. The reason why we assume the vector $|\Psi(V)\rangle$ to be of sharp particle number is that it is intended for the ground state in a finite volume V. The nonconservation of the particle number can take place only when $V\to\infty$.

In the case of the Huang model, we find in Appendix 2 that the fluctuation of the number of the $\mathbf{k}=0$-particles, $n_0 = N-\nu$, is of the order of $N^{\frac{1}{2}}$. It seems reasonable to take this property as the definition of the Bose–Einstein condensation in the interacting system together with the obvious property that the average number $\langle N_0\rangle_{\mathrm{av}} \approx N$ is macroscopic (proportional to the volume V). In order to simplify the discussion, however, we have to assume that[37]

$$|\Psi^{(\nu)}(V)\rangle = 0 \quad \text{unless} \quad \nu \leq \sigma N^{\frac{1}{2}-\delta} \qquad (9.19)$$

with some positive numbers, σ and δ. We hope that it will be meaningful to take the limit $\delta\to 0$ after the whole computation.

Now, our task is to compute the Wightman functional first for a finite V,

$$E_V(f,g) = \sum_{\mu,\nu} \langle N-\mu;\Psi^{(\mu)}(V)| \times U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |N-\nu;\Psi^{(\nu)}(V)\rangle, \qquad (9.20)$$

and then to examine what representation of field operators comes out in the limit $V\to\infty$ with $\rho = N/V$ kept constant.[38] Because of the assumption (9.19), the summation over (μ,ν) can give an infinite series when $N\to\infty$. Instead of taking the limit $V = N/\rho\to\infty$ of Eq. (9.20) as a whole, we shall simply assume that the same limit can be reached through the following two-step procedure:

$$\lim_{V\to\infty} E_V(f,g) = \lim_{V'\to\infty} \sum_{\mu,\nu}^{(V')} \lim_{V\to\infty} \langle N-\mu;\Psi^{(\mu)}(V)| \times U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |N-\nu;\Psi^{(\nu)}(V)\rangle. \qquad (9.21)$$

In this paper, we do not want to enter the discussion of this conventional procedure but just to assume its validity. The mathematical details will be discussed elsewhere.

By introducing the Fourier transform

$$\tilde{f}(\mathbf{k}) = \int_V d\mathbf{x}\, f(\mathbf{x}) e^{i\mathbf{k}\mathbf{x}}, \qquad (9.22a)$$

and a conventional notation

$$\tilde{f}_V(\mathbf{k}) = (2V)^{-\frac{1}{2}}\tilde{f}(\mathbf{k}), \qquad (9.22b)$$

we can easily see that

$$U_{\mathrm{F}}(f)V_{\mathrm{F}}(g) = E_{\mathrm{F}}(f,g;V) : U_{\mathrm{F}}(f)V_{\mathrm{F}}(g) :, \qquad (9.23)$$

where

$$: U_{\mathrm{F}}(f)V_{\mathrm{F}}(g) : = \prod_{\mathbf{k}} \exp\left[\{i\tilde{f}_V^*(\mathbf{k}) - \tilde{g}_V^*(\mathbf{k})\}a_{\mathbf{k}}^\dagger\right] \times \prod_{\mathbf{k}} \exp\left[\{i\tilde{f}_V(\mathbf{k}) + \tilde{g}_V(\mathbf{k})\}a_{\mathbf{k}}\right], \qquad (9.24)$$

is the normal product and the notation $E_{\mathrm{F}}(f,g;V)$ will be self-explanatory. In particular,

$$\lim_{V\to\infty} E_{\mathrm{F}}(f,g;V) = E_{\mathrm{F}}(f,g), \qquad (9.25)$$

with the right-hand side being given by Eq. (9.11). Accordingly, the matrix elements in Eq. (9.21) can be split into three factors:

$$\langle N-\mu;\Psi^{(\mu)}(V)|\, U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |N-\nu;\Psi^{(\nu)}(V)\rangle = E_{\mathrm{F}}(f,g;V)\cdot\langle N-\mu|\, :U_{\mathrm{F}}(f)V_{\mathrm{F}}(g):\, |N-\nu\rangle \cdot\langle\Psi^{(\mu)}(V)|\, :U_{\mathrm{F}}(f)V_{\mathrm{F}}(g):\, |\Psi^{(\nu)}(V)\rangle.$$

The first factor can be absorbed by the third:

$$\langle N-\mu;\Psi^{(\mu)}(V)|\, U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |N-\nu;\Psi^{(\nu)}(V)\rangle = \langle N-\mu|\, :U_{\mathrm{F}}(f)V_{\mathrm{F}}(g):\, |N-\nu\rangle \cdot\langle\Psi^{(\mu)}(V)|\, U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |\Psi^{(\nu)}(V)\rangle. \qquad (9.26)$$

We shall see in Appendix III that, under the assumption (9.19) we have

$$\lim_{V\to\infty} \langle N-\mu|\, :U_{\mathrm{F}}(f)V_{\mathrm{F}}(g):\, |N-\nu\rangle = \int_0^{2\pi} e^{i(\nu-\mu)\alpha} \times \exp\left[i(2\rho)^{\frac{1}{2}}\{\tilde{f}(0)\cos\alpha + \tilde{g}(0)\sin\alpha\}\right]\frac{d\alpha}{2\pi}. \qquad (9.27)$$

This formula will play a central role in the present analysis. Then, the Wightman functional (9.20) can

[37] The generalization to the case of $\delta = 0$ is discussed in Appendix III.

[38] The same sort of argument was used to construct the representation for the BCS model of a superconductor. See Ref. 12 and R. Haag, Nuovo Cimento **25**, 287 (1962).

be written as

$$\lim_{V\to\infty} E_V(f, g) = \int_0^{2\pi} E_\alpha(f, g)\frac{d\alpha}{2\pi}, \qquad (9.28)$$

where

$$E_\alpha(f, g) = \hat{E}_\alpha(f, g) \times \exp\left[i(2\rho)^{\frac{1}{2}}\{\tilde{f}(0)\cos\alpha + \tilde{g}(0)\sin\alpha\}\right] \qquad (9.29)$$

with

$$\hat{E}_\alpha(f, g) = \lim_{V'\to\infty} \sum_{\mu,\nu}^{(V')} e^{i(\nu-\mu)\alpha} \times \lim_{V\to\infty} \langle\Psi^{(\mu)}(V)|\ U_F(f)V_F(g)\ |\Psi^{(\nu)}(V)\rangle. \qquad (9.30)$$

One should notice that Eq. (9.28) is of the same form as Eq. (9.14) for the free bosons. If we show that $E_\alpha(f, g)$ describes a representation of canonical variables, then we can conclude therefrom that the infinite volume limit of the sharp-particle number representation is decomposable in the case of the interacting bosons, too.

It is convenient to begin our argument with the proof that $\hat{E}_\alpha(f, g)$, the first factor on the right-hand side of Eq. (9.29), provides a cyclic representation of canonical pair of field operators. Namely, the functional shall be proved to define a pair of field operators, $\hat{\phi}_\alpha(\mathbf{x})$ and $\hat{\pi}_\alpha(\mathbf{x})$, together with a cyclic vector $\hat{\Psi}_\alpha$ such that

$$\langle\hat{\Psi}_\alpha|\ \hat{U}_\alpha(f)\hat{V}_\alpha(g)\ |\hat{\Psi}_\alpha\rangle = \hat{E}_\alpha(f, g), \qquad (9.31)$$

where $\hat{U}_\alpha$ and $\hat{V}_\alpha$ are constructed from $\hat{\phi}_\alpha(\mathbf{x})$ and $\hat{\pi}_\alpha(\mathbf{x})$, respectively.

Now, according to the Gelfand construction of the representation,[14] the desired proof is accomplished if we show that the Wightman functional $\hat{E}_\alpha(f, g)$ satisfies the conditions (9.10a–c). Let us introduce a vector

$$|\hat{\Psi}_\alpha(V)\rangle \equiv \sum_{\nu}^{(V)} e^{i\nu\alpha}\ |\Psi^{(\nu)}(V)\rangle; \qquad (9.32)$$

then

$$\hat{E}_\alpha(f, g) = \lim_{V\to\infty} \langle\hat{\Psi}_\alpha(V)|\ U_F(f)V_F(g)\ |\hat{\Psi}_\alpha(V)\rangle. \qquad (9.33)$$

The point of our proof is to refer to the fact that the functional

$$\langle\hat{\Psi}_\alpha(V)|\ U_F(f)V_F(g)\ |\hat{\Psi}_\alpha(V)\rangle$$

for $V < \infty$ satisfies the above three conditions in an obvious way. In fact, we can prove the commutation relation (9.10a) by recalling the properties of the Fock operators,

$$\hat{E}^*_\alpha(f, g) = \lim_{V\to\infty} \langle\hat{\Psi}_\alpha(V)|\ V_F^\dagger(g)U_F^\dagger(f)\ |\hat{\Psi}_\alpha(V)\rangle = \lim_{V\to\infty} \langle\hat{\Psi}_\alpha(V)|\ V_F(-g)U_F(-f)\ |\hat{\Psi}_\alpha(V)\rangle, \qquad (9.34)$$

and their commutation relation (9.8). The condition (9.10b) is obvious. Finally, it is clear that the positivity condition (9.10c) is satisfied by

$$\langle\hat{\Psi}_\alpha(V)|\ U_F(f)V_F(g)\ |\hat{\Psi}_\alpha(V)\rangle$$

because the finiteness of V guarantees it to describe the Fock representation. Then, going to the limit $V \to \infty$, we find that the positivity condition is in fact satisfied by $\hat{E}_\alpha(f, g)$. This concludes the argument that the functional $\hat{E}_\alpha(f, g)$ defines a representation of canonical commutation relations.

We now turn to the complete functional $E_\alpha(f, g)$, which carries an additional exponential factor related to the zero-momentum operator; see Eq. (9.29). It is not difficult to prove that this functional satisfies the canonical commutation relations, etc., when reference is made to the corresponding properties of $\hat{E}_\alpha(f, g)$. But, the shortest way is to borrow the cyclic vector $|\hat{\Psi}_\alpha\rangle$ and the field operators, $\hat{\phi}_\alpha(\mathbf{x})$ and $\hat{\pi}_\alpha(\mathbf{x})$, from the above representation. In fact, the new representation defined by $E_\alpha(f, g)$ is readily realized when we take the cyclic vector and the field operators to be $|\hat{\Psi}_\alpha\rangle$ and

$$\begin{aligned}\phi_\alpha(\mathbf{x}) &= \hat{\phi}_\alpha(\mathbf{x}) + (2\rho)^{\frac{1}{2}}\cos\alpha,\\ \pi_\alpha(\mathbf{x}) &= \hat{\pi}_\alpha(\mathbf{x}) + (2\rho)^{\frac{1}{2}}\sin\alpha,\end{aligned} \qquad (9.35)$$

respectively. This procedure of generating a new representation from an old one is the same as Araki and Woods have adopted in the case of free bosons. In particular, Eq. (9.35) corresponds exactly to Eq. (9.16). Then, Eq. (9.28) tells us that the representation defined for an infinite system by

$$\lim_{V\to\infty} E_V(f, g)$$

is decomposable into the direct sum of representations realized by the operators in Eq. (9.35) together with the cyclic vector $|\hat{\psi}_\alpha\rangle$. Whether or not the latter representations are further decomposable constitute a different question, to which we will come back later.

Now, we have to emphasize that the zero-momentum part of $\hat{E}_\alpha(f, g)$ is the same as that of $E_F(f, g)$. In fact, the cyclic vector $\hat{\Psi}_\alpha(V)$ has no particle in the $\mathbf{k} = 0$-level. From this observation, we can conclude that the matrix element of the zero-momentum creation, annihilation operators, $\hat{a}^\dagger_{\alpha 0}$ and $\hat{a}_{\alpha 0}$, of $\hat{\phi}_\alpha(\mathbf{x})$ are not macroscopic. The definition (9.35) tells us then that the corresponding opera-

tors, $a^{\dagger}_{\alpha 0}$ and $a_{\alpha 0}$, of $\phi_\alpha(\mathbf{x})$ have just the same character as those operators in the previous sections have. Namely,

$$a_{\alpha 0} = \hat{a}_{\alpha 0} + N^{\frac{1}{2}} e^{i\alpha} \tag{9.36}$$

and the matrix elements of $\hat{a}_{\alpha 0}$ are not macroscopically large.

It should be noticed here that, under the assumption (9.19) the density of the $\mathbf{k} = 0$-particles is equal to the total density at $V \to \infty$.

Some remarks are in order about the representation defined by $\hat{E}_\alpha(f, g)$. In the special case of $\sigma = 0$ in Eq. (9.19) we have $\hat{E}_\alpha(f, g) = E_{\mathrm{F}}(f, g)$ coming back to the Fock representation. Even when $\sigma > 0$, the functional defines the Fock representation if and only if the strong limit $V \to \infty$ of $|\hat{\Psi}_\alpha(V)\rangle$ exists in the Fock space. If this is the case, then $\hat{\phi}_\alpha(\mathbf{x}) = \phi_{\mathrm{F}}(\mathbf{x})$ and $\hat{\pi}_\alpha(\mathbf{x}) = \pi_{\mathrm{F}}(\mathbf{x})$ and therefore the representation is irreducible.

In the realistic model of Huang, however, we can show that the limit $V \to \infty$ of the ground state does not exist in the Fock space even when we take care of the Bose–Einstein condensation by the "c-number addition." Therefore, the representation cannot be Fock's. We have good reason to suspect that the representation of $\{\hat{\phi}_\alpha(\mathbf{x}), \hat{\pi}_\alpha(\mathbf{x})\}$ is decomposable when we remember that the "finite temperature case" of Araki and Woods provides an example in which the representation of the operators corresponding to our $\{\hat{\phi}_\alpha(\mathbf{x}), \hat{\pi}_\alpha(\mathbf{x})\}$ is in fact decomposable.

In the previous sections, we have not differentiated $\{\hat{\phi}_\alpha(\mathbf{x}), \hat{\pi}_\alpha(\mathbf{x})\}$ from $\{\phi_{\mathrm{F}}(\mathbf{x}), \pi_{\mathrm{F}}(\mathbf{x})\}$ using a common notation a^{F}_0 for the annihilation operators, for example. The reason for this is that we have been only emphasizing the fact that the matrix elements of $\hat{a}_{\alpha 0}$ are not macroscopic at $V \to \infty$. The "c-number addition" or the replacement such as in Eq. (9.35) is the characteristic feature of the macroscopic occupation of the $\mathbf{k} = 0$-level (Bose–Einstein condensation) regardless whether the particles are interacting or not. We have to keep in mind that the argument in this section is limited to a fictitious model and therefore the study of a realistic case is left for the future investigation.

In conclusion, we have seen in this section that the "c-number addition" is a necessary step when one wants to get an irreducible representation for some[39] systems (and probably for any system) under Bose–Einstein condensation. This is the mathematical background we can give at present to the replacement (4.2).

[39] We are referring to the assumptions of Eq. (9.19) and of the validity of the limiting procedure in Eq. (9.21).

X. DISCUSSION

First, let us summarize the main results of this paper.

We have investigated the behavior of the Huang model near the ground state by applying the quantum mechanical adaptation of the method of small oscillation. Here, oscillation refers to the fluctuation of the number of the $\mathbf{k} = 0$-particles which are in the state of Bose–Einstein condensation.

It has been found that, in some range of the particle density and the parameters of the interparticle force, the oscillation is unstable. On the assumption that the oscillation is stable and has small amplitude, we have computed the total energy of the system as a function of the particle density. The total energy has been found to have a minimum at some density ρ_{L}. What is important is that the density ρ_{L} lies in the region where the above-mentioned oscillation is actually stable. In the physically accessible range of the density $\rho > \rho_{\mathrm{L}}$, the oscillation is found to be always stable and its amplitude not macroscopically large.

This result shows that the Huang model can be treated without any serious error by the Bogoliubov approximation in which the fluctuation of the condensed particles is neglected. In general, our method can provide the validity criterion of the Bogoliubov approximation. By the use of our method, we can estimate the errors committed by the Bogoliubov approximation. It will be interesting to apply our method to the model recently discussed by Foldy and Bassichis.

In addition to the excitation spectrum that Huang obtained, we have found a new one related to the fluctuation of the condensed particles [see Eq. (6.15b)]. The excitation energy of such fluctuations cannot be neglected when we take into account the phonon mode of $\mathfrak{N}_{\mathrm{I}}$-particles, because they are comparable in orders of magnitude.

Within these arguments, it is not quite clear whether or not the ground state obtained by our method is really the state of the lowest energy. When we tried to answer this question, we have been led naturally to a consideration of the limit of an infinitely large system. Taking advantage of the physically plausible assumption that the lowest energy should be attained by the state of Bose–Einstein condensation, we have tried to formulate a mathematical reasoning for the inevitability of our method. We have analyzed the representations of canonical variables to be applied to some models which are intended for simulating the Huang model. So far as these fictitious models are concerned, we have

established the statement that, in the limit of infinitely large system, it is imperative to use the method of small oscillation if the system is in the state of Bose–Einstein condensation.

Some further investigation is necessary to generalize this statement so as to apply the Huang model. First of all, we have to analyze the state vector of the Huang model in more detail: We have to see the structure of the sharp-particle-number ground state to attain the better simulation. In order to discuss the limit of infinitely large system, we have to analyze the limit Wightman functional. We have seen in the text that the infinite volume limit of the ground state of Huang model does not exist within the Fock representation even if the Bose–Einstein condensation is properly managed. This difficulty will be resolved in a natural way when we obtain the representation of the canonical variables suitable in the infinite system. These mathematical problems are left open for the future investigation.

The question of the higher excited states will be interesting both from physical and mathematical point of view. The physical part would not be so difficult. Anyhow, this is also an open question.

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APPENDIX I. THE BOGOLIUBOV TRANSFORMATION, ETC.

When we want to diagonalize the operator,

$$\mathcal{K} = Pa_{\mathbf{k}}^{\dagger}a_{-\mathbf{k}}^{\dagger} + Q(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger}a_{-\mathbf{k}}) + Pa_{\mathbf{k}}a_{-\mathbf{k}}. \quad \text{(I.1)}$$

we have to treat the cases $Q^2 - P^2 > 0$ and $Q^2 - P^2 \leq 0$ separately.

A. $Q^2 - P^2 > 0$

In this case, the operator $\mathcal{K}$ can be diagonalized by the Bogoliubov transformation ($\mathbf{k}$ can be equal to 0),

$$\left.\begin{aligned} a_{\mathbf{k}} &= b_{\mathbf{k}} \cosh\theta_{\mathbf{k}} - b_{-\mathbf{k}}^{\dagger} \sinh\theta_{\mathbf{k}} \\ a_{\mathbf{k}}^{\dagger} &= b_{\mathbf{k}}^{\dagger} \cosh\theta_{\mathbf{k}} - b_{-\mathbf{k}} \sinh\theta_{\mathbf{k}} \end{aligned}\right\} (\theta_{\mathbf{k}} = \theta_{-\mathbf{k}}), \quad \text{(I.2)}$$

to be

$$\mathcal{K} = \omega_{\mathbf{k}} \cdot \tfrac{1}{2}(b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}} + b_{-\mathbf{k}}^{\dagger}b_{-\mathbf{k}}) + C_{\mathbf{k}},$$

where

$$\omega_{\mathbf{k}} = \pm 2(Q^2 - P^2)^{\frac{1}{2}}, \quad C_{\mathbf{k}} = \pm(Q^2 - P^2)^{\frac{1}{2}} - Q, \quad \text{(I.3)}$$

with the upper and the lower signs referring to the cases $Q > 0$ and $Q < 0$, respectively. Due to the presumption $Q^2 - P^2 > 0$, the case of $Q = 0$ is excluded. The angle $\theta_{\mathbf{k}}$ can be determined by some of the following relations. The sign convention is the same as above:

$$\begin{aligned} \tanh\theta_{\mathbf{k}} &= [Q \mp (Q^2 - P^2)^{\frac{1}{2}}]/P, \\ \cosh\theta_{\mathbf{k}} \sinh\theta_{\mathbf{k}} &= \pm\tfrac{1}{2}P/(Q^2 - P^2)^{\frac{1}{2}}, \\ \cosh^2\theta_{\mathbf{k}} + \sinh^2\theta_{\mathbf{k}} &= \pm Q/(Q^2 - P^2)^{\frac{1}{2}}. \end{aligned} \quad \text{(I.4)}$$

For a while we assume $\mathbf{k} \neq 0$. Then, the transformation (I.2) is generated by

$$\mathfrak{U}(\theta_{\mathbf{k}}) = \exp[\theta_{\mathbf{k}}(A_{\mathbf{k}} - A_{\mathbf{k}}^{\dagger})] \quad \text{(I.5)}$$

as

$$\begin{aligned} b_{\mathbf{k}} &= a_{\mathbf{k}} \cosh\theta_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger} \sinh\theta_{\mathbf{k}} \\ &= \mathfrak{U}(\theta_{\mathbf{k}}) a_{\mathbf{k}} \mathfrak{U}^{\dagger}(\theta_{\mathbf{k}}). \end{aligned} \quad \text{(I.6)}$$

The operator $A_{\mathbf{k}}$ satisfies the following commutation relations:

$$[A_{\mathbf{k}}, A_{\mathbf{k}}^{\dagger}] = B_{\mathbf{k}}, \qquad [A_{\mathbf{k}}, B_{\mathbf{k}}] = 2A_{\mathbf{k}}, \quad \text{(I.7)}$$

where

$$A_{\mathbf{k}} = a_{\mathbf{k}}a_{-\mathbf{k}}, \qquad B_{\mathbf{k}} = a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger}a_{-\mathbf{k}} + 1.$$

For the sake of convenient reference, we note the ordering theorem

$$\begin{aligned} \mathfrak{U}(\theta_{\mathbf{k}}) &= \exp[-A_{\mathbf{k}}^{\dagger} \tanh\theta_{\mathbf{k}}] \exp[-B_{\mathbf{k}} \log\cosh\theta_{\mathbf{k}}] \\ &\times \exp[A_{\mathbf{k}} \tanh\theta_{\mathbf{k}}] = \exp[A_{\mathbf{k}} \tanh\theta_{\mathbf{k}}] \\ &\times \exp[B_{\mathbf{k}} \log\cosh\theta_{\mathbf{k}}] \exp[-A_{\mathbf{k}}^{\dagger} \tanh\theta_{\mathbf{k}}]. \end{aligned} \quad \text{(I.8)}$$

In order to prove the first relation, for example, we put

$$\mathfrak{U}(\theta_{\mathbf{k}}) = \exp[A_{\mathbf{k}}^{\dagger}f(\theta_{\mathbf{k}})] \exp[B_{\mathbf{k}}g(\theta_{\mathbf{k}})] \exp[A_{\mathbf{k}}h(\theta_{\mathbf{k}})],$$

and require it to satisfy the same differential equation and the same initial condition as $\mathfrak{U}(\theta_{\mathbf{k}})$ in Eq. (I.5) does:

$$(d/d\theta_{\mathbf{k}})\mathfrak{U}(\theta_{\mathbf{k}}) = (A_{\mathbf{k}} - A_{\mathbf{k}}^{\dagger})\mathfrak{U}(\theta_{\mathbf{k}}), \quad \mathfrak{U}(0) = 1.$$

Then, we obtain simultaneous differential equations for three unknowns $f(\theta_{\mathbf{k}})$, $g(\theta_{\mathbf{k}})$, and $h(\theta_{\mathbf{k}})$. These can easily be solved to lead us to Eq. (I.8).

In the case of $\mathbf{k} = 0$, we have to change the notation,

$$A_0 = \tfrac{1}{2}a_0a_0, \qquad B_0 = a_0^{\dagger}a_0 + \tfrac{1}{2}, \quad \text{(I.9)}$$

so that the commutation relations take the same form as those in Eq. (I.7). Then, we see that Eqs. (I.5), (I.6), and (I.8) also hold for $\mathbf{k} = 0$.

B. $Q^2 - P^2 \leq 0$

In this case, it is more convenient to use a continuous representation in terms of

$$x_{\mathbf{k}} = 2^{-\frac{1}{2}} i(a_{\mathbf{k}} - a_{\mathbf{k}}^{\dagger}), \qquad p_{\mathbf{k}} = 2^{-\frac{1}{2}}(a_{\mathbf{k}} + a_{\mathbf{k}}^{\dagger}) \tag{I.10}$$

which obey the canonical commutation relations for the coordinates and their conjugate momenta:

$$[x_{\mathbf{k}}, p_{\mathbf{k}'}] = i\delta_{\mathbf{k},\mathbf{k}'}, \qquad [x_{\mathbf{k}}, x_{\mathbf{k}'}] = [p_{\mathbf{k}}, p_{\mathbf{k}'}] = 0. \tag{I.11}$$

Then, the operator $\mathcal{K}$ [Eq. (I.1)] becomes

$$\mathcal{K} = Pp_{\mathbf{k}}p_{-\mathbf{k}} + \tfrac{1}{2}Q(p_{\mathbf{k}}^2 + p_{-\mathbf{k}}^2) - Px_{\mathbf{k}}x_{-\mathbf{k}} + \tfrac{1}{2}Q(x_{\mathbf{k}}^2 + x_{-\mathbf{k}}^2), \tag{I.12}$$

which can be cast into a normal form of harmonic oscillator Hamiltonian by the following canonical transformation

$$\xi_{\mathbf{k}+} = 2^{-\frac{1}{2}}(x_{\mathbf{k}} + x_{-\mathbf{k}}), \quad \eta_{\mathbf{k}+} = 2^{-\frac{1}{2}}(p_{\mathbf{k}} + p_{-\mathbf{k}}),$$
$$\xi_{\mathbf{k}-} = 2^{-\frac{1}{2}}(p_{\mathbf{k}} - p_{-\mathbf{k}}), \quad \eta_{\mathbf{k}-} = -2^{-\frac{1}{2}}(x_{\mathbf{k}} - x_{-\mathbf{k}}). \tag{I.13}$$

ξ's stand for the canonical coordinates and η's for their conjugate momenta. In fact, these operators satisfy the canonical commutation relations

$$[\xi_{\mathbf{k}-}, \eta_{\mathbf{k}-}] = i, \quad [\xi_{\mathbf{k}-}, \xi_{\mathbf{k}+}] = 0 \quad \text{etc.}, \tag{I.14}$$

and we have

$$\mathcal{K} = \tfrac{1}{2}(Q + P)\left[\eta_{\mathbf{k}+}^2 + \frac{Q - P}{Q + P}\xi_{\mathbf{k}+}^2 + \eta_{\mathbf{k}-}^2 + \frac{Q - P}{Q + P}\xi_{\mathbf{k}-}^2\right]. \tag{I.15}$$

This form will be convenient for treating the case $Q + P > 0$, which we assume hereafter.

Now, we see that, if $Q - P = 0$ then $\mathcal{K}$ describes two "free particles" and if $Q - P < 0$, then $\mathcal{K}$ describes two "harmonic oscillators" with the potential functions concave downwards. In any case, the spectrum of $\mathcal{K}$ is continuous and the wavefunction not normalizable.

APPENDIX II. THE FLUCTUATION OF THE PARTICLE NUMBER

As a preparatory step to the construction of a mathematical model in Sec. 9, let us compute the mean-square fluctuation,

$$(\Delta n_0)^2 \equiv \langle\Omega_0|\, n_0^2\, |\Omega_0\rangle - [\langle\Omega_0|\, n_0\, |\Omega_0\rangle]^2, \tag{II.1}$$

of the number $n_0 = a_0^{\dagger}a_0$ of the $\mathbf{k} = 0$-particles in the vacuum $|\Omega_0\rangle$ of the operator b_0, when the following transformations are made:

$$a_0 = a_0^{\mathrm{F}} + N^{\frac{1}{2}}$$

followed by

$$a_0^{\mathrm{F}} = b_0 \cosh\theta_0 - b_0^{\dagger}\sinh\theta_0. \tag{II.2}$$

The computation can be carried out in the same way as in Eq. (6.3b). We get

$$\langle\Omega_0|\, n_0\, |\Omega_0\rangle = N + \sinh^2\theta_0. \tag{II.3}$$

$$\langle\Omega_0|\, n_0^2\, |\Omega_0\rangle = (N + \sinh^2\theta_0)^2 + (\cosh\theta_0 - \sinh\theta_0)^2 N + 2\cosh^2\theta_0 \sinh^2\theta_0, \tag{II.4}$$

and therefore

$$(\Delta n_0)^2 = (\cosh\theta_0 - \sinh\theta_0)^2 N + O(1), \tag{II.5}$$

where we have assumed that $\cosh\theta_0$ and $\sinh\theta_0$ are of order 1 (when $N \to \infty$). We find that the fluctuation is proportional to $N^{\frac{1}{2}}$.

In the same way, we can compute the fluctuation of the total number of the $\mathbf{k} \neq 0$-particles finding again that it is proportional to $N^{\frac{1}{2}}$.

The models in Sec. 9 are the abstraction from these results.

APPENDIX III. DECOMPOSITION OF $\lim_{N\to\infty}\langle N - \mu\,|{:}\, U_{\mathrm{F}}(f)\, V_{\mathrm{F}}(g)\, {:}|\, N - \nu\rangle$

To begin with, we consider the case $\mu \geq \nu$. It is easy to get

$$\langle N - \mu|\, U_{\mathrm{F}}(f)V_{\mathrm{F}}(g)\, |N - \nu\rangle = \left[\frac{(N - \nu)!}{(N - \mu)!}\right]^{\frac{1}{2}}\left(\frac{-\bar{z}}{N^{\frac{1}{2}}}\right)^{\nu-\mu} L_{N-\nu}^{(\nu-\mu)}\left(\frac{z\bar{z}}{N}\right), \tag{III.1}$$

where

$$z = (\tfrac{1}{2}\rho)^{\frac{1}{2}}[\tilde{g}(0) + i\tilde{f}(0)], \quad (\tilde{f}(0),\ \tilde{g}(0)\text{: real}) \tag{III.2}$$
$$\bar{z} = (\tfrac{1}{2}\rho)^{\frac{1}{2}}[\tilde{g}(0) - i\tilde{f}(0)],$$

and $L_N^{(\nu)}(x)$ is the associated Laguerre polynomial:

$$L_{N-\nu}^{(\nu-\mu)}\left(\frac{z\bar{z}}{N}\right) = \sum_{r=0}^{N-\nu}\frac{(-1)^r}{r!(\nu - \mu + r)!}\frac{(N - \mu)!}{(N - \nu - r)!}\left(\frac{z\bar{z}}{N}\right)^r. \tag{III.3}$$

Now, we proceed to take the limit $N \to \infty$. For a while, we assume the condition (9.19) with $\delta > 0$. Then, we have

$$[(N - \nu)!/(N - \mu)!]^{\frac{1}{2}} \sim N^{-\frac{1}{2}(\nu-\mu)} \quad (N \to \infty). \tag{III.4}$$

Also, as is shown at the end of this Appendix, the factorials under the summation (III.3) can be

approximated as

$$(N-\mu)!/(N-\nu-r)! \sim N^{\nu-\mu+r} \quad (N\to\infty). \quad \text{(III.5)}$$

Thus, we get

$$\lim_{N\to\infty} \langle N-\mu| : U_F(f)V_F(g) : |N-\nu\rangle = \left(\frac{-\bar{z}}{[z\bar{z}]^{\frac{1}{2}}}\right)^{\nu-\mu} J(2[z\bar{z}]^{\frac{1}{2}}) \quad (\mu\le\nu), \quad \text{(III.6)}$$

where $J_n(x)$ is the Bessel function

$$J_n(x) = \left(\frac{x}{2}\right)^n \sum_{r=0}^{\infty} \frac{(-1)^r}{r!(n+r)!}\left(\frac{x}{2}\right)^{2r}.$$

Now, by the use of the relation

$$[\langle N-\mu| U_F(f)V_F(g) |N-\nu\rangle]^\dagger = \langle N-\nu| V_F(-g)U_F(-f) |N-\mu\rangle = \langle N-\nu| U_F(-f)V_F(-g) |N-\mu\rangle \exp[i(f,g)],$$

which follows from Eq. (9.8) and the self-adjointness of the Bose operators, we can conclude that Eq. (III.6) holds also for $\mu \ge \nu$ if we notice

$$J_{-n}(x) = (-1)^n J_n(x), \quad (n\text{: integer}).$$

In order to attain the decomposition, we notice

$$\frac{d}{dx}\left[\frac{1}{x^n}J_n(x)\right] = -\frac{1}{x^n}J_{n+1}(x), \quad (n\ge 0)$$

and the integral representation of $J_0(x)$,

$$J_0(2[z\bar{z}]^{\frac{1}{2}}) = \int_0^{2\pi} \exp[ze^{i\alpha} - \bar{z}e^{-i\alpha}]\frac{d\alpha}{2\pi}. \quad \text{(III.7)}$$

Then for $n \ge 0$,

$$\left(\frac{-\bar{z}}{[z\bar{z}]^{\frac{1}{2}}}\right)^n J_n(2[z\bar{z}]^{\frac{1}{2}}) = \left(\frac{\partial}{\partial z}\right)^n J_0(2[z\bar{z}]^{\frac{1}{2}}) = \int_0^{2\pi} e^{in\alpha}\exp[ze^{i\alpha} - \bar{z}e^{-i\alpha}]\frac{d\alpha}{2\pi}.$$

The case of $n = -m < 0$ can be dealt with as

$$\left(\frac{-\bar{z}}{[z\bar{z}]^{\frac{1}{2}}}\right)^{-m} J_{-m}(2[z\bar{z}]^{\frac{1}{2}}) = \left(\frac{z}{[z\bar{z}]^{\frac{1}{2}}}\right)^m J_m(2[z\bar{z}]^{\frac{1}{2}}) = \left(-\frac{\partial}{\partial\bar{z}}\right)^m J_0(2[z\bar{z}]^{\frac{1}{2}}).$$

Therefore, referring to the integral representation of $J_0(x)$, we obtain

$$\lim_{N\to\infty} \langle N-\mu| : U_F(f)V_F(g) : |N-\nu\rangle = \int_0^{2\pi} e^{i(\nu-\mu)\alpha}\exp[ze^{i\alpha} - \bar{z}e^{-i\alpha}]\frac{d\alpha}{2\pi}. \quad \text{(III.8)}$$

This is the desired result, Eq. (9.27).

The functional for the free Bose gas can be obtained as a special case when we put $\mu = \nu = 0$ and switch the normal product into the ordinary one thus recovering $E_F(f, g)$ [see Eq. (9.23)]:

$$\lim_{N\to\infty} \langle N| U_F(f)V_F(g) |N\rangle = \int_0^{2\pi} E_\alpha(f,g)\frac{d\alpha}{2\pi}, \quad \text{(III.9)}$$

where

$$E_\alpha(f,g) = E_F(f,g) \times \exp[i(2\rho)^{\frac{1}{2}}\{\tilde{f}(0)\cos\alpha + \tilde{g}(0)\sin\alpha\}]. \quad \text{(III.10)}$$

Now, we have to show the validity of the approximation (III.5). Let's consider the case of $(N-\mu)!$ first. If $\mu \le \sigma N^{\frac{1}{2}-\delta}$ as assumed in Eq. (9.19), then the Stirling formula tells us that

$$\log(N-\mu)! = (N-\mu+\tfrac{1}{2})\log(N-\mu) - (N-\mu) + \tfrac{1}{2}\log 2\pi + O\left(\frac{1}{N}\right) = (N-\mu+\tfrac{1}{2})\log N - N + \tfrac{1}{2}\log 2\pi + \frac{\mu^2}{N} + O\left(\frac{1}{N}\right), \quad \text{(III.11)}$$

where we have made use of an approximation $\log(1-[\mu/N]) = -\mu/N + O(\mu^2/N^2)$. The reason why we assume $\delta > 0$ is that the term μ^2/N can be neglected at $N\to\infty$. Thus,

$$(N-\mu)! = (2\pi N)^{\frac{1}{2}}e^{-N}N^{N-\mu}\left(1 + O\left[\frac{1}{N^{2\delta}}\right]\right). \quad \text{(III.12)}$$

In order to apply the same argument to $(N-\nu-\gamma)!$, we have to confirm the inequality $\nu+\gamma \le (\sigma+\sigma')N^{\frac{1}{2}-\delta}$ for some positive number σ' by showing that the series (III.4) gets a negligible contribution from the sequence of terms beyond r_0, $r \ge r_0$ with $r_0 \equiv \sigma' N^{\frac{1}{2}-\delta}$. To begin with, we show that the sequence in the series (III.4) is of monotonic decrease for $r_0 \le r \le N-\nu$ and for a sufficiently large N. In fact,

$$\left|\frac{(r+1)\text{th term}}{r\text{th term}}\right| \le \frac{1}{(r_0+1)(\nu-\mu+r_0+1)}\frac{z\bar{z}}{N}, \quad \text{(III.13)}$$

and the right-hand side becomes smaller than one for large N. The contribution from the r_0th term can be computed by the use of the Stirling formula. It is inversely proportional to something like $N^{\frac{1}{2}-\delta}$th power of N, or more precisely,

$$\frac{1}{r_0!(\nu-\mu+r_0)!}\frac{(N-\mu)!}{(N-\nu+r_0)!}\left(\frac{z\bar{z}}{N}\right)^{r_0} \sim \exp[\{-2\sigma'(\tfrac{1}{2}-\delta)N^{\frac{1}{2}-\delta} + (\tfrac{1}{2}+\delta)(\nu-\mu)\}\log N]. \quad \text{(III.14)}$$

Thus, we see that the total contribution from the terms with $r_0 \leq r \leq N - \nu$ vanishes quicker than Eq. (III.14) $\times N$ does as $N \to \infty$. This is the desired result.

We close this Appendix by mentioning what happens if $\delta = 0$ is assumed. If so, we must keep μ^2/N in Eq. (III.11) and therefore we have

$$(N - \mu)! = (2\pi N)^{\frac{1}{2}} N^{N-\mu} \exp[-N + (\mu^2/N)] \quad \text{(III.15)}$$

in place of Eq. (III.12). In the series (III.4), we can still neglect the terms with $r_0 \leq r \leq N - \nu$. For $r < r_0$, we have

$$(N - \nu - r)! = (2\pi N)^{\frac{1}{2}} N^{N-\nu-r} \exp[-N + (\nu^2/N)].$$

Thus, the correction to (III.5) is independent of r:

$$(N - \mu)!/(N - \nu - r)! \sim N^{\nu-\mu+r} \exp[-(\nu^2 - \mu^2)/N]. \quad \text{(III.16)}$$

Also, we have

$$[(N - \nu)!/(N - \mu)!]^{\frac{1}{2}} \sim N^{-\frac{1}{2}(\nu-\mu)} \exp[+\tfrac{1}{2}(\nu^2 - \mu^2)/N]. \quad \text{(III.17)}$$

These equations are used in the case of $\mu \leq \nu$. In general $\nu^2 - \mu^2$ in the above must be replaced by $|\mu^2 - \mu^2|$. Therefore, Eq. (III.8) must be replaced by

$$\lim_{N\to\infty} \langle N - \mu| : U_F(f)V_F(g) : |N - \nu\rangle = [\text{rhs of Eq. (III.8)}] \cdot \exp[-|\nu^2 - \mu^2|/(2N)], \quad \text{(III.18)}$$

and Eqs. (9.28)–(9.30) should be corrected accordingly.

Now, the reason why we avoided this case of $\delta = 0$ in the text is that the positivity condition is difficult to prove. In fact, if we adopt Eq. (III.18) we cannot put $\hat{E}_\alpha(f, g)$ in the form of Eq. (9.33) on which we have been relying in proving the positivity condition. It should, however, be noticed here that, if it is meaningful to take the limit $\delta \to 0$ after the whole computation, the positivity of the $\delta = 0$-Wightman functional follows from the positivity of the $\delta > 0$-functional.

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Dynamics of a Simple Many-Body System of Hard Rods

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General formulas are given for the exact calculation of the nonequilibrium properties of the one-dimensional system of equal-mass hard rods both for a finite but large system and in the limit of infinite size. Only properties which depend upon labeling one or more of the particles are nontrivial in this system. Various results are obtained on Poincaré cycles, delocalization of a particle with time and electrical conductivity when one particle is charged.

INTRODUCTION

IN order to understand the dynamical behavior of systems containing a large number of particles, it is important to have a number of sample systems in which the dynamical equations can be handled exactly. We give here a study of Poincaré cycles, pseudostochastic behavior, and nonequilibrium properties of the one-dimensional hard-rod system, which is perhaps the simplest model that can be considered. Some of the simpler properties have been considered previously by Frisch and others.[1] The other studies of this type in the literature that we have seen are restricted to various harmonic oscillator assemblies, and we feel that a study of a system whose mechanics are not based on the theory of normal modes should be important for contrast, in spite of the fact that it is less physical than these other models.

The discussion of many ergodic properties in this system is quite convenient. We also obtain some results on Poincaré cycles not really restricted to this system and compare them with other known results. It appears to be possible to calculate almost any desired property of this system, although, of course, some calculations are messy. Unfortunately, most of the most interesting properties of real many-body systems are both degenerate and untypical in this system. However, the Brownian-motion-like path of a given particle appears to be one property that does bear attention.

DESCRIPTION OF THE DYNAMICS OF THE SYSTEM

We consider N point particles, all of the same mass, constrained to move along a line like beads on a string. The particles do not penetrate each other, so that they retain their ordering along the line. When a pair of particles collide, their energy and momentum are conserved so that they merely exchange velocities. We assume that there are no three-body collisions or that they are so improbable as to have negligible effect during the time in which we are observing the system. This can be achieved by assuming hard-sphere or other very sharp repulsive forces between the particles and negligible attraction. We assume, as stated above, that the particles are mass points; the same procedure can also be used for particles of finite size simply by subtracting off the distances of closest approach from the interparticle distances and relating these new distances to the mass-point model. If the system has periodic boundary conditions, as we assume in this work, this equivalence is not quite exact because after these new distances are introduced, the center of mass of the system (to the extent that it can be defined) should still move in a box of the original size.

In order to follow the dynamics of the system in complete detail we make use of the following trick. We plot the positions of the particles versus time as shown in Fig. 1. If no collision occurs, the motion of one of the particles is represented by a straight line, or "trajectory", starting on the X axis at the initial position of the particle, and with a slope equal to the reciprocal of its velocity. When a collision occurs, two of these lines cross, and since collisions are elastic, the two particles merely exchange trajectories. Neither trajectory is changed in direction. This makes the dynamics of the system simple to follow; we need only keep track of which particle is on each line in the diagram at any given time.

To this end, we number the particles and the trajectories. We pick one of the particles, number it zero, and put our origin of coordinates at the position of this particle at the initial time. We number the rest of the particles 1, 2, $\cdots$, $N-1$, starting with the neighbor to the right of particle zero, and continuing from left to right. Since one particle never passes through another, this ordering

[1] H. L. Frisch, Phys. Rev. **104**, 1 (1956); E. Teramoto and C. Suzuki, Progr. Theoret. Phys. (Kyoto) **14**, 411 (1955).

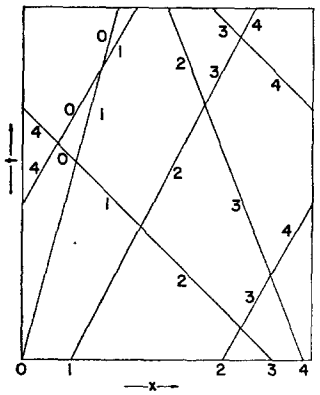

FIG. 1. Diagram showing the nature of the dynamics of the system.

is maintained for all time. We give each trajectory a number equal to the number of the particle occupying it at the initial time.

We now define $A_{jk}(t)$ to be equal to one if particle j is on trajectory k at time t and to be zero otherwise. A knowledge of $A_{jk}(t)$ for each j and k constitutes a complete solution of the dynamics of the system in a very convenient form. If, instead of studying a single system, we form an ensemble over the initial conditions, the average $\langle A_{jk}(t)\rangle$ of $A_{jk}(t)$ becomes the probability that particle j is on trajectory k at time t.

Since the particles remain in the same order around the ring (we assume periodic boundary conditions), it is possible to determine which particle is on a given trajectory simply by counting how many trajectories have crossed this trajectory from each side up to the given time. Each time a trajectory crosses it from the right, the particle on the given trajectory at this time is replaced by its neighbor to the right, which is numbered one higher. Similarly, after a collision from the left, the number of the particle on the trajectory is decreased by 1. Notice that this is true independent of the history of each of the trajectories involved. We shall refer to a collision from the left as a "negative" collision. As a result of these considerations we find that after trajectory k has been crossed n times by other trajectories (in the special sense where the number of negative crossings is subtracted), it will be occupied by particle number $k + n$. In this discussion particle zero is the particle with number one larger than $N - 1$ and $N - 1$ is one smaller than zero, i.e., we must count the particles modulo N.

We now show how these considerations can be used to calculate the $A_{jk}(t)$'s. We define $r_n(h, k, t)$ to be equal to 1 if trajectory h crosses trajectory k exactly n times between the initial time and time t, and to be zero otherwise. The number n can be positive, negative, or zero. If we average r_n over an ensemble of initial conditions, $\bar{r}_n$ will give the probability that trajectory h crosses trajectory k a total of n times. Next we define the characteristic functions for the probability distributions,

$$s(u; h, k, t) \equiv \sum_{n=-\infty}^{\infty} r_n(h, k, t)e^{inu}. \tag{1}$$

In terms of these quantities, $A_{jk}(t)$ is given by

$$A_{jk}(t) = \frac{1}{N}\sum_{l=0}^{N-1} \exp\left[-\frac{2\pi i}{N}(j-k)l\right] \times s\left(\frac{2\pi l}{N}; 0, k, t\right)s\left(\frac{2\pi l}{N}; 1, k, t\right) \times s\left(\frac{2\pi l}{N}; 3, k, t\right)\cdots s\left(\frac{2\pi l}{N}; N-1, k, t\right)$$

with

$$s(u, k, k, t) \equiv 1. \tag{2}$$

To show this, we replace the s's by the sums containing the r_n's and use the fact that

$$\frac{1}{N}\sum_{l=0}^{N-1} \exp\left[-\frac{2\pi i}{N}nl\right] = \begin{cases} 1 & n = 0 \pmod N, \\ 0 & \text{otherwise}; \end{cases} \tag{3}$$

$$A_{jk} = \sum_{n_0, n_1, \cdots = \infty}^{\infty} \left[\frac{1}{N}\sum_{l=0}^{N-1} \exp\left\{\frac{2\pi i}{N}l(n_0 + n_1 + \cdots n_{N-1} - j + k)\right\}\right] r_{n_0}r_{n_1}\cdots r_{n_{N-1}}. \tag{4}$$

We state the argument in terms of probabilities, since a single system is actually a special case in which the probabilities are either zero or one. If the expression in the brackets is left out for the moment, the resulting sum adds together the probabilities of all the possible combinations of crossings which trajectory k could undergo between the initial time and time t. Putting in the expression in brackets restricts the summation to those combinations which put particle j on trajectory k. The sum of these probabilities is just $A_{jk}(t)$.

The expression for $s(u; h, k, t)$ to be used in this equation takes two forms depending upon whether h is greater than or less than k. If particle h starts to the right of k, s can be written in the form

$$s(u; h, k, t) = S[u, w_{kh}], \quad k < h, \tag{5}$$

with

$$S[u, w] = e^{inu} \quad \text{when} \quad (n-1)L < w \leq nL \quad \text{for each } n \tag{6}$$

and

$$w_{kh} = x_k - x_h + (v_k - v_h)t, \tag{7}$$

where x_i and v_i are the initial position and the velocity of the ith trajectory. If h starts to the left of k we have

$$s(u; h, k, t) = e^{-iu}S[u, w_{kh}], \quad h < k. \tag{8}$$

In terms of S, Eq. (4) becomes

$$A_{jk} = \frac{1}{N}\sum_u \exp[-iju]\prod_{h=0}^{N-1} S[u, w_{kh}]$$

with

$$u = \frac{2\pi l}{N}, \quad \text{and} \quad \sum_u = \sum_{l=0}^{N-1}. \tag{9}$$

We note that S satisfies the equation

$$S[u, w + L] = e^{iu}S[u, w]. \tag{10}$$

Since $\exp[iu]$ is always taken equal to one of the Nth roots of unity, $S[u, w]$ is periodic in w with period NL.

Unfortunately the fact that the dynamics of the system are so simple makes most of the characteristics important in the usual many-body systems trivial and degenerate in this one. For example, the velocity distribution does not change with time since there is always one particle with each of the initial velocities. More generally it can be stated that the only properties of this system that will be interesting are those which depend upon attaching labels to one or more of the particles. If the particles are not distinguishable we may treat the system more simply by allowing them to exchange identities during collision, which in turn is equivalent to allowing them to pass through each other without interaction. Hence in this case we may expect the same results as for a noninteracting gas.

CALCULATIONS WITH A FIXED SET OF INITIAL CONDITIONS

Although we cannot study the approach of the velocity distribution toward equilibrium we may assume that the velocities at the initial time have already been randomized by some otherwise unconsidered process such as three-body collision and study randomization in configuration space. This is of some interest even for noninteracting gases. The procedures illustrated first on the noninteracting gas will later also be applied on properties of the hard-particle system.

It is convenient to make the assumption that the velocities of the N particles satisfy no relation of the form

$$\sum_{i=0}^{N-1} n_i v_i L = 0, \tag{11}$$

where the n_i's are positive or negative integers with perhaps some, but not all, of them zero. When this assumption is fulfilled we may apply a theorem due to Kronecker and Weyl to calculate time averages of various properties of this system following the procedure used by Montroll and Mazur[2] for a harmonic oscillator system. By the time average expectation we mean the expectation

$$\langle f[x_0(t) \cdots x_{N-1}(t)]\rangle = \lim_{T\to\infty}\frac{1}{T}\int_0^T f[x_0(t) \cdots x_{N-1}(t)]\, dt \tag{12}$$

with $x_i(t) = x_i + v_i t$. The Kronecker–Weyl theorem states that if a bounded Riemann integrable function of N variables, $f(x_0 \cdots x_{N-1})$, is periodic in each argument with period 2π and if the previously stated assumption holds then

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T f\, dt = \frac{1}{(2\pi)^N}\int_0^{2\pi} dx_0 \cdots \int_0^{2\pi} dx_{N-1}\, f. \tag{13}$$

This theorem justifies the use of the usual uniform average in the configuration space of this system.

We use the theorem first to describe the Poincaré cycle behavior of the trajectories. We say that a set M of trajectories has returned to an ϵ neighborhood of their original positions, or alternatively has suffered a recurrence, at time t if the inequality

$$f(t) = \sum_{i\in M} \dashv x_i(t) - x_i(0)\vdash < \epsilon \tag{14}$$

is satisfied. By $\dashv y \vdash$ we mean the function which is equal to the absolute value of y for $-L/2 < y \leq L/2$ and is defined outside this interval by the requirement that it be periodic with period L.

We may calculate the number of recurrences in a given period of time by counting the number of zeros of the function $f(t) - \epsilon$ and dividing by two. For this reason following Montroll and Mazur we define the recurrence time T_r by the equation

$$\frac{1}{T_r} = \frac{1}{2}\lim_{T\to\infty}\frac{1}{T}\int_0^T \sum_\alpha \delta(t - t_\alpha)\, dt, \tag{15}$$

where the t_α are the zeros of $f(t) - \epsilon$. This can be transformed to

$$\frac{1}{T_r} = \frac{1}{2}\lim_{T\to\infty}\frac{1}{T}\int_0^T \delta[f(t) - \epsilon]\, |f'(t)|\, dt. \tag{16}$$

The theorem can be applied to this expression if we replace the delta function with any well-behaved

[2] P. Mazur and E. Montroll, J. Math. Phys. **1**, 70 (1960).

approximation. This gives

$$\frac{1}{T_r} = \frac{1}{2}\frac{1}{L^M}\int_{-L/2}^{L/2} dx_1 \cdots \int dx_M\, \delta\Big(\sum_{i\in M} |x_i| - \epsilon\Big) \times \Big|\sum_{i\in M} v_i \operatorname{sgnp} x_i\Big| \qquad (17)$$

where

$$\operatorname{sgnp} y = 1 \quad 0 < x < L/2$$
$$-1 \quad -L/2 < x < 0. \qquad (18)$$

Sgnp y is defined outside this interval by the requirement that it be periodic with period L. This formula is easily evaluated to give

$$\frac{1}{T_r} = \frac{1}{2(M-1)!\,L}\left(\frac{\epsilon}{L}\right)^{M-1} \sum_{\pm} \Big|\sum_i \pm v_i\Big|, \qquad (19)$$

provided $\epsilon \leq L/2$. In this formula we take the sum over all combinations of + and − signs in the sum of velocities inside the absolute value sign. It can be shown using the central-limit theorem of probability theory that if the number of trajectories is large and a small number of v's are not much larger than the rest that

$$\sum_{\pm} \Big|\sum_i \pm v_i\Big| \sim 2^M\left(\frac{2\sigma^2}{\pi}\right)^{\frac{1}{2}}, \qquad \sigma^2 = \sum_i v_i^2, \qquad (20)$$

and hence the recurrence time approaches

$$T_r \sim (2\epsilon\pi/M^{\frac{1}{2}}\sigma)(ML/2\epsilon e)^M. \qquad (21)$$

Hemmer, Maximon, and Wergeland[3] have also given a method for finding the recurrence time in a problem equivalent to this one. Their definition of the recurrence time is the same as ours except that a recurrence is defined to be a return to the volume in M space defined by

$$\dashv x_i(t) - x_i(0)\vdash < a_i \quad i = 1, 2, 3, \cdots, M \qquad (22)$$

for any set of positive a_i's rather than the volume defined by (14). The recurrence time that they obtain for this volume is

$$T_r = \prod_{i=1}^{M}\left(\frac{L}{2a_i}\right) \Big/ \sum_{i=1}^{M} \frac{|v_i|}{2a_i}. \qquad (23)$$

If we choose the a_i's all equal and adjust the common value so that the volume of this hypercube is equal to that of the "2^M-a hedron" of (14), this formula gives

$$T_r = (L/2\epsilon)^M[2\epsilon M!/(M!)^{1/M} \sum_i |v_i|]. \qquad (24)$$

If we further assume a Maxwell distribution of velocities so that $\bar{v} = (8/3\pi M)^{\frac{1}{2}}\sigma$, we find that this formula differs from (21) by an additional factor

$$(3M)^{\frac{1}{2}}/2(M!)^{1/M} \cong \tfrac{1}{2}e(3/M)^{\frac{1}{2}} \quad \text{for large } M. \qquad (25)$$

This difference is not large considering that the formula contains factors as large as $(LM/2\epsilon)^M$. The method of Hemmer, Maximon, and Wergeland can also be adapted to the region of Eq. (14) to yield precisely Eq. (19). A third method of defining the recurrence time due to Smoluchowski has been shown by Kac[4] to give the same result as Hemmer, Maximon, and Wergeland.

These same methods can be used to determine properties of the system which depend upon knowing which particle is on which trajectory except that the expressions to be evaluated are periodic in the usual variables with a period NL reflecting this property of $S(u, x)$. Single-particle properties are easily calculated. We find that the time average single-particle distribution is uniform throughout the system independent of the initial spatial distribution. A particle spends $1/N$th of its time on each trajectory, consequently the probability that it will have a velocity in a given range is the fraction of the trajectories with a velocity in this range. On the average, particle i requires a time of NL/v_i to return to its original position on its original trajectory. The time required for a particle to return to a set of velocities θ is given by

$$\tau \cong \left[\rho \int_{\bar{\theta}} P(v_1)\, dv_1 \int_{\theta} P(v_2)\, dv_2\, |v_1 - v_2|\right]^{-1}, \qquad (26)$$

where $P(v)$ is the probability density for finding trajectories in a range about v, $\rho = N/L$ is the density of the system, and where $\bar{\theta}$ is the compliment of the set θ.

Properties of the system which depend upon two-particle correlations are only slightly more difficult to calculate. The recurrence time for two particles to come back to their original trajectories and close to their original positions is given approximately by

$$\frac{1}{T_r^{(2)}} = \lim_{T\to\infty} \frac{1}{2}\frac{1}{T}\int_0^T \sum_\alpha \delta(t - t_\alpha) A_{ij}(t) A_{kk}(t)\, dt, \qquad (27)$$

where the t_α's are the roots of the function

$$f(t) - \epsilon = \dashv x_i(t) - x_i(0)\vdash + \dashv x_k(t) - x_k(0)\vdash - \epsilon. \qquad (28)$$

This formula counts only those zeros of $f(t) - \epsilon$ which occur when A_{ij} and A_{kk} are both equal to 1. The formula is approximate because it is not clear

[3] P. C. Hemmer, L. C. Maximon, and H. Wergeland, Phys. Rev. **111**, 689 (1958).

[4] M. Kac, Phys. Rev. **115**, 1 (1959).

whether we should assume that there are one or two zeros of the function for each recurrence. Equation (27) can be transformed to

$$\frac{1}{T_r^{(2)}} = \frac{1}{2(NL)^N}\int_0^{NL}\cdots\int_0^{NL} dx_0\cdots dx_{N-1} \times \delta(|x_i| + |x_k| - \epsilon) \times |v_i \operatorname{sgnp} x_i + v_k \operatorname{sgnp} x_k|\, A_{ii}A_{kk} \tag{29}$$

where in each of the A's w_{kh} is set equal to $x_k - x_h$. This expression contains a special case of the quantity $\mathfrak{A}_{j'jk'k}$

$$\mathfrak{A}_{j'jk'k} = \frac{1}{(NL)^{N-2}}\int_0^{NL}\cdots\int_0^{NL} A_{j,j}A_{k,k}\prod_{\substack{h\neq j,k\\ h=0}}^{h=N-1} dx_h \tag{30}$$

to be evaluated, which is of some interest in itself. It gives the time average probability of finding particle j' on trajectory j which is at a given position and particle k' on trajectory k at another given position. Written out more fully, the expression for $\mathfrak{A}_{j'jk'k}$ is

$$\mathfrak{A}_{j'jk'k} = \frac{1}{(NL)^{N-2}} \times \int_0^{NL}\cdots\int_0^{NL}\frac{1}{N^2}\sum_{u_1u_2}\exp\left[-i(j'u_1 + k'u_2)\right] \times \prod_{h=0}^{N-1} S[u_1, x_j - x_h]S[u_2, x_k - x_h]\prod_{h\neq j,k} dx^h. \tag{31}$$

The integral over a typical x_h in this expression has the form

$$I = \frac{1}{NL}\int_0^{NL} S[u_1, x_i - x_h]S[u_2, x_k - x_h]\, dx_h \tag{32}$$

and using Eq. (10),

$$I = e^{i(u_1+u_2)}\frac{1}{NL}\int_0^{NL} S[u_1, x_i - x_h + L] \times S[u_2, x_k - x_h + L]\, dx_h.$$

In this expression we may introduce $x_h' = x_h - L$ as a new variable of integration and maintain the same limits because the integral is over a full period to obtain

$$I = e^{i(u_1+u_2)}I$$

or

$$I = 0 \quad \text{unless} \quad u_2 = -u_1 \bmod (2\pi). \tag{33}$$

We use this formula to eliminate u_2 from the expression and find that the result is now clearly periodic in each x_h with period L so that each spacial average can now be carries out over this shorter range. Following this the evaluation can be carried out straightforwardly to obtain

$$\mathfrak{A}_{j'jk'k} = \frac{1}{N}\frac{(N-2)!}{(N-k'+j'-1)!\,(k'-j'-1)!} \times \left(\frac{x_k - x_i}{L}\right)^{k'-j'-1}\left(1 - \frac{x_k - x_i}{L}\right)^{N+j'-k'-1} \quad \text{for } k' > j' \text{ and } x_k > x_i \tag{34}$$

and

$$\mathfrak{A}_{j'jk'k} = \frac{(N-2)!}{N(N-k'+j'-1)!\,(k'-j'-1)!} \times \left(\frac{x_j - x_k}{L}\right)^{N-k'+j'-1}\left(1 - \frac{x_j - x_k}{L}\right)^{k'-j'-1} \quad \text{for } k' > j' \text{ and } x_k < x_j. \tag{35}$$

The results for $j' < k'$ are obtained by interchanging labels. In terms of $\mathfrak{A}$ the two particle recurrence time is

$$\frac{1}{T_r^{(2)}} = \frac{1}{2L^2}\int_{-L/2}^{L/2} dx_i\int_{-L/2}^{L/2} dx_k\,\delta(|x_i| + |x_k| - \epsilon) \times |v_i \operatorname{sgnp} x_i + v_k \operatorname{sgnp} x_k|\,\mathfrak{A}_{jjkk}. \tag{36}$$

To simplify the work, we consider only the limit of an infinite system so that N and L approach infinity in such a way that $\rho = N/L$, the density of the system remains finite. Then $\mathfrak{A}$ is given for $k' > j'$ by

$$\mathfrak{A}_{j'jk'k} \sim \frac{1}{N}\frac{[\rho(x_k - x_i)]^{k'-j'-1}}{(k'-j'-1)!}e^{-(x_k-x_i)\rho}, \quad x_k > x_i,$$
$$\mathfrak{A}_{j'jk'k} \sim 0 \qquad (x_k < x_i). \tag{37}$$

This second expression becomes zero because the particles cannot change their order along the line in an infinite system. Substituting this in Eq. (36) we obtain the result

$$\frac{1}{T_r^{(2)}} = \frac{\rho}{2N^3}|v_k - v_i|\frac{(\rho\epsilon)^{\nu+1}}{\nu!}e^{-\rho\epsilon} + \frac{\rho^{\nu+2}}{2N^3\nu!}|v_k + v_i|\int_0^{\epsilon} y^{\nu}e^{-\rho y}\, dy$$

where $\nu = k - j - 1$ and

$$\frac{1}{\nu!}\int_0^{\epsilon} y^{\nu}e^{-\rho y}\, dy = \frac{1}{\rho^{\nu+1}}\left[1 - \sum_{i=0}^{\nu}\frac{(\rho\epsilon)^i}{i!}e^{-\rho\epsilon}\right]. \tag{38}$$

The result which we have given for $\mathfrak{A}_{j'jk'k}$ can actually be obtained more simply. We note that $\mathfrak{A}_{j'jk'k}$ is the probability that particle j' is on trajectory j at a given position x_i and that there are exactly $\nu = k' - j' - 1$ trajectories between this point and the given point x_k where trajectory k is

located, so that particle k' falls on this trajectory. From (13) the probability that there are ν trajectories between these points is given by

$$\frac{(N-2)!}{\nu!\,(N-\nu-2)!}\left(\frac{x_k-x_j}{L}\right)^{\nu}\left(1-\frac{x_k-x_j}{L}\right)^{N-\nu-2}, \quad (39)$$

and the probability that particle j' is on trajectory j is just $1/N$ no matter how the trajectories are arranged by a study of the single-particle average we have discussed. Combining these results gives (34) and (35). The extension from two particles to M particles is obvious.

ENSEMBLE CALCULATIONS

We now consider the calculation of the properties of an ensemble of systems obtained by assuming suitable spatial and velocity distributions for the particles at the initial time. It might appear that any results found in this way should be obtainable from the formalism we have already given by virtue of the equivalence of time and ensemble averages. This is not the case, however, because we are able to study the dynamics of an ensemble in the limit of a large volume and large number of particles. For this infinite system the Kronecker–Weyl theorem is not available. Perhaps this is one of the more interesting points to be illustrated by a model. Unfortunately the mathematics becomes somewhat messy so we limit the discussion to properties which can be written in the form

$$F = \langle f[v_0(0);\, x_j(t), v_j[t]\rangle. \quad (40)$$

We assume, as indicated, the f is a function of the coordinate and momentum of the jth particle at time t and also of the velocity of particle zero at the initial time. Note that we have assumed that particle zero starts at the origin at zero time. The function f may also depend on t explicitly without causing trouble. The quantity F can be written quite simply in terms of the A_{jk}'s and the initial values of the variables of the system,

$$F = \sum_k \langle f(v_0;\, x_k + v_k t, v_k) A_{jk}\rangle. \quad (41)$$

We assume that at the initial time the particles are uniformly distributed in space except that the zeroth particle is at the origin and that each has the velocity distribution $g(v)$. The thermal distribution g_T,

$$g_T(v) = (m\beta/2\pi)^{\frac{1}{2}} \exp\,[-m\beta v^2/2], \quad (42)$$

is of particular interest. Since the velocities of the particles are independent, it is possible to simplify formulas by expressing them in terms of the quantity

$$R[u,\, x_k + v_{kt} - x_h] \equiv \int_{-\infty}^{\infty} g(v_h) S[u,\, x_k + v_k t - x_h - v_h t]\, dv_h. \quad (43)$$

Thus we have

$$\begin{aligned} F = {} & \frac{1}{N}\sum_u \frac{(N-1)!}{L^{N-1}} \int_0^L dx_{N-1} \\ & \times \int_0^{x_{N-1}} dx_{N-2} \cdots \int_0^{x_2} dx_1 \Big\{ \sum_{k\neq 0} \int_{-\infty}^{\infty} g(v_k)\, dv_k \\ & \times \prod_{\substack{h=1 \\ h\neq k}}^{N-1} (R[u,\, x_k + v_k t - x_h]) \int_{-\infty}^{\infty} g(v_0)\, dv_0 \\ & \times S[u,\, x_k + v_k t - v_0 t] f(v_0;\, x_k + v_k t, v_k) \\ & + \int_{-\infty}^{\infty} g(v_0)\, dv_0 \int_0^L dx_{N-1} \cdots \int_0^{x_2} dx_1 \\ & \times \prod_{h=1}^{N-1} (R[u, +v_0 t - x_h]) f(v_0;\, v_0 t, v_0) \Big\}. \end{aligned} \quad (44)$$

This can be simplified by using the fact that

$$\int_0^L dx_n \int_0^{x_n} dx_{n-1} \cdots \int_0^{x_2} dx_1 = \frac{1}{n!} \int_0^L dx_n \int_0^L dx_{n-1} \cdots \int_0^L dx_1 \quad (45)$$

if the integrand is symmetric in these arguments. By interchanging integrations, using this relation and carrying out the sum over k explicitly the expression can be simplified considerably:

$$\begin{aligned} F = {} & \frac{1}{N}\sum_u \frac{N-1}{L} \exp\,[-iju] \\ & \times \int_0^L dx_k \int_{-\infty}^{\infty} g(v_k)\, dv_k Q(u,\, x_k + v_k t, v_k) \\ & \times \left[\frac{1}{L}\int_0^L R[u,\, x_k + v_k t - x_h]\, dx_k\right]^{N-2} \\ & + \frac{1}{N}\sum_u \exp\,[-iju] \int_{-\infty}^{\infty} g(v_0)\, dv_0 f(v_0, v_0 t, v_0) \\ & \times \left[\frac{1}{L}\int_0^L R[u,\, x_k + v_k t - x_h]\, dx_h\right]^{N-1} \\ Q(u,\, x_k + v_k t, v_k) \equiv {} & \int_{-\infty}^{\infty} g(v_0) f(v_0,\, x_k + v_k t, v_k) \\ & \times S[u,\, x_k + v_k t - v_0 t]\, dv_0. \end{aligned} \quad (46)$$

Next it is convenient to consider the origin to be at the center of the interval. This is accomplished by the transformation,

$$\int_0^L dx_k = \int_0^{L/2} dx_k + \int_{L/2}^L dx_k,$$

$x_k' = x_k - L$ in second integral,

$$S(u, w' + L) = e^{+iu}S[u, w'],$$

$$\int_0^L dx_k = \int_0^{L/2} dx_k + e^{-iu}\int_{-L/2}^0 dx_k', \qquad (47)$$

where the integrand is now the original function in both integrals. Now

$$\frac{1}{L}\int_0^L R[u, w - x_k]\, dx_k$$

$$= \int_{-\infty}^{\infty} g(v_k)\, dv_k \frac{1}{L}\int_0^L S(u, w - v_k t - x_k)\, dx_k \qquad (48)$$

and

$$\frac{1}{L}\int_0^L S[u, w' - x_k]\, dx_k = 1 + (w'/L)(1 - e^{-iu}) \times S[u, w'] \quad \text{for} \quad -L < w' < L, \qquad (49)$$

hence if contributions from outside this range are negligible, as is true if $g(v_k) \cong 0$ when $|w - v_k t| > L$, we have

$$\frac{1}{L}\int_0^L R[u, w - x_k]\, dx_k \cong 1 + \frac{1}{L}(1 - e^{-iu})T[u, w], \qquad (50)$$

with

$$T[u, w] = \int_{-\infty}^{\infty} (w - v_k t)S[u, w - v_k t]g(v_k)\, dv_k. \qquad (51)$$

We expect these conditions to be fulfilled for large L and N.

Now consider the limit as N and L approach infinity with $\rho = N/L$ held finite. This gives

$$F = \rho\frac{1}{2\pi}\int_0^{2\pi} du\, e^{-iju} \times \left[\int_0^{\infty} dx_k + e^{-iu}\int_{-\infty}^0 dx_k\right]\int_{-\infty}^{\infty} g(v_k)\, dv_k \times Q(u, x_k + v_k t, v_k)\exp\{\rho(1 - e^{-iu})T[u, x_k + v_k t]\} + \frac{1}{2\pi}\int_0^{2\pi} du\, e^{-iju}\int_{-\infty}^{\infty} g(v_0)\, dv_0\, f(v_0, v_0 t, v_0) \times \exp\{\rho(1 - e^{-iu})T[u, v_0 t]\}, \qquad (52)$$

where we have used the fact that

$$\frac{1}{N}\sum_u \to \frac{1}{2\pi}\int_0^{2\pi} du, \qquad (53)$$

and have assumed that $Q \to 0$ for x_k large in order that we have the limit

$$[1 + (1/L)(1 - e^{-iu})T]^N \to \exp\{\rho(1 - e^{-iu})T\} \qquad (54)$$

for all values of x_k which contribute.

The integration over u can be carried out if the expressions for T and Q are simplified.

$$T(u, w) = -A(w) + (w + A)e^{iu},$$
$$Q(u, w, v_k) = B + Ce^{iu},$$

with

$$A(w) = \int_{w/t}^{\infty} (-w + v_k t)g(v_k)\, dv_k,$$
$$B = \int_{w/t}^{\infty} g(v_0)f(v_0, w, v_k)\, dv_0, \qquad (55)$$
$$C = \int_{-\infty}^{w/t} g(v_0)f(v_0, w, v_k)\, dv_0,$$

where we have used the assumption

$$\int_{-\infty}^{\infty} vg(v)\, dv = 0. \qquad (56)$$

We make use of the formula

$$J^{(m)} \equiv \frac{1}{2\pi}\int_0^{2\pi} du\, e^{-imu} \times \exp\{\rho(1 - e^{-iu})(-A + Ge^{+iu})\} = (G/A)^{m/2}I_m[2\rho(AG)^{\frac{1}{2}}]e^{-(A+G)\rho}, \qquad (57)$$

where I_m is a Bessel function of imaginary argument. This formula is easily obtained by integrating the usual generating function for Bessel functions,

$$\exp\left[\frac{x(t - t^{-1})}{2}\right] = \sum_{n=-\infty}^{\infty} t^n J_n(x), \qquad (58)$$

around the origin with a t^{-m-1} factor and changing variables.

The results obtained by using $\delta[y - x_j(t)]$ for f are particularly interesting. This gives the probability $P(y)$ of finding particle j at position y at time t. The result is

$$P(y) = \{2\rho(1 - B_0)B_0 H^j I_j + \rho(1 - B_0)^2 H^{j-1}I_{j-1} + \rho B_0^2 H^{j+1}I_{j+1} + (1/t)H^j g(y/t)I_j\}\exp[-(2A(y) + y)\rho]$$

where

$$B_0 = \int_{y/t}^{\infty} g(v_0)\, dv_0 \quad H = \left[\frac{y + A(y)}{A(y)}\right]^{\frac{1}{2}}$$
$$I_n = I_n(2\rho\{A(y)[y + A(y)]\}^{\frac{1}{2}}) \qquad (59)$$

We examine the behavior described by this complicated formula only asymptotically in the limit of large time so that we may set $y/t \simeq 0$ throughout the expression. However we shall assume that y is also large of order $t^{\frac{1}{2}}$ to keep in certain contributions

which would otherwise be neglected. In this limit

$$A \simeq t \int_0^\infty vg(v)\, dv,$$
$$B_0 \simeq \int_0^\infty g(v)\, dv. \tag{60}$$

A standard asymptotic formula for the Bessel function of large argument gives

$$J^{(m)} \cong \left(\frac{G}{A}\right)^{m/2} \frac{1}{[4\pi\rho(AG)^{\frac{1}{2}}]^{\frac{1}{2}}} e^{2(AG)^{\frac{1}{2}}\rho-(A+G)\rho}$$
$$= \left(\frac{G}{A}\right)^{m/2} \frac{1}{[4\pi\rho(AG^{\frac{1}{2}})]^{\frac{1}{2}}} e^{-(A^{\frac{1}{2}}-G^{\frac{1}{2}})^2\rho} \tag{61}$$

and since $G = y + A \simeq A$,

$$J^{(m)} \cong (4\pi\rho A)^{-\frac{1}{2}} e^{-y^2\rho/4A}$$

and if

$$D = \frac{1}{\rho}\int_0^\infty vg(v)\, dv,$$

we have

$$P(y) \simeq (4\pi Dt)^{-\frac{1}{2}} e^{-y^2/4Dt}. \tag{62}$$

Thus the long-time effect of the motion is to cause the particles about the origin to appear to diffuse away. This, of course, is not true diffusion since there is no way for a particle to get past its nearest neighbors. This delocalization phenomenon is not unexpected here since it also occurs in one-dimensional harmonic-oscillator assemblies.[5]

We can obtain precisely this value of D from an extremely crude statistical model of this process. We assume that the trajectories are "on the average" side by side with a distance $1/\rho$ between them. The particle we are observing performs a random walk on these trajectories, stepping right or left with equal probability at a rate equal to the rate at which the trajectories move this distance to collide with each other. This rate is

$$\rho \int_{-\infty}^\infty |v|\, g(v)\, dv = 2\rho \int_0^\infty vg(v)\, dv. \tag{63}$$

The usual theory described, for example, by Chandrasekhar[6] gives for the "diffusion constant" of this motion the expression

$$D = \tfrac{1}{2}nl^2;$$
$$n = \text{rate of stepping}, \quad l = \text{length of step}. \tag{64}$$

Now if we assume that the process is such a random walk over a line of points a distance $1/\rho$ apart with a jumping rate of $\rho\langle|v|\rangle$ as above we get the same result as in the foregoing analysis.

Another quantity of interest is the correlation function $\langle v_0(0)v_j(t)\rangle$. The behavior of correlations of this type is of general interest because of the role they play in the theory of stochastic processes. A trick is required to calculate this quantity using the general formalism we have given because there are contributions to the integral over x_k for large values of the argument, and we are required to make a transformation on the expression in Eq. (46) before taking the limit of an infinite system. We restrict the $g(v)$ under consideration to the thermal distribution $g_T(v)$ given in Eq. (42). Then the expression of Eq. (46) with f taken as $v_0(0)v_j(t)$ has the general form

$$F = \left(\frac{m\beta}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^\infty v_k\, dv_k\, e^{-(m\beta/2)v_k^2} \int_0^L dx_k\, \phi(x_k + v_k t) \tag{65}$$

+ second term.

Integrating by parts in v_k we obtain

$$F = \frac{1}{m\beta}\left(\frac{m\beta}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^\infty e^{-(m\beta/2)v_k^2}\, dv_k$$
$$\times \int_0^L dx_k \frac{\partial}{\partial v_k}\phi(x_k + v_k t) + \text{second term} \tag{66}$$

and, since in this expression $\partial/\partial v_k = t\partial/\partial x_k$, we have

$$F = \frac{t}{m\beta}\int_{-\infty}^\infty dv_k\, g_T(v_k)[\phi(L + v_k t) - \phi(v_k t)]$$
$$+ \text{second term}. \tag{67}$$

Here we may make use of Eq. (10) and then take the limit as N approaches infinity with ρ finite as before. The final result can be written as

$$\langle v_0(0)v_j(t)\rangle$$
$$= \frac{\rho t}{2\pi m\beta}\int_{-\infty}^\infty dv[H^{j+1}I_{j+1} + H^{j-1}I_{j-1} - 2H^jI_j]$$
$$\times \exp\left[-m\beta v^2 - (2A(vt) + vt)\right] + \left(\frac{m\beta}{2\pi}\right)^{\frac{1}{2}}$$
$$\times \int_{-\infty}^\infty v^2\, dv\, H^jI_j \exp\left\{-(m\beta/2)v^2 - [2A(vt) + vt]\rho\right\},$$

with

$$H = [A(vt) + vt/A(vt)]^{\frac{1}{2}},$$
$$I_n = I_n(2\rho\{A(vt)[vt + A(vt)]\}^{\frac{1}{2}}). \tag{68}$$

We note from the definition of A in Eq. (60) that H is actually independent of t and that the argument of the Bessel function is linear in t.

[5] R. J. Rubin, J. Math. Phys. **1**, 309 (1960); **2**, 373 (1961).
[6] S. Chandrasekhar, Rev. Mod. Phys. **15**, 5 (1943).

A rather messy calculation shows that for large t,

$$\langle v_0(0)v_0(t)\rangle \cong \left(\frac{m\beta}{2\pi}\right)^{\frac{1}{2}}\left(-1+\frac{5}{2\pi}\right)\frac{1}{\rho^3 t^3}. \tag{69}$$

Unlike harmonic oscillators this correlation approaches an asymptotic value even for a finite system and without oscillation. The initial thermal average appears to be responsible for the loss of Poincaré cycles. Since this correlation goes to zero for large times $v_0(t)$ viewed as a stochastic process must be ergodic by a theorem of Montroll and Mazur.[2] In essence the vanishing of this correlation for large times indicates a type of irreversibility in this system. If a single particle of the system is given an electrical charge the motion of this particle in an external electric field will give rise to an electrical conductivity. This conductivity can be expressed in terms of the motion of the system in the absence of the external field by the Kubo formula[7]

$$\sigma(\omega) = e^2\beta\int_0^\infty e^{i\omega t}\langle v_0(0)v_0(t)\rangle\, dt. \tag{70}$$

This formula is sometimes written with an additional factor to give convergence of the integral for large t but from what we have just seen such a factor is clearly unnecessary for this system. The time integration indicated in the formula can easily be carried out on the expression for the correlation we have given, yielding a result which still contains a messy integration over v. For low frequencies we find that

$$\sigma \cong e^2\beta\Big[D + \text{linear term in } \omega + (m\beta/2\pi)^{\frac{1}{2}} \times\left(-1+\frac{5}{2\pi}\right)\frac{1}{2\rho^3}\omega^2\log\omega + O(\omega^2)\Big]. \tag{71}$$

At zero frequency the conductivity is related to the diffusion coefficient as is required by the Einstein relation[7]; the $\omega^2 \log \omega$ term is easily shown to be implied by the asymptotic dependence given in Eq. (69). It would be interesting to know whether such terms exist for actual physical systems.

[7] R. Kubo, Proc. Phys. Soc. Japan 12, 570 (1957).

Other initial conditions can also be treated. Let us assume that at the initial time the first M particles labeled from zero to $M-1$ are restricted to lie in the interval $[0, L/2]$ and that they have a Maxwellian velocity distribution with temperature T_1. The rest of the particles labeled from M to $N-1$ are assumed to be in the interval $[L/2, L]$ at time $t = 0$ and have a Maxwellian velocity distribution with temperature T_2. These initial conditions model the usual experimental arrangement used for studying gaseous or liquid diffusion. The mathematics which we have described for uniform initial conditions can also be carried through in this case with slight additional complication. The most striking feature of the analysis is that the condition that the pressures in the two regions be equal to each other, which is necessary in order to make observations of diffusion in the usual experiments, is replaced for this model by the somewhat different condition that

$$\rho_1(T_1)^{\frac{1}{2}} = \rho_2(T_2)^{\frac{1}{2}}, \tag{72}$$

where ρ_1 and ρ_2 are the initial densities in the two regions. This condition actually states that the number of trajectories crossing the boundary between the two regions per unit time be the same from the left as from the right. Given in this way, the condition is not surprising. Carrying through the analysis we find that a particle starting on the boundary of the two regions again has a Gaussian probability distribution asymptotically with time, but with the diffusion constant D given by

$$D = [4\rho_1/(\rho_1+\rho_2)^2](2\pi m\beta_2)^{-\frac{1}{2}} = [4\rho_2/(\rho_1+\rho_2)^2](2\pi m\beta_1)^{-\frac{1}{2}}. \tag{73}$$

It appears that a variety of other properties of this system could be calculated if required.

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Lepton Scattering Amplitudes in Two Model Field Theories*

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Two lepton–lepton scattering amplitudes are considered within the context of a no-recoil Bloch–Nordsieck model, with emphasis on the singularities in that configuration-space variable conjugate to momentum transfer. For the interaction $\mathfrak{L}' = -g\bar{\psi}A\psi$, renormalizable in four dimensions, and in the approximation of including only the exchange of all possible bosons between a pair of leptons, a light cone singularity no worse than that of the one-boson-exchange graph is found. Similar statements may be made for the same interaction, nonrenormalizable in six dimensions, provided certain continuations in the center-of-mass energy variable are employed; otherwise, an essential singularity appears. A remark illustrating the formation of bound states is made for the renormalizable interaction. No argument is given to establish the relevance of these models to the actual field-theoretic situations.

I. INTRODUCTION

RECENT work of Lee,[1] and of Feinberg and Pais,[2] has stimulated interest in the possibility of constructing sensible nonrenormalizable field theories.[3] An essential part of the peratization methods[2,4,5] appears to be the necessity of exhibiting a scattering amplitude damped on the light cone (lc) of that configuration-space variable x conjugate to momentum transfer. The presence of such damping suggests that the corresponding field theory may have a small but finite chance of existing; and conversely, from the appearance of, e.g., an essential lc singularity, one would infer that the corresponding interaction is not sensible, or that specific prescriptions (such as regularization) must be employed. Further, it is not known if the peratization calculations are very sensitive to their common approximation, the neglect of external 4-momenta—and hence all c.m. energy dependence—but not momentum transfer. These considerations have motivated Khuri and Pais,[6] and Pais and Wu[7] to study singular potential theory models, in a search for possible self-damping mechanisms. In a spirit somewhat similar to that of the recent calculation of Sawyer,[8] we would like to consider a singular, nonrenormalizable model within the realm of field theory.

In order to make the problem soluble, we consider lepton–lepton scattering amplitudes defined for the simplest interaction within the Bloch–Nordsieck (BN) model.[9] This model has been employed[10] in studies of lepton progagator structure, and it turns out that analogous techniques may be used to discuss scattering amplitudes as well. In such approximations there are no antileptons, and hence all closed loops vanish. We go further and neglect all lepton self-energy and vertex-type structure, in order to construct relatively simple amplitudes given by the exchange of scalar bosons in all possible combinations (ladder and crossed graphs) between a pair of BN leptons.

Our method is to first write down (Sec. II) the generic, functional form of all such approximate scattering functions, and to then apply (Sec. III) the formulas to the interaction $\mathfrak{L}' = -g\bar{\psi}A\psi$ in (A) four dimensions and in (B) six dimensions. Theory A is conventionally renormalizable; B is not. Our results indicate that, considered as a function of x,

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[1] T. D. Lee, Phys. Rev. **128**, 899 (1962).
[2] G. Feinberg and A. Pais, Phys. Rev. **131**, 2724 (1963); Phys. Rev. **133**, B477 (1964).
[3] These theories differ from those discussed previously (e.g., L. N. Cooper, Phys. Rev. **100**, 362 (1955), and other references quoted there) in that the S-matrix is not unity.
[4] K. Bardakci, M. Bolsterli, and H. Suura, Phys. Rev. **133**, B1273 (1964).
[5] H. M. Fried, Phys. Rev. **133**, B1562 (1964); and "Functional Methods in the Peratization Theory of Weak Interactions," CIMS preprint.
[6] N. N. Khuri and A. Pais, Rev. Mod. Phys. **36**, 590 (1964).
[7] A. Pais and T. T. Wu, J. Math. Phys. **5**, 799 (1964); Phys. Rev. **134**, B1303 (1964).
[8] R. F. Sawyer, Phys. Rev. **134**, B448 (1964).
[9] F. Bloch and A. Nordsieck, Phys. Rev. **52**, 54 (1937).
[10] See, for example, N. N. Boguliubov and D. V. Shirkov, *Introduction to the Theory of Quantum Fields* (Interscience Publishers, Inc., New York, 1959).

these configuration space amplitudes may each possess a Fourier transform if certain continuations of the c.m. energy variable are judiciously performed during the process of integration. In particular, such continuations are necessary to avoid an essential singularity in Case B; by essential singularity we here mean an exponential divergence of form $\exp(1/z)$, $z \to 0+$. These remarks may be illustrated by stating the nature of these amplitudes near the lc ($x^2 = r^2 - x_0^2 \sim 0$), and, when appropriate, near the apex of the lc ($r \sim 0$). (A) A singularity of form $(x^2)^{-1}(r^2)^{-\bar{\alpha}(s)}$. If certain linear combinations of the external 4-momenta, denoted by $L(q)$, are initially set equal to zero, this changes to $(x^2)^{-1}\ |x^2|^{-\bar{\alpha}(s)}$. (B) A singularity of form $|x^2|^{-2+a/r^2}\ \{1 + b/r^2\}$, $a > 0$. If the approximation $L(q) = 0$ is initially made, this changes to $(x^2)^{-3} \exp\{\bar{\alpha}(s)/\pi x^2\}$. Here $\bar{\alpha}(s)$ depends upon the total c.m. energy s in such a manner that Re $\bar{\alpha}(s) < 0$ for $s > 4m^2$, where m denotes the lepton mass. In fact, $\bar{\alpha}(s)$ is closely related to the lowest g^2 order approximation $\alpha_1(s)$ of the Regge function $\alpha(s)$, appropriate to this interaction, which has been discussed by many authors[11,12]; here, $\bar{\alpha} = 1 + \alpha_1$.

For interaction (A), in the physical region for scattering, we thus find a certain measure of "damping at the origin" when integration over r is performed, during the calculation of the Fourier transform. For $s < 4m^2$, however, $\bar{\alpha}(s)$ is real and positive, with the effect of introducing a pole into the continuation of the scattering amplitude whenever $\bar{\alpha}(s)$ passes through an integer. Hence the behavior of the configuration space model amplitude near the origin acts to produce bound states (Sec. IV) in a manner completely analogous to the small-impact-parameter behavior of the (Coulomb) potential theory model of Ref. 11.

The drastic nature of the approximation which initially sets $L(q) = 0$ is apparent for interaction B unless one has the possibility of continuing in s; for example, if s is fixed such that $s = s_0 > 4m^2$, an exponential divergence appears on the interior of the lc. The reason for this is that this model distinguishes between interactions A and B by exhibiting an exponential factor whose argument near the lc is proportional either to $\ln|x^2|$ or to $1/x^2$, respectively. In the latter case, spacelike and timelike regions have opposite signs; and since this dependence is exponentiated, an exponential divergence can occur. The same conclusion may also be valid for the essential singularities encountered in previous peratization calculations.[4,5] Our result, however, is certainly model dependent, and hence without general applicability.

We also emphasize that we know of no argument relating these models to each field-theoretic situation. In fact, we think that the no-recoil models, while approximating the appropriate Feynman graphs with expressions having the correct degree of divergence or convergence, as the case may be, can yield results which have nothing to do with the interactions they purport to model. This is because such expressions contain the combinations associated with infrared behavior; or put another way, they give the structure expected in a real field theory when virtual momenta are very small. However, as used here, a typical virtual momentum may appear conjugate to the coordinate x, and it probably makes little physical sense to use these models for small x, or x^2. Rather than pursue this subject we here forego all claim to physical significance, and merely present the models; solubility is their *raison d'être*.

Most arithmetical details have been put into a brief Appendix. We thought it worthwhile, however, to include the elementary manipulations of Sec. II in the text, since they do not seem to be very well known.

II. MODEL SCATTERING AMPLITUDES

We begin by writing down the functional statement of the four-point Green's function corresponding to the exchange of all possible scalar bosons (mass M) between a pair of distinguishable leptons (mass m),

$$M(x_1y_1, x_2y_2) = M(x;y) = \exp[-i(\delta/\delta J)\Delta_F\delta/\delta J'] \times G_{\mathrm{I}}(x_1y_1 \mid J)G_{\mathrm{II}}(x_2y_2 \mid J')|_{J=J'=0}, \quad (1)$$

where the specific choice of interaction is expressed by the dependence of the Green's functions $G_{\mathrm{I,II}}$ upon the external source $J(z)$. Coordinates with subscript 1 shall always refer to lepton I, and subscript 2 denotes lepton II. Within the stated approximations, (1) can be obtained directly from Schwinger's functional solution for the unrenormalized four-point Green's function, but it is easy to see that the expansion of the exponential operator of (1) yields the sum of all ladder and crossed graphs. The nth term of that expansion produces n boson propagators Δ_F, which link a pair of $(n + 2)$-point Green's functions; each of the latter is symmetric in its n boson coordinates, and may be written as a permutation sum over $n!$ distinct terms. The

[11] R. Blankenbecler and M. L. Goldberger, Phys. Rev. **126**, 766 (1962).
[12] B. W. Lee and R. Sawyer, Phys. Rev. **127**, 2266 (1962).

combination of these two Green's functions then produces a total of $(n!)^2$ terms which rearrange themselves into the desired $n!$ topologically distinct graphs, each of which occurs $n!$ times; and the $(n!)^{-1}$ factor coming from the expansion of the exponential just restores the proper counting.

All the complexity of the problem has been put into the Green's functions $G_{I,II}$, and we first write down their differential equation, without approximation,

$$[m + \gamma\cdot\partial_x + \mathcal{J}(x)]G(xy \mid J) = \delta(x - y), \tag{2}$$

where $\mathcal{J}(x) = \mathcal{J}[J(x)] = gJ(x)$ for the interactions A and B. It may be noted that the interaction $\mathcal{L}' = -g\bar{\psi}A^2\psi$, corresponding to the choice $\mathcal{J} = gJ^2$, is nonrenormalizable in four dimensions and can also be studied in a BN model; closed-form solutions for the configuration-space scattering amplitudes are here obtained in terms of quadratures over the logarithm of a Fredholm-type determinant.

The BN approximation[9] replaces the Dirac γ matrices by constant 4-vectors iv_μ, with $v^2 = -1$; this effectively neglects "radiative recoil" variations of the lepton's momentum. In this model, the Green's functions satisfy

$$[m + iv\cdot\partial_x + \mathcal{J}(x)]G(xy \mid J) = \delta(x - y), \tag{3}$$

which can be solved immediately[10]:

$$G(xy \mid J) = i\int_0^\infty d\xi e^{-i\xi m} \times \left\{\exp\left[-i\int_0^\xi d\xi'\mathcal{J}(x + \xi'v)\right]\right\}\delta(x - y - \xi v), \tag{4}$$

where m is understood to have a small, negative, imaginary part. The momentum-space Green's functions, defined by

$$\tilde{G}(qp \mid J) = (2\pi)^{-4}\int dx\, dy\, e^{i[qx+py]}G(xy \mid J),$$

are then given by

$$\tilde{G}(qp \mid J) = i(2\pi)^{-4}\int dx\, e^{i[q+p]x}\int_0^\infty d\xi \times \exp -i\xi[m - v\cdot p] \times \exp\left[-i\int_0^\xi d\xi'\mathcal{J}(x + \xi'v)\right]. \tag{5}$$

The amplitude $M(x; y)$ of (1) is related to the configuration-space scattering amplitude $T(x; y)$ by

$$M(x; y) = S_F^I(x_1 - y_1)S_F^{II}(x_2 - y_2) + \int S_F^I(x_1 - u_1)S_F^{II}(x_2 - u_2)T(u; v) \times S_F^I(v_1 - y_1)S_F^{II}(v_2 - y_2), \tag{6}$$

where the $S_F^{I,II}$ are free (because of our neglect of self-energy structure) lepton propagators; the Fourier transform of $T(x; y)$, evaluated on the mass shell of all 4-momenta, represents the conventional momentum-space scattering amplitude. Hence it is convenient to discuss the amputated form of (5), which we do in the following way. Amputating first on p, we denote by $\tilde{G}(q\bar{p} \mid J)$ the product $(m - v\cdot p)\tilde{G}(qp \mid J)$; and a single integration-by-parts on the variable ξ then yields

$$\tilde{G}(q\bar{p} \mid J) = \delta(q + p) + \tilde{H}(q\bar{p} \mid J),$$

$$\tilde{H}(q\bar{p} \mid J) = (2\pi)^{-4}\int_0^\infty d\xi\, e^{-i\xi[m - v\cdot p]}\int dx\, e^{i[q+p]x}\frac{\partial}{\partial\xi} \times \exp\left[-i\int_0^\xi d\xi'\mathcal{J}(x + \xi'v)\right]. \tag{7}$$

The $\delta(q + p)$ term of (7) corresponds to the disconnected term of (1), which may be removed by considering the functional $H(xy \mid J) = G(xy \mid J) - S_F(x - y)$.

Amputation on q is most easily performed by defining a new variable $x' = x + \xi v$, such that $\tilde{H}$ becomes

$$\tilde{H}(q\bar{p} \mid J) = (2\pi)^{-4}\int dx' e^{i[q+p]x'} \times \int_0^\infty d\xi\, e^{-i\xi[m + v\cdot q]}\mathfrak{F}(\xi \mid x'), \tag{8}$$

with

$$\mathfrak{F}(\xi \mid x') = \frac{\partial}{\partial\xi}\exp\left[-i\int_0^\xi d\xi'\mathcal{J}(x + \xi'v)\right]\Big|_{x=x'-\xi v} = -i\mathcal{J}(x')\exp\left[-i\int_0^\xi d\xi'\mathcal{J}(x' - \xi'v)\right]. \tag{9}$$

Again employing an integration by parts, and denoting by $\tilde{H}(\bar{q}\bar{p} \mid J)$ the combination $(m + v\cdot q)\tilde{H}(q\bar{p} \mid J)$, we obtain

$$\tilde{H}(\bar{q}\bar{p} \mid J) = -i(2\pi)^{-4}\int dx\, e^{i[q+p]x} \times \left\{\mathfrak{F}(0 \mid x) + \int_0^\infty d\xi\, e^{-i\xi[m + v\cdot q]}\frac{\partial}{\partial\xi}\mathfrak{F}(\xi \mid x)\right\}, \tag{10}$$

where the prime on the x coordinate of (9) has been dropped.

A marked simplification, corresponding to "going to the mass shell," can be achieved here; but it is

first worthwhile to consider the type of lepton progagators we are producing. For an exact treatment of interaction A or B we would use, in the construction of any Feynman graph linking leptons I and II, lepton progagators given by the denominator function

$$D(q + \sum_i k_i) = m + i\gamma\cdot(q + \sum_i k_i),$$

where k_i denote internal, virtual boson momenta. In the BN model, in contrast, we are producing functions of form

$$D_{\mathrm{BN}}(q + \sum_i k_i) = m + v\cdot(q + \sum_i k_i).$$

To see the comparison, rationalize the correct denominators and take the infrared limit $\sum_i k_i \ll q$,

$$D^{-1} \to D_{\mathrm{IR}}^{-1}(q, \sum_i k_i)$$
$$= (m - i\gamma\cdot q)[m^2 + q^2 + 2q\cdot\sum_i k_i]^{-1}. \quad (11)$$

For a scalar interaction (the kind we consider here), there is no difficulty in replacing each factor of $-i(\gamma\cdot q)$ by m; hence, on the mass shell, $q^2 + m^2 = 0$, (11) may be replaced by

$$D_{\mathrm{IR}}^{-1} = m(q\cdot\sum_i k_i)^{-1}. \quad (12)$$

Exactly the same form is obtained within the BN model if we make the mass-shell replacement $v = q/m$; with this identification of v, the model just duplicates the infrared structure of each Feynman graph. It should be remarked that the use of the BN model as an initial step of an approximation scheme is, apparently, the antithesis of the peratization approximations,[2,4,5] where external momenta are neglected compared to internal momenta.

The procedure of "going to the mass shell," in (10), can now be trivially performed, since the combination $(m + v\cdot q)$ appears only in the exponential factor of the ξ integrand of $\tilde{H}$. We may therefore write

$$\tilde{H}^{MS}(\bar{q}\bar{p} \mid J) = -i(2\pi)^{-4}\int dx\, e^{i(q+p)x}$$
$$\times\left\{\mathfrak{F}(0 \mid x) + \int_0^\infty d\xi\,\frac{\partial}{\partial\xi}\mathfrak{F}(\xi \mid x)\right\}, \quad (13)$$

provided that the upper limit convergence of each ξ-integration, occurring in the perturbation expansion of $\mathfrak{F}(\xi \mid x)$, is assured. But this will be the case if the Fourier transform of $\mathcal{J}(x + \xi v)$ is supplied with a convergence factor,

$$\mathcal{J}(x + \xi v) \to \int dk\tilde{\mathcal{J}}(k)e^{ik[x+\xi v]}e^{-\epsilon\xi}\big|_{\epsilon\to 0+},$$

and with this understanding, we obtain the simple answer

$$\tilde{H}^{MS}(\bar{q}\bar{p} \mid J) = -i(2\pi)^{-4}\int dx\, e^{i[q+p]x}\mathfrak{F}(\infty \mid x). \quad (14)$$

In the perturbative expansion of (14) combinations have occurred such that the sum over $n!$ permutations of the n symmetric boson coordinates, entering into an $(n + 2)$-point function, has been replaced on the mass shell by an equivalent sum over n permutations of related denominator factors; this is written down explicitly in Appendix I.

Our model scattering amplitude may now be written in the form

$$\tilde{T}(q; p) = (2\pi)^4 \exp\,[-i(\delta/\delta J)\Delta_F\delta/\delta J']$$
$$\times \tilde{H}_{\mathrm{I}}^{MS}(\bar{q}_1\bar{p}_1 \mid J)\tilde{H}_{\mathrm{II}}^{MS}(\bar{q}_2\bar{p}_2 \mid J')|_{J=J'=0}. \quad (15)$$

In (15) we have two functionals $\mathfrak{F}_{\mathrm{I,II}}$, depending upon the variables $x_{1,2}$ and $v_{1,2} = q_{1,2}/m$. Substituting (14) and (9) into (15) there results

$$\tilde{T}(q; p) = \delta(q_1 + p_1 + q_2 + p_2)$$
$$\times\int dx\, e^{i(q_1+p_1)x}\psi(x \mid q_{1,2}), \quad (16)$$

where

$$\psi(x \mid q_{1,2}) = \exp\,[-i(\delta/\delta J)\Delta_F\delta/\delta J']\mathcal{J}(x_1)\mathcal{J}'(x_2)$$
$$\times\exp\left[-i\int_0^\infty d\xi_1\mathcal{J}(x_1 - \xi_1 v_1)\right]$$
$$\times\exp\left[-i\int_0^\infty d\xi_2\mathcal{J}'(x_2 - \xi_2 v_2)\right]\Bigg|_0, \quad (17)$$

with $\mathcal{J}' = \mathcal{J}[J']$ and $x = x_1 - x_2$. This is as far as we can go without specifying $\mathcal{J}[J]$.

III. SPECIFIC MODEL APPROXIMATIONS

The functional dependence of the scattering amplitude given by (16) and (17) can be evaluated immediately for the interactions A and B; one finds

$$\psi(x \mid q_{1,2}) = \left\{-ig^2\Delta_{\mathrm{F}}(x) - g^4\int_0^\infty d\xi_1\Delta_{\mathrm{F}}(x - \xi_1 v_1)\right.$$
$$\left.\times\int_0^\infty d\xi_2\ \Delta_{\mathrm{F}}(x + \xi_2 v_2)\right\}e^{f(x\mid q_{1,2})}, \quad (18)$$

where

$$f(x \mid q_{1,2}) = ig^2\iint_0^\infty d\xi_1\, d\xi_2\Delta_{\mathrm{F}}(x - \xi_1 v_1 + \xi_2 v_2),$$

and $v_{1,2} = q_{1,2}/m$.

A remark concerning the structure of this result may be pertinent here. The lowest-order term of

ψ, $-ig^2\Delta_F$, gives just the one-boson-exchange graph, while the two-rung ladder graph is given by the Fourier transform of $-ig^2\Delta_F(x)f(x \mid q_{1,2})$. Thus "exponentiation" has occurred, in (18); but in configuration space, rather than in momentum space.

The existence of a well-defined transform for (16) depends upon the behavior of the various parts of (18) near the lc and near the apex of the lc. We next describe the relevant properties of these functions for the cases A and B, treating the renormalizable interaction first; all arithmetical details have been put into Appendix II.

(A) Near the lc ($|x^2|\ M^2 \ll 1$) the one-boson-exchange contribution behaves according as

$$-ig^2\Delta_F(x) \sim \left(\frac{g}{2\pi}\right)^2 \frac{1}{x^2}, \tag{19}$$

while the second term in the curly bracket of (18) (which, by itself, corresponds to the simplest crossed graph) is less singular,

$$g^4 \int_0^\infty d\xi_1\Delta_F \int_0^\infty d\xi_2\Delta_F \sim \left(\frac{mg}{8\pi^2}\right)^2 (x\cdot q_1)^{-1}(x\cdot q_2)^{-1} \ln^2 |x^2|. \tag{20}$$

It should be remarked that the factors $x\cdot q_{1,2}$ of (20) can never vanish, on the lc, if $m \neq 0$, $r \neq 0$.

The function $f(x \mid q_{1,2})$ is finite on the lc. However, near the apex of the lc a logarithmic singularity appears which plays a central role in the subsequent discussion of bound states,

$$f(x \mid q_{1,2})|_{x^2=0,\, r\sim 0} \sim -\bar{\alpha}(s) \ln (rM)^2, \tag{21}$$

where

$$\bar{\alpha}(s) = \left(\frac{mg}{2\pi}\right)^2 \int_{4m^2}^\infty \frac{ds'}{s'-s}\,[s'(s'-4m^2)]^{-\frac{1}{2}}. \tag{22}$$

The properties of $\bar{\alpha}(s)$ have already been described in the Introduction. We have retained the boson mass dependence of (21) to emphasize that it is this mass which provides the scale; this is not surprising in an infrared model.

We now consider the effect on these estimates of prior approximations. For this, we write $f(x \mid q_{1,2}) = f(x^2, x\cdot q_{1,2}, s)$, where $s = -(q_1+q_2)^2$. The components of $q_{1,2}$ may, of course, be simply related to s, but it is convenient to treat them separately in order to parody similar peratization approximations when $m \neq 0$. We denote by $L(q) = 0$ the approximation of neglecting the external momenta $q_{1,2}$ appearing in the combinations $x\cdot q_{1,2}$, in all terms of (18); for massless fermions, the approximations $L(q) = 0$ and $s = 0$ are identical. The estimate of (20), when $L(q) = 0$, is now changed to read

$$g^4 \int_0^\infty d\xi_1\Delta_F \cdot \int_0^\infty d\xi_2\Delta_F \sim \left(\frac{g^2}{8\pi}\right)^2 \frac{1}{x^2}, \tag{23}$$

contributing a singularity of the same type as that of (19), while that of (21) is now logarithmically divergent over the entire lc,

$$f(x^2, 0, s)|_{x^2\sim 0} \sim -\bar{\alpha}(s) \ln (|x^2|\ M^2). \tag{24}$$

Hence the lc singularity of (18) remains of polynomial form,

$$\psi \sim (1/x^2)\cdot(1/|x^2|)^{\bar{\alpha}(s)}, \tag{25}$$

but the strength of the singularity depends upon s, and in particular on whether s is above or below threshold.

(B) The boson propagators in (18) are here defined in six dimensions (five spatial, one time). Depending upon the approximations, exponential divergences can now appear on the lc or at the apex of the lc. Independent of any approximation, we have

$$ig^2\Delta_F(x)|_{x^2\sim 0} \sim -(g^2/4\pi^3)(1/x^2)^2. \tag{26}$$

Consider first the simplest situation which results from the approximation $L(q) = 0$. The second term in the curly bracket of (18) is then even more singular than (26),

$$g^4 \int_0^\infty d\xi_1\Delta_F \cdot \int_0^\infty d\xi_2\Delta_F|_{x^2\sim 0} \sim \left(\frac{g}{4\pi}\right)^4 \left(\frac{1}{x^2}\right)^3, \tag{27}$$

but the dominant behavior arises from

$$f(x^2, 0, s)|_{x^2\sim 0} \sim \bar{\alpha}(s)/\pi x^2, \tag{28}$$

since (28) is to be exponentiated. Thus, to avoid an exponential singularity when approaching the exterior of the lc, $x^2 \to 0+$, s must be in the physical region for scattering; and conversely, when approaching the interior of the lc, $x^2 \to 0-$, s should be considered below threshold.

When the approximation $L(q) = 0$ is not made, the singularity at all points of the lc following from (28) is removed, but care must be taken to avoid one at the apex of the lc, as $r \to 0$. For $r \neq 0$, one finds

$$f(x^2, x\cdot q_{1,2}, s)|_{x^2\sim 0} \sim a \ln |x^2|, \qquad a > 0, \tag{29}$$

which, together with the behavior

$$g^4 \int_0^\infty d\xi_1\Delta_F \int_0^\infty d\xi_2\Delta_F\Big|_{x^2\sim 0} \sim (mg^2/8\pi^3)^2(1/x^2)^2(x\cdot q_1)^{-1}(x\cdot q_2)^{-1}, \tag{30}$$

characterizes the lc singularity, as $x^2 \to 0^\pm$,

$$\psi \sim (1/x^2)^2\ |x^2|^a, \qquad a > 0, \tag{31}$$

which is completely different and far gentler than that of (26), (27), and (28).

Approaching the apex of the lc at a fixed angle such that $x^2 \neq 0$, it is shown in Appendix II that, as $r \to 0$, the condition $\mathrm{Re}\, f \leq 0$ may be guaranteed when continuations to s values below threshold are performed in at least one special way. These statements do not guarantee the existence of the Fourier transform (16) but they do provide well-defined rules of continuation to prevent the appearance of exponential infinities which could otherwise occur. As such they stand as an example of the danger involved in neglecting the dependence on external momenta, when calculating amplitudes in a non-renormalizable theory.

IV. APPEARANCE OF BOUND STATES

The previous discussion concerning the continuation of s below threshold suggests that one may be able to see explicitly any bound states present in such models, and for the renormalizable interaction at least, this is the case. Specifically, we can isolate a part of the Fourier transform, (16), which arises from the lc behavior of (18), near the apex of the lc, $r \sim 0$. We first indicate how this comes about starting from the result of (21), which when exponentiated, leads to a factor $(rM)^{-2\bar{\alpha}(s)}$. An equivalent calculation will also be made based on the prior approximation $L(q) = 0$.

The lc dependence of $-ig^2\Delta_F(x)$ contributes a factor $(g^2/4\pi)\delta(x^2)$ to (18), and hence a contribution $\delta(q_1 + p_1 + q_2 + p_2)T^{1c}(s, t)$ to (16), where

$$T^{1c}(s, t) = \frac{g^2}{4\pi} \int dx\, e^{i(q_1+p_1)\cdot x}\delta(x^2)e^{f(0, x\cdot q_{1,2}, s)}, \tag{32}$$

with $t = -(q_1 + p_1)^2$. The contribution to (16) due to the behavior of the remaining off-the-lc dependence of $-ig^2\Delta_F$ is much more difficult to ascertain, and is not considered here. If we now perform the x_0 integration, in (32),

$$T^{1c}(s, t) = \frac{g^2}{4\pi} \int \frac{d^3r}{r} e^{i\mathbf{Q}\cdot\mathbf{r}} \cdot \frac{1}{2} \sum_{\pm} e^{f(0, r\gamma_\pm, s)} \tag{33}$$

where, in the c.m., $(q_1 + p_1)_0 = 0$, $\mathbf{q}_1 + \mathbf{p}_1 = \mathbf{Q}$, $\gamma_\pm = (\mathbf{r}\cdot\mathbf{q}_{1,2}/r) \mp q_{1,2}^{(0)}$; and if we then consider the contribution to (33) coming from the behavior of $f(0, r\gamma_\pm, s)$ in the region $rM \ll 1$, we find a term

$$\delta T^{1c}(s, t) = \frac{g^2}{4\pi} \int_0^{1/M} \frac{r\, dr}{(rM)^{2\bar{\alpha}}} \int d\Omega\, e^{i\mathbf{Q}\cdot\mathbf{r}}$$

$$= \frac{g^2}{M(-t)^{\frac{1}{2}}} \int_0^1 \frac{du}{u^{2\bar{\alpha}}} \sin\left[\frac{u}{M}(-t)^{\frac{1}{2}}\right]. \tag{34}$$

The point of this discussion is now evident: for $\bar{\alpha}(s) \geq 1$, the integral of (34) diverges at its lower limit. This situation can occur for $s < 4m^2$; and we therefore expect the bound state poles of $T(s, t)$ to show up as singularities in the continuation of (34) from values of s above threshold. These singularities can be immediately identified by extending the upper limit of integration, in (34), to $+\infty$; this merely adds to δT^{1c} a finite part such that (34) is replaced by

$$\delta T^{1c}(s, t) = (g^2/M^{2\bar{\alpha}(s)})\Gamma[1 - 2\bar{\alpha}(s)]$$

$$\times [-t]^{\bar{\alpha}(s)-1} \cos[\pi\bar{\alpha}(s)]. \tag{35}$$

Equation (35) displays poles, with the appropriate momentum transfer dependence, every time $\bar{\alpha}$ passes through a positive integer, $\bar{\alpha}(s) = n$, a situation which occurs only for $s < 4m^2$. In a nonrelativistic approximation, with $s = (2m - E)^2$, $E/m \ll 1$, such poles appear whenever

$$E = E_n = (g^2/8\pi)^2(1/2n^2)(m/2),$$

corresponding to the infinite number of bound states characteristic of an attractive, scalar Coulomb potential between a pair of equal-mass fermions; these bound states exist here because we are calculating with an infrared model. The central question of particle physics then presents itself in new guise: can the model be improved (e.g., by taking recoil at least partially into account) such that (21) and (34) are retained and a modified $\bar{\alpha}(s)$ found which no longer diverges at threshold? A successful calculation of this sort would then provide a field-theoretic approximation method which yields a finite number of bound states and possibly also resonances; that is, one which includes the effect of short-range forces between fermions.

The approximation used in arriving at (34) should really be justified. The passage to (34) is incomplete because corrections to the small r behavior of $f(0, r\gamma_\pm, s)$ should be taken into account. However, the effect of doing this would be only to change the residues of the poles which occur when $\bar{\alpha} = n$; and while it is not impossible to manufacture an r dependence such that certain residues vanish, these possibilities appear to be rather artificial. It is interesting to note that additional (but not necessarily expected) r dependence of the form $r^p \ln^q r$, in $f(0, r\gamma_\pm, s)$, would lead to subsequent poles of degree $q + 1$ whenever $\bar{\alpha} = (p + 1)/2$, for odd p.

An alternate method of obtaining results equivalent to (35) is to initially adopt the approximation $L(q) = 0$; then, the use of (25) in the region

$M^2 |x^2| \ll 1$ provides a contribution to (16) expressible as an integral over a single invariant variable $\lambda = x^2$,

$$\Delta T^{\mathrm{lc}}(s, t) \sim M^{-2\bar{\alpha}} \int_{-1/M^2}^{+1/M^2} \frac{d\lambda}{\lambda} |\lambda|^{-2\bar{\alpha}} \times \int d^4x\, \delta(x^2 - \lambda) e^{i(q_1+p_1)x}. \quad (36)$$

We have assumed, in writing (36), that $s > 4m^2$, Re $\bar{\alpha}(s) < 0$; and the continuation to values of s below threshold will be made from the result of the integral of (36). It is again convenient to add to (36) a nonsingular part obtained by extending the range of integration to $\pm\infty$. This yields

$$\Delta T^{\mathrm{lc}}(s, t) \sim \frac{i\pi^2}{M^{2\bar{\alpha}}} \frac{\Gamma(1-\bar{\alpha})}{\Gamma(1+\bar{\alpha})} \left[\frac{-t}{4}\right]^{\bar{\alpha}-1}, \quad (37)$$

which is equivalent to (35) as far as the bound states are concerned.

In summary, this model possesses bound states whose energy eigenvalues may be determined by "sliding down the lc," testing the r dependence of that function which multiplies the configuration space one-boson-exchange term, as in (21). Under the approximation $L(q) = 0$, the lc behavior of the amplitude is seen to produce similar results. One might hope that these procedures could be used to test for bound states in more realistic models.

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APPENDIX I

Here and in Appendix II, we collect some supplementary, and for the most part arithmetical, remarks relevant to and in roughly the same sequence as the topics covered in the preceding discussion.

Explicit evaluation of (8) and (9) for the fully amputated $(n+2)$-point Green's function yields

$$\tilde{H}(\bar{q}\bar{p} \mid \bar{k}_1, \cdots, \bar{k}_n) = (-ig)^n \delta(q_1 + p_1 + k_1 + \cdots + k_n) \Delta \int_0^\infty d\xi e^{-i\xi\Delta} \times \sum_{P=1}^{n} \int_0^\xi d\xi_1 e^{-i\xi_1 a_1} \cdots \int_0^\xi d\xi_{n-1} e^{-i\xi_{n-1} a_{n-1}}, \quad (A1)$$

where $\Delta = m + v\cdot q$, $a_i = k_i v$, and $\sum_{P=1}^{n}$ denotes a cyclic permutation of n terms over the indices $k_1, \cdots, k_n$. Performing n successive integrations by parts, and going to the mass shell, $\Delta = 0$, one obtains

$$\tilde{H} = (-g)^n \cdot \delta \cdot \sum_{P=1}^{n} \cdot \sum_{P=1}^{n-1} (a_1)^{-1} \cdot \sum_{P=1}^{n-2} (a_1 + a_2)^{-1} \cdots \times \sum_{P=n-2}^{n-1} (a_1 + \cdots + a_{n-2})^{-1} \cdot (a_1 + \cdots + a_{n-1})^{-1}. \quad (A2)$$

The basic simplicity of the BN model is now evident, since the sum of the $n!$ permutations of (A2) is reducible to a sum over n related factors. If one goes directly to the mass shell in (A1), the only portion of each of the factors

$$\int_0^\infty d\xi_i\, e^{-i\xi_i a_i},$$

which can contribute comes from the lower limit, $-i(a_i)^{-1}$; and in place of (A2) one obtains the equivalent form

$$\tilde{H} = (-g)^n \cdot \delta \cdot \sum_{P=1}^{n} (a_1 a_2 \cdots a_{n-1})^{-1}. \quad (A3)$$

Since the factors $-i(a_i)^{-1}$ may also be obtained from the integrals

$$\int_0^\infty d\xi e^{-i\xi a_i - \epsilon\xi}\big|_{\epsilon\to 0+},$$

an alternate way of writing the amputated, mass-shell Green's functions is simply given by (14).

APPENDIX II

The analysis of Secs. II and III follows from the properties of Δ_f in (A) four or (B) six dimensions,

$$\Delta_{F4}(x; M^2) = (2\pi)^{-4} \int d^4k\, e^{ikx}(k^2 + M^2 - i\epsilon)^{-1} \quad (A4)$$

$$= (16\pi^2)^{-1} \int_0^\infty dt\, t^{-2} e^{-itM^2 + ix^2/4t} \quad (A5)$$

$$= \frac{iM}{4\pi^2} \frac{\theta(x^2)}{(x^2)^{\frac{1}{2}}} K_1[M(x^2)^{\frac{1}{2}}] - \frac{M}{8\pi} \frac{\theta(-x^2)}{(-x^2)^{\frac{1}{2}}} \times H_1^{(2)}[M(-x^2)^{\frac{1}{2}}] + \frac{1}{4\pi}\delta(x^2) \quad (A6)$$

for four dimensions, and

$$\Delta_{F6}(x; M^2) = (2\pi)^{-6} \int d^6k\, e^{ikx}(k^2 + M^2 - i\epsilon)^{-1} \quad (A7)$$

$$= -i(4\pi)^{-3} \int_0^\infty dt\, t^{-3} e^{-itM^2 + ix^2/4t} \quad (A8)$$

$$= -(1/\pi)(\partial/\partial x^2)\Delta_{F4}(x; M^2) \quad (A9)$$

$$= \frac{iM^2}{8\pi^3}\frac{\theta(x^2)}{x^2}K_2[M(x^2)^{\frac{1}{2}}]$$
$$-\frac{M^2}{16\pi^2}\frac{\theta(-x^2)}{x^2}H_2^{(2)}[M(-x^2)^{\frac{1}{2}}]$$
$$-(M^2/16\pi)\delta(x^2)-(1/4\pi^2)\delta'(x^2)$$

for six dimensions. It should be noted that the propagators Δ_F have previously been called Δ_C; but we here follow the usage of Ref. 2. Subsequent reductions are based upon these formulas.

(a) $$\int_0^\infty d\xi\Delta_{F4}(x-\xi v)$$
$$= -2im(2\pi)^{-4}\int d^4k\, e^{ikx}(k^2+M^2)^{-1}(2k\cdot q)^{-1}. \quad \text{(A10)}$$

By combining denominators,

$$(k^2+M^2)^{-1}(2k\cdot q)^{-1} = \int_0^\infty du[k^2+M^2+2uk\cdot q]^{-2},$$

and shifting to a new variable $k' = k + uq$, (A10) may be written in the form

$$-2im(2\pi)^{-4}\int_0^\infty du\int dk' e^{ix(k'-uq)}$$
$$\times[k'^2+M^2+u^2m^2]^{-2}$$
$$= 2im\int_0^\infty du\, e^{-iuq\cdot x}\frac{\partial}{\partial M^2}\Delta_{F4}(x;M^2+u^2m^2)$$
$$= \frac{m}{8\pi^2}\int_0^\infty du\, e^{-iuq\cdot x}\{2\theta(x^2)K_0([x^2(M^2+u^2m^2)]^{\frac{1}{2}})$$
$$-\pi i\theta(-x^2)H_0^{(2)}([-x^2(M^2+u^2m^2)]^{\frac{1}{2}})\}. \quad \text{(A11)}$$

Hence, as $x^2 \to 0^\pm$, for $q\cdot x \neq 0$, we obtain

$$\int_0^\infty d\xi\Delta_{F4}(x-\xi v) \sim \frac{im}{8\pi^2}(x\cdot q)^{-1}\ln|x^2|,$$

due to the logarithmic singularity of K_0 and H_0. A similar result for $\int_0^\infty d\xi\ \Delta_F(x+\xi v)$ leads to (20).

If, however, we make the prior approximation $L(q) = 0$, which here corresponds to setting $q = 0$ in (A11), the parametric integration of the latter can be performed, yielding

$$\int_0^\infty d\xi\Delta_{F4}|_{q=0} = \frac{1}{8\pi}\left\{\frac{\theta(x^2)}{(x^2)^{\frac{1}{2}}}e^{-M(x^2)^{\frac{1}{2}}}\right.$$
$$\left.-i\frac{\theta(-x^2)}{(-x^2)^{\frac{1}{2}}}e^{-iM(-x^2)^{\frac{1}{2}}}\right\}. \quad \text{(A12)}$$

The square of (A12) then gives, near the lc, the dependence of (23).

(b) In six dimensions, representations analogous to those of (A10) and (A11) may be used to obtain

$$\int_0^\infty d\xi\Delta_{F6}(x-\xi v)$$
$$= -\frac{im}{2\pi}\int_0^\infty du\, e^{-iuq\cdot x}\Delta_{F4}(x;M^2+u^2m^2), \quad \text{(A13)}$$

from which the dominant behavior near the lc may be inferred,

$$-\frac{i}{8\pi^3}\left(\frac{m}{q\cdot x}\right)\frac{1}{x^2}, \quad \text{(A14)}$$

where, again, $q\cdot x \neq 0$ for $m \neq 0$, $r \neq 0$. Thus, the lc behavior of the second term in the curly bracket of (18) becomes

$$g^4\int_0^\infty d\xi_1\Delta_{F6}\cdot\int_0^\infty d\xi_2\Delta_{F6}\Big|_{x^2\sim 0}$$
$$\sim (mg^2/8\pi^3)^2(x\cdot q_1)^{-1}(x\cdot q_2)^{-1}(x^2)^{-2}, \quad \text{(A15)}$$

which is no worse than that of (26).

If the prior approximation $L(q) = 0$ is made, we obtain, by setting $q = 0$ in (A13), the lc dependence

$$\int_0^\infty d\xi\Delta_{F6}(x-\xi v)|_{q=0} \sim \frac{1}{16\pi^2}(x^2)^{-\frac{1}{2}}, \quad \text{(A16)}$$

which leads to the result of (27).

(c) The four-dimensional estimate of $f(x \mid q_{1,2})$ is obtained by performing the $\xi_{1,2}$ integrations of (18),

$$f(x^2, x\cdot q_{1,2}, s) = ig^2m^2(2\pi)^{-4}$$
$$\times\int dk\, e^{ikx}(k^2+M^2)^{-1}(k\cdot q_1)^{-1}(k\cdot q_2)^{-1}. \quad \text{(A17)}$$

When the ξ denominators are combined according to

$$(k\cdot q_1)^{-1}(k\cdot q_2)^{-1} = -4\int_0^1 dz(2k\cdot\bar{q})^{-2},$$

with $\bar{q} = zq_1 - (1-z)q_2$, and $\bar{q}^2 = -m^2 + z(1-z)s$, (A17) becomes

$$f = -4ig^2m^2(2\pi)^{-4}\int_0^1 dz$$
$$\times\int dk\, e^{ik\cdot x}(k^2+M^2)^{-1}(2k\cdot\bar{q})^{-2}. \quad \text{(A18)}$$

Combining denominators again, we can identify the dependence on x^2 and $x\cdot q_{1,2}$:

$$f = -8ig^2m^2(2\pi)^{-4}\int_0^1 dz\int_0^\infty u\, du\, e^{-iu\bar{q}\cdot x}$$
$$\times\int dk' e^{ik'x}[k'^2+M^2-u^2\bar{q}^2]^{-3}$$
$$= -4ig^2m^2\int_0^1 dz\int_0^\infty u\, du\, e^{-iu\bar{q}\cdot x}\left(\frac{\partial}{\partial M^2}\right)^2$$
$$\times\Delta_{F4}(x;M^2-u^2\bar{q}^2)$$

$$= \frac{iq^2m^2}{4\pi^2}\int_0^1 dz\int_0^\infty u\,du\,e^{-iu\bar{q}\cdot x} \times \int_0^\infty dt\,e^{ix^2/4t - it[M^2-u^2\bar{q}^2]}. \quad \text{(A19)}$$

Since $-\bar{q}^2 \geq 0$ for $s < 4m^2$, we consider s below threshold when performing the parametric integrations of (A19). Calling $\bar{\gamma}_\pm = (\mathbf{r}\cdot\mathbf{q}/r) \mp \bar{q}_0$, on the lc (A19) becomes

$$f(0, r\bar{\gamma}_\pm, s) = \left(\frac{mg}{2\pi}\right)^2 \int_0^1 \frac{dz}{[-\bar{q}^2]} \times \int_0^\infty \frac{w\,dw}{1+w^2} e^{-irM\bar{\gamma}_\pm w[-\bar{q}^2]^{\frac{1}{2}}}, \quad \text{(A20)}$$

and for very small values of rM, the last integral of (A20) produces a logarithmic dependence,

$$f(0, r\bar{\gamma}_\pm, s)|_{r\sim 0} \sim -\left(\frac{mg}{2\pi}\right)^2 \ln(rM)\int_0^1 \frac{dz}{[-\bar{q}^2]}. \quad \text{(A21)}$$

The function $\bar{\alpha}(s)$ is here defined by the comparison of (A21) with (21), or directly by (22); the integral of (22) is well known, and we include it here for completeness,

$$\bar{\alpha}(s) = \frac{m^2g^2}{2\pi^2}(4m^2-s)^{-\frac{1}{2}}\left\{\frac{\theta(s)\theta(4m^2-s)}{s^{\frac{1}{2}}}\sin^{-1}\left(\frac{s}{4m^2}\right)^{\frac{1}{2}} + \theta(-s)(-s)^{-\frac{1}{2}}\sinh^{-1}(-s/4m^2)^{\frac{1}{2}}\right\} \quad \text{(A22)}$$

and

$$\bar{\alpha}(s) = \frac{m^2g^2}{2\pi^2}\frac{\theta(s-4m^2)}{[s(s-4m^2)]^{\frac{1}{2}}} \times \left\{i\frac{\pi}{2} - \sinh^{-1}\left(\frac{s}{4m^2}-1\right)^{\frac{1}{2}}\right\} \quad \text{(A23)}$$

when the continuation $s \to z \to s + i\epsilon$ has been performed.

When the initial approximation $L(q) = 0$ is made, which corresponds to setting $\bar{q}\cdot x = 0$ in (A19), the parametric integrals there can be calculated immediately,

$$f(x^2, 0, s) = \bar{\alpha}(s)\int_0^\infty dt\,t^{-1}e^{-itM^2+ix^2/4t} = \bar{\alpha}(s)\{2\theta(x^2)K_0[M(x^2)^{\frac{1}{2}}] - i\pi\theta(-x^2)H_0^{(2)}[M(-x^2)^{\frac{1}{2}}]\}. \quad \text{(A24)}$$

For small values of $M^2\,|x^2|$, (A24) provides the logarithmic dependence quoted in (24).

(d) The six-dimensional version of (A19) follows easily from (A9) and (A19),

$$f(x^2, x\cdot q_{1,2}, s) = \left(\frac{mg}{4\pi}\right)^2\frac{1}{\pi}\int_0^1 dz\int_0^\infty u\,du\,e^{-iu\bar{q}\cdot x} \times \int_0^\infty \frac{dt}{t}e^{ix^2/4t - it[M^2-u^2\bar{q}^2]}, \quad \text{(A25)}$$

and corresponding representations may be written, as in (A11), in terms of K_0 and H_0. For the approximation $L(q) = 0$, it is easy to see that (28) is valid near the lc. The situation is more complicated when $L(q) \neq 0$, but it is not difficult to see that as the lc is approached from either direction,

$$f(x^2, x\cdot q_{1,2}, s)|_{x^2\sim 0} \sim -a\ln(1/|x^2|), \qquad a = \frac{1}{\pi}\left(\frac{mg}{4\pi}\right)^2\int_0^1 dz(x\cdot\bar{q})^{-2} \geq 0. \quad \text{(A26)}$$

Hence the exponential of (A26) vanishes in this limit, and the bad singularity of (28) is removed.

When $x^2 \neq 0$ similar results may be demonstrated, provided that we continue the s dependence of the factor $[-\bar{q}^2]$ of (A25) below threshold; the s dependence of the $\bar{q}\cdot x$ factor should not be continued. Under these conditions $\bar{q}\cdot x$ is real and $[-\bar{q}^2]$ is positive. There may well exist other prescriptions for avoiding exponential infinities at the apex of the lc; the ones stated here have only the virtue of simplicity.

For $x^2 < 0$, we set $x_0 = \xi r$, $\xi^2 > 1$, and rewrite (A25) in the form

$$f = -i\left(\frac{mg}{4\pi}\right)^2\frac{1}{r^2(\xi^2-1)}\int_0^1\frac{dz}{[-\bar{q}^2]}\int_0^\infty v\,dv\,e^{-ib\nu} \times H_0^{(2)}([r^2(\xi^2-1)M^2+v^2]^{\frac{1}{2}}), \quad \text{(A27)}$$

where $b = \bar{\gamma}[(-\bar{q}^2)(\xi^2-1)]^{\frac{1}{2}}$, $\bar{\gamma} = (1/r)(\bar{q}\cdot x) = \eta(s/4-m^2)^{\frac{1}{2}} - \xi(2z-1)(s/4)^{\frac{1}{2}}$, and $\eta = \mathbf{r}\cdot\mathbf{q}_1/r\,|\mathbf{q}_1|$ in the c.m. The important r dependence is exhibited as a multiplicative factor in front of the integrals of (A27), and the limit $r \to 0$ may be taken inside the latter,

$$f \sim -i\left(\frac{mg}{4\pi}\right)^2\frac{1}{r^2(\xi^2-1)}\int_0^1\frac{dz}{[-\bar{q}^2]} \times \int_0^\infty v\,dv\,e^{-ib\nu}H_0^{(2)}(v). \quad \text{(A28)}$$

The v integration of (A28) may be carried out explicitly to show that the corresponding f is, in this limit, real and negative for all real values of b; but perhaps the simplest way of seeing this is to rewrite (A28) in the form of (A25),

$$f \sim \left(\frac{mg}{4\pi}\right)^2 \frac{1}{\pi r^2} \int_0^1 dz \int_0^\infty u\, du\, e^{-iu\bar{\gamma}} \times \int_0^\infty \frac{dt}{t} e^{-it-i(\xi^2-1)u^2[-\bar{q}^2]/4t}, \quad \text{(A29)}$$

which, for real γ and positive $-\bar{q}^2$, permits (i) a counterclockwise rotation of the t integration contour through an angle of 90°, and (ii) a counterclockwise (clockwise) rotation of the u integration contour through an angle of 90° for positive (negative) values of $\bar{\gamma}$. [The situation for $\bar{\gamma} = 0$ is identical with that of the $L(q) = 0$ approximations previously discussed.] The result may then be written in the form

$$f \sim -\frac{1}{\pi r^2}\left(\frac{mg}{4\pi}\right)^2 \int_0^1 dz \int_0^\infty w\, dw\, e^{-w|\bar{\gamma}|} \times \int_0^\infty \frac{d\tau}{\tau} e^{-\tau-(\xi^2-1)w^2[-\bar{q}^2]/4\tau}, \quad \text{(A30)}$$

and it is clear that this quantity is real and negative. Hence, in this limit, exp (f) does not diverge.

For $x^2 > 0$, a slightly more stringent condition on $\bar{\gamma}$ is required, namely, that its s dependence shall be considered well above threshold; the s dependence of $[-\bar{q}^2]$ is again to be considered below $4m^2$. For $\xi^2 < 1$, (A25) may be written in the form

$$f = \frac{2}{r^2(1-\xi^2)} \frac{1}{\pi}\left(\frac{mg}{4\pi}\right)^2 \int_0^1 \frac{dz}{[-\bar{q}^2]} \times \int_0^\infty v\, dv\, e^{-ic_0 v} K_0([r^2M^2(1-\xi^2)+v^2]^{\frac{1}{2}}), \quad \text{(A31)}$$

and the $r \to 0$ limit may be taken inside the integral of (A31). One finds a complex function whose real part is given by

$$\mathrm{Re}\, f \sim \frac{2}{r^2(1-\xi^2)} \frac{1}{\pi}\left(\frac{mg}{4\pi}\right)^2 \int_0^1 \frac{dz}{[-\bar{q}^2]} \frac{1}{1+c^2} \times \left[1 - \frac{c \sinh^{-1} c}{\sqrt{1+c^2}}\right], \quad \text{(A32)}$$

where $c = \bar{\gamma}/[(1-\xi^2)(-\bar{q}^2)]^{\frac{1}{2}}$, and we may consider c, or $\bar{\gamma}$, as positive, since (A32) is a function of c^2 only. For fixed values of ξ, η, z, $-\bar{q}^2$, a sufficiently large value of c ($c > 2.24$) can always be found by choosing s sufficiently large such that the bracket of (A32) will be negative; and this is all that is needed to avoid an exponential infinity near the apex of the lc.

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Asymptotic Expansion of the Intensity of the Small-Angle X-Ray Scattering from Cylinders of Arbitrary Cross Section*

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From a previously developed expression for the intensity of the small-angle x-ray scattering from randomly oriented right cylinders of arbitrary cross section and with uniform electron density, an asymptotic expansion is developed which can be used to approximate the scattered intensity at relatively large angles of the small-angle region. The asymptotic expansion is useful for numerical calculations at these large angles, where calculations by the usual techniques of numerical integration and series expansion are most difficult. The terms in the asymptotic expansion are found to be determined by the behavior of the characteristic function $\beta(r)$ of the cross section at certain values of r. The general asymptotic expansion is used to calculate asymptotic expressions for the scattering from right circular cylinders and rectangular parallelepipeds.

INTRODUCTION

In order to study the size and shape of colloidal particles by small-angle x-ray scattering, it is necessary to know how the particle size and shape are related to the angular distribution of the scattered intensity. Even when one assumes that the sample being studied consists of independent randomly oriented identical particles with uniform electron density, the problem is too complicated to allow a general solution. Although the approximate methods which have been developed are ordinarily adequate for analysis of experimental data, further studies can provide a better understanding of the effect of particle structure on the scattered intensity, thus permitting more information to be gained from a given experiment and also allowing scattering techniques to be applied to a broader range of problems.

In recent years interest has arisen in the nature of the scattering curve at relatively large angles of the small-angle region—that is, at angles such that $hL \gg 1$, where L is a dimension characteristic of the particle being studied, λ is the x-ray wavelength, θ is the scattering angle, and $h = 4\pi\lambda^{-1} \sin \frac{1}{2}\theta$. Since the scattered intensity can be represented as a Fourier integral, techniques for asymptotic expansion of Fourier integrals prove to be useful for studying the behavior of the scattering for this range of angles. Previous publications from this laboratory have been concerned with some general techniques for calculating the scattered intensity at relatively large scattering angles[1] and with the scattering from generalized cylinders—that is, from right cylinders of arbitrary cross section.[2]

In the present paper, a general expression is derived for the asymptotic expansion of the scattered intensity for generalized cylinders of arbitrary cross section. Since asymptotic expansions of this type can be used most easily in the range of angles in which numerical integration and series expansion are most difficult, the general asymptotic expansion should be particularly convenient for numerical calculation at relatively large angles of the small-angle region.

In addition, the general expansion answers a question raised in previous work[2] on generalized cylinders. In the earlier calculations, the scattered intensity for right circular cylinders, unlike the scattering from bodies of all other known shapes, appeared not to be proportional to h^{-4} at large h. Since the h^{-4} dependence of the scattered intensity at large h was believed to be a very general result,[3] the indications that the relation might not be satisfied for right circular cylinders were rather surprising. Thus it is gratifying that the asymptotic expansion for right circular cylinders shows, in contradiction to the previous suggestions, that the scattering at large h is proportional to h^{-4}, as expected from general principles.

THE GENERAL ASYMPTOTIC EXPANSION

For a randomly oriented particle with uniform electron density, the scattered intensity $I(h)$ can be expressed[2]

$$I(h) = \frac{1}{h}\int_0^{D_3} dr\, H(r) \sin hr,$$

where D_3, which will be called the maximum diameter of the particle, is the length of the longest line that can be contained in the particle, and $H(r)$ is a func-

* Work supported by the National Science Foundation.
[1] P. W. Schmidt and R. Hight, Jr., J. Appl. Phys. 30, 866 (1959).
[2] A. Miller and P. W. Schmidt, J. Math. Phys. 3, 92 (1962).
[3] Reference 1, p. 867.

tion which is determined by the size and shape of the particle. The intensity is assumed to be normalized so that $I(0) = 1$. As only the scattering from a single particle is considered, the calculations can be applied only to assemblies of independent particles, for which the scattering is not affected by interparticle interactions.

Erdélyi,[4] in his discussion of the asymptotic expansion of Fourier integrals, has shown that the asymptotic expansion of $I(h)$ will be determined by the values of $H(r)$ and its derivatives at $r = 0$ and $r = D_3$, and by the behavior of $H(r)$ at any finite or infinite discontinuities it or any of its derivatives may have in the interior of the interval of integration. The problem of calculating the asymptotic expansion of $I(h)$ thus reduces to the determination of the behavior of $H(r)$ in the neighborhood of $r = 0$, of $r = D_3$, and of any interior points at which $H(r)$ or its derivatives are discontinuous.

In Ref. 2, $H(r)$ was expressed in terms of an integral over a function $\beta(r)$, called the two-dimensional characteristic function and having the property that the scattered intensity $J(h)$ for a randomly oriented plane lamina of negligible thickness and uniform electron density and with the shape of the cylinder cross section is given by

$$J(h) = \frac{1}{A}\int_0^D 2\pi r\beta(r)\frac{\sin hr}{hr}\,dr,$$

where D, the maximum diameter of the cross section, is the length of the longest line that can be contained in the two-dimensional cross section, and A is the cross-section area. The intensity $J(h)$ is normalized so that $J(0) = 1$. For small r,[5]

$$\beta(r) = 1 - P(\pi A)^{-1}r + \cdots,$$

where P is the perimeter of the cross section. Also,[6] one expects that quite generally, $\beta(D) = \beta'(D) = 0$, and that $\beta(r)$ and $\beta'(r)$ are continuous. Higher derivatives, however, can ordinarily be expected to have discontinuities. Rearrangement of Eq. (3) of Ref. 2 shows that for a generalized cylinder, $H(r)$ can be expressed by the relation

$$H(r) = M(r) + N(r),$$

where

$$\begin{aligned}
&0 \le r \le D,\\
&\quad M(r) = \frac{4\pi}{V}\int_0^r dx\, x\beta(x)Q[(r^2 - x^2)^{\frac{1}{2}}],\\
&D \le r \le D(1+v^2)^{\frac{1}{2}},\\
&\quad M(r) = \frac{4\pi}{V}\int_0^D dx\, x\beta(x)Q[(r^2 - x^2)^{\frac{1}{2}}],\\
&0 \le r \le vD,\\
&\quad N(r) = 0,\\
&vD \le r \le D(1+v^2)^{\frac{1}{2}},\\
&\quad N(r) = -\frac{4\pi}{V}\int_0^{(r^2-v^2D^2)^{\frac{1}{2}}} dx\, x\beta(x)Q[(r^2 - x^2)^{\frac{1}{2}}],\\
&\quad Q(x) = 1/x - 1/vD,
\end{aligned} \tag{1}$$

and where V is the particle volume, and v, the axial ratio, represents the ratio of cylinder height to the maximum diameter D of the cross section. Thus $D_3/D = (1 + v^2)^{\frac{1}{2}}$. A consequence of (1) is that calculation of the discontinuities in $H(r)$ requires knowledge of the discontinuities in the derivatives of $\beta(r)$. Since at present it is not possible to state generally the types of discontinuities to be expected, the calculations are carried out for types of discontinuities which, although they do not represent an exhaustive list of all possible types, nevertheless include most types of discontinuity that have been encountered when exact calculation of $\beta(r)$ has been possible.

According to Erdélyi's general calculation of the asymptotic expansions of Fourier integrals, if at an interior point a of the interval of integration, $H(r)$ can be written $H(r) = F(r) + G(r)$, where $F(r)$ and all its derivatives are continuous at $r = a$, then only $G(r)$ will contribute to the asymptotic expansion, and $F(r)$ need not be considered in the calculation of the asymptotic expansion. This result will be used many times to simplify the calculations.

The discontinuities in the derivatives of $\beta(r)$ will be assumed to fall into two classes and will be considered to occur at points called Type-I and Type-II points. For a Type-I point, $r = a_{2i+1}$, $\beta(r)$ will be assumed to be expressible in the form

$$\begin{aligned}
r \ge a_{2i+1}, &\qquad \beta(r) = L_{2i+1}(r) + K_{2i+1}(r),\\
r \le a_{2i+1}, &\qquad \beta(r) = L_{2i+1}(r),
\end{aligned}$$

where

$$K_{2i+1}(r) = \sum_{n=0}^{\infty} A_n^{2i+1}\left[\frac{r^2}{(a_{2i+1})^2} - 1\right]^{n+\alpha_{2i+1}},$$

and where all derivatives of the function $L_{2i+1}(r)$ are continuous at $r = a_{2i+1}$. Type-II points are designated by $r = a_{2i}$. At these points, the form of $\beta(r)$ are assumed to be

$$\begin{aligned}
r \le a_{2i}, &\qquad \beta(r) = L_{2i}(r) + K_{2i}(r),\\
r \ge a_{2i}, &\qquad \beta(r) = L_{2i}(r),
\end{aligned}$$

[4] A. Erdélyi, *Asymptotic Expansions* (Dover Publications, Inc., New York, 1956), p. 49.
[5] Reference 1, Eq. (8).
[6] Reference 2, p. 93.

where

$$K_{2i}(r) = \sum_{n=0}^{\infty} A_n^{2i}\left[1 - \frac{r^2}{(a_{2i})^2}\right]^{n+\alpha_{2i}},$$

and where $L_{2i}(r)$ is a function with all derivatives continuous at $r = a_{2i}$. With this scheme of notation, odd subscripts refer to quantities calculated for Type-I points, while even subscripts denote quantities related to Type-II points.

The subscript i is allowed to have integral values ranging from $i = 1$ to $i = 2n + 1$, where the value of the integer n is determined by the number of Type-I and Type-II points for a given cross section shape. The subscript 0 refers to quantities determined by the behavior of $\beta(r)$ in the neighborhood of $r = 0$, where the Taylor expansion

$$\beta(r) = \sum_{n=0}^{\infty} \frac{\beta^{(n)}(0)}{n!} r^n \tag{2}$$

is assumed to converge, with

$$\beta^{(n)}(0) = d^n\beta(r)/dr^n|_{r=0}.$$

The exponents α_i occurring in the above series expansions are determined by the form of the cross section. For $\beta(r)$ and $\beta'(r)$ to be continuous, all the α_i must be greater than 1.

From the Taylor expansion (2), $M(r)$ is seen to be expressible by the series

$$M(r) = M_0(r),$$

where

$$M_0(r) = \sum_{n=0}^{\infty} B_n^0 r^{n+1},$$

$$B_n^0 = \frac{4\pi}{V}\frac{1}{(n+1)!} \times \left[\frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2}n + 1)\beta^{(n)}(0)}{\Gamma(\frac{1}{2}n + \frac{1}{2})} - \frac{n}{vD}\beta^{(n-1)}(0)\right].$$

In the neighborhood of $r = vD$, (2) can be used to show that

$$N(r) = N_0(r),$$

where

$$N_0(r) = \sum_{n=0}^{\infty}\left[C_n^0\left(\frac{r^2}{v^2D^2} - 1\right)^{n+2} + D_n^0\left(\frac{r^2}{v^2D^2} - 1\right)^{n+5/2}\right]$$

$$C_n^0 = \frac{2\pi}{V\Gamma(n+3)}\sum_{m=0}^{n}\frac{(-1)^m\Gamma(m+\frac{3}{2})\Gamma(n-m+1)\beta^{(2n-2m)}(0)(vD)^{2n+1-2m}}{\Gamma(\frac{1}{2})\Gamma(2n-2m+1)}$$

$$D_n^0 = \frac{2\pi}{V}\sum_{m=0}^{n}\frac{(-1)^m\Gamma(m+\frac{3}{2})\Gamma(n-m+\frac{3}{2})\beta^{(2n-2m+1)}(0)(vD)^{2n+2-2m}}{\Gamma(\frac{1}{2})\Gamma(n+\frac{7}{2})\Gamma(2n+2-2m)}.$$

When there is a Type-II point at $r = a_{2i}$, then, in the neighborhood of $r = [(a_{2i})^2 + v^2D^2]^{\frac{1}{2}}$, $N(r)$ can be written

$$N(r) = F_{2i}(r) + N_{2i}(r),$$

where

$$F_{2i}(r) = -\frac{4\pi}{V}\left[\int_0^{(r^2-v^2D^2)^{\frac{1}{2}}} dx\, xL_{2i}(x)Q[(r^2 - x^2)^{\frac{1}{2}}] + \int_0^{a_{2i}} dx\, xK_{2i}(x)Q[(r^2 - x^2)^{\frac{1}{2}}]\right],$$

$$r \geq [v^2D^2 + (a_{2i})^2]^{\frac{1}{2}}, \qquad N_{2i}(r) = 0,$$

$$r \leq [v^2D^2 + (a_{2i})^2]^{\frac{1}{2}},$$

$$N_{2i}(r) = \frac{4\pi}{V}\int_{(r^2-v^2D^2)^{\frac{1}{2}}}^{a_{2i}} dx\, xK_{2i}(x)Q[(r^2 - x^2)^{\frac{1}{2}}].$$

As $F_{2i}(r)$ and all its derivatives are continuous at $t = [v^2D^2 + (a_{2i})^2]^{\frac{1}{2}}$, $F_{2i}(r)$ can be neglected in computing the asymptotic expansion.

In the expression for $N_{2i}(r)$ for $r \leq [v^2D^2 + (a_{2i})^2]^{\frac{1}{2}}$, let

$$S = \left[\frac{(a_{2i})^2 - x^2}{v^2D^2 + (a_{2i})^2 - r^2}\right]^{\frac{1}{2}}.$$

Then, after making series expansions of K_{2i} and Q, one finds that

$$r \leq [(vD)^2 + (a_{2i})^2]^{\frac{1}{2}},$$

$$N_{2i}(r) = \sum_{n=0}^{\infty} C_n^{2i}\left(1 - \frac{r^2}{v^2D^2 + (a_{2i})^2}\right)^{n+2+\alpha_{2i}},$$

where

$$C_n^{2i} = \frac{2\pi}{V}\frac{[v^2D^2 + (a_{2i})^2]^{n+2+\alpha_{2i}}}{\Gamma(n+3+\alpha_{2i})} \times \sum_{m=0}^{n}\frac{A_{n-m}^{2i}\Gamma(m+\frac{3}{2})\Gamma(n-m+1+\alpha_{2i})}{\Gamma(\frac{1}{2})(vD)^{2m+3}(a_{2i})^{2n-2m+2\alpha_{2i}}}.$$

If there is a Type-I point at $r = a_{2i+1}$, $N(r)$ can be expressed

$$N(r) = F_{2i+1}(r) + N_{2i+1}(r),$$

where

$$F_{2i+1}(r) = -\frac{4\pi}{V}\int_0^{(r^2-v^2D^2)^{\frac{1}{2}}} dx\, xL_{2i+1}(x)Q[(r^2-x^2)^{\frac{1}{2}}]$$

$$r \le [v^2D^2 + (a_{2i+1})^2]^{\frac{1}{2}}, \qquad N_{2i+1}(r) = 0,$$

$$r \ge [v^2D^2 + (a_{2i+1})^2]^{\frac{1}{2}},$$

$$N_{2i+1}(r) = -\frac{4\pi}{V}\int_{a_{2i+1}}^{(r^2-v^2D^2)^{\frac{1}{2}}} dx\, xK_{2i+1}(x)Q[(r^2-x^2)^{\frac{1}{2}}].$$

Using a method similar to the technique used to evaluate $N_{2i}(r)$, one finds that

$$r \ge [v^2D^2 + (a_{2i+1})^2]^{\frac{1}{2}}$$

$$N_{2i+1}(r) = \sum_{n=0}^{\infty} C_n^{2i+1}\left[\frac{r^2}{v^2D^2 + (a_{2i+1})^2} - 1\right]^{n+2+\alpha_{2i+1}},$$

where

$$C_n^{2i+1} = \frac{2\pi}{\Gamma(\frac{1}{2})V}\frac{[v^2D^2 + (a_{2i+1})^2]^{n+2+\alpha_{2i+1}}}{\Gamma(n+3+\alpha_{2i+1})}$$

$$\times \sum_{m=0}^{n}\frac{(-1)^m A_{n-m}^{2i+1}\Gamma(m+\frac{3}{2})\Gamma(n-m+1+\alpha_{2i+1})}{(vD)^{2m+3}(a_{2i+1})^{2n-2m+2\alpha_{2i+1}}}.$$

When there is a Type-I point at $r = a_{2i+1}$, $M(r)$ can be written

$$M(r) = E_{2i+1}(r) + M_{2i+1}(r),$$

where

$$E_{2i+1}(r) = \frac{4\pi}{V}\int_0^r dx\, xL_{2i+1}(x)Q[(r^2-x^2)^{\frac{1}{2}}]$$

$$r \le a_{2i+1}, \qquad M_{2i+1}(r) = 0,$$

$$r \ge a_{2i+1},$$

$$M_{2i+1}(r) = \sum_{n=0}^{\infty} B_n^{2i+1}\left[\frac{r^2}{(a_{2i+1})^2} - 1\right]^{n+\frac{1}{2}+\alpha_{2i+1}}$$

$$+ \sum_{n=0}^{\infty} D_n^{2i+1}\left[\frac{r^2}{(a_{2i+1})^2} - 1\right]^{n+1+\alpha_{2i+1}}$$

$$B_n^{2i+1} = \frac{2\pi a_{2i+1}\Gamma(\frac{1}{2})\Gamma(n+1+\alpha_{2i+1})}{V\Gamma(n+\frac{3}{2}+\alpha_{2i+1})}A_n^{2i+1}$$

$$D_n^{2i+1} = -[2\pi/V][(a_{2i+1})^2/vD(n+1+\alpha_{2i+1})]A_n^{2i+1}.$$

For a Type-II point at $r = a_{2i}$, by rearrangement involving partial integration, in the neighborhood of $r = a_{2i}$, $M(r)$ can be expressed

$$M(r) = E_{2i}(r) + M_{2i}(r),$$

where ϵ is a number such that $\epsilon > |r - a_{2i}|$, and

$$E_{2i}(r) = J_{2i}(r) + \frac{4\pi}{V}\int_0^r dx\, xL_{2i}(x)Q[(r^2-x^2)^{\frac{1}{2}}] + \frac{4\pi}{V}$$

$$\times \int_{\epsilon}^{a_{2i}} dx\, xQ\{[r^2+x^2-(a_{2i})^2]^{\frac{1}{2}}\}K_{2i}\{[(a_{2i})^2-x^2]^{\frac{1}{2}}\},$$

$$M_{2i}(r) = -\frac{2\pi a_{2i}}{V}\sum_{n=0}^{\infty}\frac{(-1)^n\Gamma(\frac{1}{2})\Gamma(n+\alpha_{2i}+1)A_n^{2i}}{\Gamma(n+\alpha_{2i}+\frac{3}{2})\cos(\alpha_{2i}\pi)}$$

$$\times\left[\frac{r^2}{(a_{2i})^2} - 1\right]^{n+\alpha_{2i}+\frac{1}{2}},$$

$$J_{2i}(r) = -M_{2i}(r) + \frac{4\pi}{V}$$

$$\times \int_0^{\epsilon} dx\, xK_{2i}\{[(a_{2i})^2-x^2]^{\frac{1}{2}}\}Q\{[r^2-(a_{2i})^2+x^2]^{\frac{1}{2}}\}$$

for $r > a_{2i}$. When $r < a_{2i}$, the same expression holds for $E_{2i}(r)$, and

$$M_{2i}(r) = \frac{2\pi(a_{2i})^2}{VvD}\sum_{n=0}^{\infty}\frac{A_n^{2i}[1 - r^2/(a_{2i})^2]^{n+\alpha_{2i}+1}}{(n+1+\alpha_{2i})}$$

$$+ \frac{2\pi a_{2i}}{V}\frac{\sin(\alpha_{2i}\pi)}{\cos(\alpha_{2i}\pi)}$$

$$\times \sum_{n=0}^{\infty}\frac{\Gamma(\frac{1}{2})\Gamma(n+1+\alpha_{2i})A_n^{2i}}{\Gamma(n+\frac{3}{2}+\alpha_{2i})}\left[1 - \frac{r^2}{(a_{2i})^2}\right]^{n+\frac{1}{2}+\alpha_{2i}}$$

$$J_{2i}(r) = -M_{2i}(r)$$

$$+ \frac{4\pi}{V}\int_{[(a_{2i})^2-r^2]^{\frac{1}{2}}}^{\epsilon} dx\, xK_{2i}\{[(a_{2i})^2-x^2]^{\frac{1}{2}}\}$$

$$\times Q\{[r^2-(a_{2i})^2+x^2]^{\frac{1}{2}}\}.$$

It can be shown that $E_{2i}(r)$ and all its derivatives are continuous at a_{2i}. Thus, for a Type-II point at $r = a_{2i}$, only $M_{2i}(r)$ contributes to the asymptotic expansion.

These expressions of $M_{2i}(r)$ do not hold when $\alpha_{2i} = n + \frac{1}{2}$, where n is a positive integer. For these values of α_{2i}, the derivatives of M_{2i} have logarithmic discontinuities. But when the effect of these logarithmic terms on the asymptotic expansion of the intensity is calculated by the method of Jones and Kline,[7] one obtains the same results as are found by computing the asymptotic expansion for the scattered intensity for arbitrary α_{2i} and then letting $\alpha_{2i} = n + \frac{1}{2}$. Thus this value of α_{2i} does not need special treatment when one is concerned only with computation of the asymptotic expansion.

For a function $f(x)$ which in the neighborhood of point a can be written (for $x > a$),

$$F(x) = \sum_{n=0}^{\infty} c_n\left(\frac{x^2}{a^2} - 1\right)^{n+\alpha}.$$

Erdélyi's theorem for the asymptotic expansion of Fourier integrals shows that the contribution of the point $r = a$ to the asymptotic expansion of the integral

$$\frac{1}{h}\int_a^b dx\, F(x)\sin hx$$

[7] D. S. Jones and M. Kline, J. Math. and Phys. 37, 27 (1958).

is given by

$$a^2 \sum_{n=0}^{N-1} \frac{d_n}{(ha)^{n+2+\alpha}} \cos\left(ha + \frac{n+\alpha}{2}\pi\right),$$

where

$$d_n = \sum_{m=0}^{n} \frac{2^{2m+\alpha-n}\Gamma(m+1+\alpha)\Gamma(n+1+\alpha)}{(n-m)!\Gamma(2m+\alpha+1-n)} c_m.$$

Similarly, if in the neighborhood of point a the function $g(x)$ can be written for $x < a$,

$$g(x) = \sum_{n=0}^{\infty} c_n \left(1 - \frac{x^2}{a^2}\right)^{n+\alpha},$$

the contribution of point a to the asymptotic expantion of

$$\frac{1}{h}\int_b^a dx\, g(x) \sin hx$$

is given by

$$-a^2 \sum_{n=0}^{N-1} \frac{d_n}{(ha)^{n+2+\alpha}} \cos\left(ha - \frac{n+\alpha}{2}\pi\right),$$

where

$$d_n = \Gamma(n+1+\alpha) \times \sum_{m=0}^{n} \frac{(-1)^{n-m}2^{2m+\alpha-n}\Gamma(1+m+\alpha)c_m}{(n-m)!\Gamma(2m+\alpha+1-n)}.$$

[When $g(x)$ is expressed as a power series

$$g(x) = \sum_{l=0}^{\infty} b_l (1-x)^{l+\alpha},$$

this series can be rearranged to give, for $x > 0$,

$$g(x) = \sum_{l=0}^{\infty} \frac{b_l(1-x^2)^{l+\alpha}}{(1+x)^{l+\alpha}} = \sum_{l=0}^{\infty} \frac{b_l(1-x^2)^{l+\alpha}}{\{1+[1-(1-x^2)]^{\frac{1}{2}}\}^{l+\alpha}} = \sum_{n=0}^{\infty} \frac{(1-x^2)^{n+\alpha}}{\Gamma(n+\alpha+1)} \times \sum_{l=0}^{n} \frac{(l+\alpha)b_l\Gamma(2n+\alpha-l)}{(n-l)!2^{2n+\alpha-l}}.$$

The c_n thus can be expressed in terms of the b_n. A similar procedure is possible for the c_n in the above series for $f(x)$.]

Application of these results to the $M_i(r)$ and $N_i(r)$ shows that the asymptotic expansion of the intensity $I(h)$ has the form

$$I(h) = I_0(h) + I_1(h) + I_2(h) + I_3(h), \qquad (3)$$

where

$$I_0(h) = \sum_{k=0}^{N} \left[\frac{(-1)^k c_k^0}{(h)^{2k+4}} + \frac{d_k^0 \cos(hvD + \frac{1}{2}k\pi)}{(hvD)^{k+4}} + \frac{b_k^0 \cos(hvD + \frac{1}{2}(k+\frac{1}{2})\pi)}{(hvD)^{k+9/2}}\right],$$

$$I_1(h) = \sum_{i=1}^{n}\sum_{k=0}^{N} \frac{b_k^i \sin(ha_i - \frac{1}{4}\pi + \gamma_i + \frac{1}{2}k\pi)}{(ha_i)^{5/2+k+\alpha_i}},$$

$$I_2(h) = \sum_{i=1}^{n}\sum_{k=0}^{N} \frac{d_k^i \sin(ha_i + \gamma_i + \frac{1}{2}k\pi)}{(ha_i)^{3+k+\alpha_i}},$$

$$I_3(h) = \sum_{i=1}^{n}\sum_{k=0}^{N} \frac{c_k^i \cos\{h[(a_i)^2 + v^2D^2]^{\frac{1}{2}} + \gamma_i + \frac{1}{2}k\pi\}}{[h\sqrt{(a_i)^2 + v^2D^2}]^{4+\alpha_i+k}},$$

where

$$\gamma_i = (-1)^{i+1}(\tfrac{1}{2}\alpha_i\pi)$$

$$c_k^0 = \frac{4\pi}{V}\left[\frac{2k+1}{vD}\beta^{(2k)}(0) - \frac{\Gamma(\frac{1}{2})\Gamma(k+\frac{3}{2})\beta^{(2k+1)}(0)}{k!}\right],$$

$$b_k^i = \frac{2\pi(a_i)^3\Gamma(\frac{1}{2})\Gamma(k+\frac{3}{2}+\alpha_i)(-1)^i}{V} \times \sum_{l=0}^{k} \frac{2^{2l+\alpha_i+\frac{1}{2}-k}(-1)^{(i+1)l}\Gamma(l+\alpha_i+1)A_i^i}{(k-l)!\Gamma(\frac{3}{2}+\alpha_i+2l-k)},$$

$$b_k^0 = -\frac{2\pi(vD)^3\Gamma(k+\frac{7}{2})}{V2^{k-5/2}\Gamma(\frac{1}{2})} \times \sum_{m=0}^{k} \frac{\Gamma(m+\frac{3}{2})(vD)^{2m+1}\beta^{(2m+1)}(0)}{(2m+1)!} \times \sum_{l=0}^{k-m} \frac{(-1)^l 2^{2l+2m}\Gamma(l+\frac{3}{2})}{(k-m-l)!\Gamma(2l+\frac{7}{2}+2m-k)},$$

$$d_k^0 = -\frac{4\pi^{\frac{1}{2}}(vD)^3\Gamma(k+3)}{V2^k}\sum_{m=0}^{k}\frac{(vD)^{2m}\beta^{(2m)}(0)}{\Gamma(m+\frac{1}{2})} \times \sum_{l=0}^{k-m} \frac{(-1)^l(2l+1)!}{(k-m-l)!l!(2l+2m+2-k)!},$$

$$d_k^i = \frac{4\pi(a_i)^4\Gamma(k+2+\alpha_i)}{VvD2^k} \times \sum_{l=0}^{k} \frac{(-1)^{(i+1)(l+1)}2^{2l+\alpha_i}\Gamma(1+l+\alpha_i)A_i^i}{(k-l)!\Gamma(2+\alpha_i+2l-k)},$$

$$c_k^i = \frac{8\pi(a_i)^3\Gamma(k+3+\alpha_i)(-1)^i}{V2^{k-\alpha_i}} \times \sum_{m=0}^{k} \frac{(-1)^{(i+1)m}\Gamma(m+\alpha_i+1)A_m^i}{\Gamma(\frac{1}{2})} \times \sum_{l=0}^{k-m} \frac{(-1)^l 2^{2l+2m}\Gamma(l+\frac{3}{2})\left[1+\frac{v^2D^2}{(a_i)^2}\right]^{l+m+3+\alpha_i}}{(k+m-l)!\Gamma(2m+2l+3+\alpha_i-k)\left(\frac{vD}{a_i}\right)^{2l+3}}.$$

RIGHT CIRCULAR CYLINDERS

For a circular cross section[8] of diameter D,

$$\beta(x) = 1 - \frac{4}{\pi}\int_0^{r/D} ds\,(1 - s^2)^{\frac{1}{2}}.$$

Thus $\beta(r)$ has a Type-II point at $r = D$, in the neighborhood of which

$$\beta(r) = \frac{2}{\pi\Gamma(\frac{1}{2})}\sum_{n=0}^{\infty}\frac{\Gamma(n+\frac{1}{2})}{(n+\frac{3}{2})n!}\left(1 - \frac{x^2}{D^2}\right)^{n+\frac{3}{2}}.$$

Also,

$$\beta^{(2n+1)}(0) = \frac{2}{\pi\Gamma(\frac{1}{2})}\frac{(2n)!\Gamma(n-\frac{1}{2})}{n!D^{2n+1}}.$$

For $n > 0$,

$$\beta^{(2n)}(0) = 0.$$

Thus, there are no Type-I points, and there is one Type-II point, at $r = D$, and with $\alpha = \frac{3}{2}$. The only i value that need be considered in (3) is $i = 2$, and therefore, substituting in (3) gives

$$I_0(h) = \frac{16(1-\cos hvD)}{(hD)^2(hvD)^2} + \sum_{k=0}^{N}\frac{(-1)^{k+1}e_k^0}{(hD)^{2k+4}} + \frac{b_k^0\cos(hvD + \frac{1}{2}(k+\frac{1}{2})\pi)}{(hvD)^{k+9/2}},$$

$$I_1(h) = \sum_{k=0}^{N}\frac{b_k^1\sin(hD + \frac{1}{2}k\pi)}{(hD)^{k+4}},$$

$$I_2(h) = \sum_{k=0}^{N}\frac{d_k^2\sin(hD + \frac{1}{4}\pi + \frac{1}{2}k\pi)}{(hD)^{k+9/2}},$$

$$I_3(h) = \sum_{k=0}^{N}\frac{c_k^2\cos(hD[1+v^2]^{\frac{1}{2}} + \frac{1}{4}\pi + \frac{1}{2}k\pi)}{[hD\{[1+v^2]^{\frac{1}{2}}\}^{k+11/2}},$$

$$e_j^0 = \frac{32}{v}\frac{(2j+1)!}{2j-1}\left[\frac{\Gamma(j+\frac{1}{2})}{\Gamma(\frac{1}{2})j!}\right]^2,$$

$$b_k^0 = -\frac{64v^2\sqrt{2}\Gamma(k+\frac{7}{2})}{\pi^2 2^k}\sum_{m=0}^{k}\frac{[\Gamma(m+\frac{1}{2})]^2v^{2m+1}}{(2m-1)m!} \times \sum_{l=0}^{k-m}\frac{(-1)^l 2^{2m+2l}\Gamma(l+\frac{3}{2})}{(k-m-l)!\Gamma(2l+2m-k+\frac{7}{2})},$$

$$b_k^2 = -\frac{64(k+2)!}{\pi v 2^k}\sum_{l=0}^{k}\frac{(-1)^l 2^{2l}\Gamma(l+\frac{3}{2})\Gamma(l+\frac{1}{2})}{(k-l)!l!(2l-k+2)!},$$

$$d_k^2 = \frac{32}{\pi v^2}\frac{\Gamma(k+\frac{1}{2})\Gamma(k-\frac{3}{2})}{2^k k!}\frac{\sqrt{2}}{\pi^{\frac{1}{2}}}\left(k^2 + 4k + \frac{3}{4}\right),$$

$$c_k^2 = -\frac{128\Gamma(k+\frac{9}{2})\sqrt{2}}{\pi^2 2^k} \times \sum_{m=0}^{k}\frac{(-1)^m\Gamma(m+\frac{3}{2})\Gamma(m+\frac{1}{2})}{m!} \times \sum_{l=0}^{k-m}\frac{(-1)^l 2^{2l+2m}\Gamma(l+\frac{3}{2})(1+v^2)^{l+m+9/2}}{v^{2l+4}(k-m-l)!\Gamma(\frac{9}{2}a + 2m + 2l - k)}.$$

Note that at large h, $I(h)$ is proportional to h^{-4}, in agreement with the general prediction for the asymptotic behavior of the scattering intensity for solid particles.

This property of the asymptotic expansion of the scattered intensity for right circular cylinders is a consequence of the result mentioned in the previous section which stated that the case $\alpha_{2i} = n + \frac{1}{2}$ produced no effects in the asymptotic expansion which were qualitatively different from the expressions for general α_{2i}.

RECTANGULAR PARALLELEPIPEDS

The function $\beta(r)$ for a rectangle with sides $2l$ and $2m$ can be found by a two-dimensional analog of the procedure used to obtain $H(r)$ for a cylinder of arbitrary cross section. From this calculation the a_i, α_i, and A_j^i are found to be

$$a_1 = 2l, \quad \alpha_1 = \tfrac{3}{2}, \quad A_j^1 = (-1)^j/\pi(j+\tfrac{3}{2}),$$
$$a_3 = 2l, \quad \alpha_3 = 2,$$
$$A_j^3 = (-1)^{j+1}l\Gamma(j+\tfrac{3}{2})/\pi m\Gamma(\tfrac{1}{2})(j+2)!,$$
$$a_5 = 2m, \quad \alpha_5 = \tfrac{3}{2}, \quad A_j^5 = (-1)^j/\pi(j+\tfrac{3}{2}),$$
$$a_7 = 2m, \quad \alpha_7 = 2,$$
$$A_j^7 = (-1)^{j+1}m\Gamma(j+\tfrac{3}{2})/\pi l\Gamma(\tfrac{1}{2})(j+2)!,$$
$$a_8 = 2(l^2+m^2)^{\frac{1}{2}}, \quad \alpha_8 = 3,$$
$$A_j^8 = [4\pi(j+3)!]^{-1}[(l^2+m^2)/lm]^3 a_j(l,m),$$
$$a_j(x,y) = \sum_{k=0}^{j}\frac{\Gamma(k+\frac{3}{2})\Gamma(j-k+\frac{3}{2})(x^2+y^2)^j}{\Gamma(\frac{3}{2})\Gamma(\frac{3}{2})x^{2k}y^{2j-2k}}.$$

Also, $\beta(0) = 1$, $\beta^{(1)}(0) = -(\pi lm)^{-1}(m+1)$, $\beta^{(2)}(0) = (2\pi lm)^{-1}$, and all higher derivatives of $\beta(r)$ are zero at $r = 0$.

Substitution in Eq. (3) gives the asymptotic expansion

$$I(h) = I_a(h) + I_b(h) + I_c(h) + I_d(h) + I_e(h) + I_f(h) + I_g(h),$$

where $2n = vD$, and

$$I_a(h) = 4\pi(mnl)^{-1}(2h)^{-4}[l^{-1}(1-\cos 2hl) + m^{-1}(1-\cos 2hm) + n^{-1}(1-\cos 2hn)],$$

$$I_b(h) = 8(lmn)^{-1}(2h)^{-5}[l\sin 2hl + m\sin 2hm + n\sin 2hn],$$

[8] A. Guinier, *et al.*, *Small Angle Scattering of X-Rays*, (John Wiley & Sons, Inc., New York, 1955), Eq. (26), p. 17.

$$I_c(h) = 24(lmn)^{-2}(2h)^{-6}[\cos 2hl + \cos 2hm + \cos 2hn - 1],$$

$$I_d(h) = \frac{8}{(lmn)(2h)^4}\frac{\pi^{\frac{1}{2}}}{\sqrt{2}} \times \sum_{k=0}^{N} s_k\left[\frac{m+n}{mn}\frac{\cos[2hl + \frac{1}{2}(k+\frac{1}{2})\pi]}{(2hl)^{k+\frac{1}{2}}} + \frac{l+n}{ln}\frac{\cos[2hm + \frac{1}{2}(k+\frac{1}{2})\pi]}{(2hm)^{k+\frac{1}{2}}} + \frac{l+m}{lm}\frac{\cos[2hn + \frac{1}{2}(k+\frac{1}{2})\pi]}{(2hn)^{k+\frac{1}{2}}}\right],$$

$$s_k = \frac{\Gamma(k+\frac{7}{2})}{2^k\Gamma(\frac{3}{2})}\sum_{j=0}^{k}\frac{(-1)^j 2^{2j}\Gamma(j+\frac{3}{2})}{(k-j)!\Gamma(\frac{7}{2}+2j-k)},$$

$$I_e(h) = \frac{8}{(lmn)(2h)^5}\frac{\pi^{\frac{1}{2}}}{\sqrt{2}} \times \sum_{k=0}^{N}\left[b_k(l,m)\frac{\sin[2h(l^2+m^2)^{\frac{1}{2}} + \frac{1}{2}(k+\frac{1}{2})\pi]}{[2h(l^2+m^2)^{\frac{1}{2}}]^{k+\frac{1}{2}}} + b_k(m,n)\frac{\sin[2h(m^2+n^2)^{\frac{1}{2}} + \frac{1}{2}(k+\frac{1}{2})\pi]}{[2h(m^2+n^2)^{\frac{1}{2}}]^{k+\frac{1}{2}}} + b_k(l,n)\frac{\sin[2h(l^2+n^2)^{\frac{1}{2}} + \frac{1}{2}(k+\frac{1}{2})\pi]}{[2h(l^2+n^2)^{\frac{1}{2}}]^{k+\frac{1}{2}}}\right],$$

$$b_k(x,y) = \frac{\Gamma(k+\frac{9}{2})(x^2+y^2)^2}{x^3y^3 2^k} \times \sum_{j=0}^{k}\frac{(-1)^j 2^{2j}a_j(x,y)}{(k-j)!\Gamma(\frac{9}{2}+2j-k)},$$

$$I_f(h) = -\frac{8}{(lmn)^2(2h)^6} \times \sum_{k=0}^{N}\left[c_k(l,m)\frac{\cos[2h(l^2+m^2)^{\frac{1}{2}} + \frac{1}{2}k\pi]}{[2h(l^2+m^2)^{\frac{1}{2}}]^k} + c_k(m,n)\frac{\cos[2h(m^2+n^2)^{\frac{1}{2}} + \frac{1}{2}k\pi]}{[2h(m^2+n^2)^{\frac{1}{2}}]^k} + c_k(l,n)\frac{\cos[2h(l^2+n^2)^{\frac{1}{2}} + \frac{1}{2}k\pi]}{[2h(l^2+n^2)^{\frac{1}{2}}]^k}\right],$$

$$c_k(x,y) = \frac{(k+4)!(x^2+y^2)^2}{2^k x^2 y^2} \times \sum_{j=0}^{k}\frac{(-1)^j 2^{2j}a_j(x,y)}{(k-j)!(2j+4-k)!},$$

$$I_g(h) = -\frac{8(l^2+m^2+n^2)^6}{(lmn)^4} \times \sum_{k=0}^{n} f_k(l,m,n)\frac{\sin[2h(l^2+m^2+n^2)^{\frac{1}{2}} + \frac{1}{2}k\pi]}{[2h(l^2+m^2+n^2)^{\frac{1}{2}}]^{k+7}},$$

$$f_k(l,m,n) = \frac{(k+5)!}{2^k}\sum_{s=0}^{k}\frac{(-1)^s 2^{2s}(l^2+m^2+n^2)^s}{(k-s)!(2s+5-k)!} \times \sum_{i=0}^{s}\sum_{j=0}^{s-i}\frac{\Gamma(i+\frac{3}{2})\Gamma(j+\frac{3}{2})\Gamma(s-i-j+\frac{3}{2})}{[\Gamma(\frac{3}{2})]^3 l^{2i}m^{2j}n^{2s-2i-2j}}.$$

The expression for $I(h)$ is unchanged by permutations of l, m, and n. This property is the result of the fact that for a parallelepiped, any face can be taken as the cross section.

The first terms of this expansion reproduce Eq. (13) of Ref. 2 and also give the additional terms shown in the thesis from which the results of Ref. 2 were taken.

DISCUSSION

In (3), $I_0(h)$ is determined by the behavior of $\beta(r)$ at $r = 0$, while $I_1(h)$, $I_2(h)$, and $I_3(h)$ depend on the nature of the discontinuities in the derivatives of $\beta(r)$ at the Type-I and Type-II points. The number of terms used in the asymptotic expansion is determined by the value of N. Ordinarily, in an asymptotic expansion, the last term retained (in this case, the term for which $k = N$) can be taken as at least a rough estimate of the error involved in using the asymptotic expansion to approximate the intensity.

At sufficiently large h, the terms of $k = 0$ will dominate. If only these terms are considered, (3) becomes

$$I_0(h) = \frac{4\pi}{VvD}\frac{1-\cos hvD}{h^4} + \frac{2\pi P}{VAh^4} + \frac{2}{V}\frac{P}{A}\left(\frac{\pi}{2vD}\right)^{\frac{1}{2}}\frac{\cos(hvD+\frac{1}{4}\pi)}{h^{9/2}},$$

$$I_1(h) = \frac{(2\pi)^{\frac{1}{2}}}{V} \times \sum_{i=1}^{n}\frac{(-1)^i 2^{\alpha_i}\Gamma(1+\alpha_i)(a_i)^3 A_0^i}{(ha_i)^{\alpha_i+5/2}}\sin\left(ha_i - \frac{\pi}{4} + \gamma_i\right),$$

$$I_2(h) = -\frac{4\pi}{VvD} \times \sum_{i=1}^{n}\frac{(-1)^i 2^{\alpha_i}\Gamma(1+\alpha_i)(a_i)^4 A_0^i}{(ha_i)^{\alpha_i+3}}\sin(ha_i + \gamma_i), \tag{4}$$

$$I_3(h) = \frac{4\pi}{V} \times \sum_{i=1}^{n}\frac{(-1)^i 2^{\alpha_i}\Gamma(1+\alpha_i)[(a_i)^2 + v^2D^2]^{1+\alpha_i/2}A_0^i}{(a_i)^{2\alpha_i}(vD)^3 h^{4+\alpha_i}} \times \cos\{h[(a_i)^2 + v^2D^2]^{\frac{1}{2}} + \gamma_i\}.$$

Note that $I_0(h)$ will always contain terms proportional to h^{-4}, while the exponents of $I_1(h)$, $I_2(h)$ and $I_3(h)$ in (4) will depend on the values of the α_i.

The terms in (4) which do not oscillate can be

written

$$\frac{2\pi}{V}\frac{2A + PvD}{AvDh^4} = \frac{2\pi S}{(V)^2h^4},$$

where S is the total surface area of the generalized cylinder. When the normalization of $I(h)$ is taken into account, this result agrees with the general expression given by Guinier, *et al.*[8]

If all terms in $I(h)$ are to decrease at large h, at least as rapidly as h^{-4}, then all the α_i must be greater than or equal to $\frac{3}{2}$. For the cross-section shapes (circle, rectangle) for which $\beta(r)$ has been calculated, the α_i are found to satisfy this relation. It would be interesting to study $\beta(r)$ to see how general this result is.

The dependence of $I(h)$ on the behavior of $\beta(x)$ in the neighborhood of the Type-I and Type-II points suggests that it would be of interest to make more detailed investigations of the effect of the cross-section shape on the existence and nature of these points. It would be especially useful to study the properties of $\beta(r)$ in the neighborhood of $r = D$, where, according to the form of $\beta(r)$ for all cross-section shapes which have been studied up to the present time, there is a very strong suggestion that a Type-II point will always occur.

It should be emphasized that the asymptotic expansions which have been developed will approximate the scattered intensity only at angles for which $ha_i \gg 1$ for all of the a_i. For highly elongated or highly flattened generalized cylinders, which can be referred to as rods or platelets, respectively, there will be angles for which the condition $ha_i \gg 1$ is satisfied for some but not all of the a_i. For these shapes, special techniques are necessary to calculate the intensity. A method applicable to rods is given in Ref. 2. Further study is necessary to develop an analogous technique for dealing with platelets.

Interacting Fermions in One Dimension. I. Repulsive Potential*

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The exact energies and wavefunctions for the ground state and low-lying excited states of a system of $N-1$ one-dimensional fermions all of the same spin and one fermion of the opposite spin are calculated in the large-volume, finite-density limit when the particles interact via a repulsive delta function potential. A number of properties of the system such as pair correlation functions and the effective mass of a certain class of excitations are also discussed.

I. INTRODUCTION

We consider the Hamiltonian

$$H = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\frac{d^2}{dx^2} + g\sum_{i>j}^{N}\sum\delta(x_i - x_j),$$

which arises when N particles of mass M interact in one dimension with equal strength delta function potentials. The exact solubility and the scattering solutions of this Hamiltonian have been discussed in Ref. 1. In order to proceed systematically, however, it is advisable to discuss the nature of the solution briefly here.

This Hamiltonian is viewed as discribing the interaction of a single particle with a fixed potential in an N-dimensional space where the coordinates of the N-dimensional space are the positions of each of the particles. The fixed potential in this mathematically equivalent space is a series of intersecting $N-1$ dimensional delta function sheets. These delta function sheets are arranged in this N-dimensional space so that they are the boundaries of $N!$ different regions where each region corresponds to one of the $N!$ possible permutations of the particles along a line. We therefore call each of the permutations of the particles along the line a "region," for example the region $x_1 < x_2 < x_3 \cdots < x_N$. If we assume that we have N wavenumbers $k_1 \cdots k_N$, we may form in each region of space $N!$ plane waves such as

$$e^{i(k_1x_1+k_2x_2+k_3x_3\cdots+k_Nx_N)}$$

or

$$e^{i(k_2x_1+k_1x_2+k_7x_3\cdots)}.$$

This particular problem is soluble because it is possible to satisfy the differential equation by assuming that the entire wavefunction is made up of a linear combination of $N!$ possible plane waves in each region of space.

As we have indicated above the delta function potential provides a barrier between regions of the multidimensional space. This barrier may be taken into account by replacing the delta function potential by a "two-sided" boundary condition. By integrating the Schrödinger equation over an infinitesimal region which spans the delta-function potential between particle 1 and 2 we find the well-known condition

$$\frac{1}{\sqrt{2}}\left[\left(\frac{\partial}{\partial x_1}-\frac{\partial}{\partial x_2}\right)_{x_1-x_2=0^+} - \left(\frac{\partial}{\partial x_1}-\frac{\partial}{\partial x_2}\right)_{x_1-x_2=0^-}\right]\psi = \sqrt{2}g; \qquad \psi(x_1 = x_2),$$

where we have chosen units so that $\hbar = M = 1$. In the next section we show explicitly that this equation, plus continuity of the wavefunction is sufficient to determine the coefficients of the $N!$ plane waves in any region given the values of the coefficients in some particular region. Although it is not obvious from this point of view, this process is internally consistent, that is, no matter how one calculates the coefficients in any given region the answer is always the same. This consistency is shown in a somewhat different form in Ref. 1.

In the sense given above the wavefunction is determined provided that we know the coefficients of the $N!$ plane waves in any particular region. We must now find the generalization of a scattering solution to a solution where the density of the interacting particles is fixed. This generalization has been carried out by Lieb[2] when the fundamental particles are bosons. The finite-density limit for Fermi particles is more difficult. It is, in fact, the central difficulty which keeps us from working a more general class of problems than that which is presented here. The only known systematic method of procedure to obtain the finite-density limit is a

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[2] E. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).

twofold process: (1) apply periodic boundary conditions to a scattering solution for a fixed number of particles; (2) allow the size of the periodic box and the number of particles to become infinite in such a way that the density remains a constant.

II. APPLICATION OF PERIODIC BOUNDARY CONDITIONS TO A PARTICULAR PROBLEM

Let us now consider a special case of the previous general problem of N particles, namely that in which $N-1$ of the particles are spin-up fermions and one particle is a spin-down fermion. Let us choose x_1 to be the coordinate of the spin-down fermion. We call region 1 the region where $x_1 < x_2 < x_3 \cdots < x_N$, that is the region which has the particles all in order with the different particle on the left. All of the particles $2 \cdots N$ are indistinguishable so we must antisymmetrize the wavefunction in this region to take this into account.

Consider the particular plane wave

$$\exp\,[i(k_1x_1 + k_2x_2 + k_3x_3 + \cdots + k_Nx_N)];$$

let its amplitude be denoted by $(1\,2\,3 \cdots N)$. [From now on we write, e.g., $(1\,2\,3 \cdots N)$ as $(123 \cdots N)$ for compactness. As no mulitple-digit numerals are used in these expressions, there should be no confusion.] Similarly the amplitude of the plane wave

$$\exp\,[i(k_9x_1 + k_7x_2 + k_4x_3 + \cdots)]$$

would be denoted by $(974 \cdots)$.

The order of the numbers inside the parenthesis dictate which particle has which k. The k in the first slot goes with the first particle, the k in the second slot goes with the second particle, etc.

Antisymmetry of the wavefunction dictates that

$$(123\cdots N) = -(1324\cdots N) = (1342\cdots N) = \text{etc.}$$

That is, all of the coefficients which have "1" in the first slot differ from the first amplitude only by a plus or minus sign, according to whether they are an even or odd permutation of the numbers $2 \cdots N$. Similar relations hold among the amplitudes which have any number in the first slot.

Now let us calculate the amplitudes in the next adjacent region. Let us consider the interaction of particles 1 and 2 and calculate the wavefunction in the region $x_2 < x_1 < x_3 < x_4 \cdots < x_N$, which we call region 2. The amplitudes must go together in pairs of the type $(1\,2\,{}^{\text{some permutation}})$ and $(2\,1\,{}^{\text{same permutation}})$ because this pair have exactly the same dependence on $x_3 \cdots x_N$ when $x_1 = x_2$. Any other plane wave will have a different dependence.

Now using Eq. (2)

$$[i(k_1 - k_2)/\sqrt{2}][(12\cdots N)_2 - (21\cdots N)_2 - (12\cdots N)_1 + (21\cdots N)_1] = \sqrt{2}g[(12\cdots N)_1 + (21\cdots N)_1].$$

And continuity of the wavefunction gives

$$(12\cdots N)_1 + (21\cdots N)_1 = (12\cdots N)_2 + (21\cdots N)_2.$$

Solving these two equations for the amplitudes in region 2 gives

$$\begin{bmatrix}(12\cdots N)\\(21\cdots N)\end{bmatrix}_2 = \begin{bmatrix}1 + 1/s_{12} & 1/s_{12}\\ -1/s_{12} & 1 - 1/s_{12}\end{bmatrix}\begin{bmatrix}(12\cdots N)\\(21\cdots N)_2\end{bmatrix}_1$$

where $s_{12} = i(k_1 - k_2)/g$.

We could have gone through a similar calculation for any pair of adjacent particles, but for the indistinguishable particles the result is trivial. If the particles which pass through one another are of the same spin the amplitudes on the right-hand side of the expression above will be equal and opposite by antisymmetry. It is then easily seen that the amplitudes in the next adjacent region are exactly the same as in the first region. This means that we can move the spin up particles through one another at will, a manifestation of the fact that these particles do not interact because the exclusion principle makes the wavefunction zero when any two particles of the same spin come together.

III. APPLICATION OF PERIODIC BOUNDARY CONDITIONS

We now wish to apply the condition $\psi(0) = \psi(L)$ for every one of the N particles. In this particular problem where $N-1$ particles are spin up and one particle is spin down there is a short-cut way of doing this. If we start in region 1 $(x_1 < x_2 < x_3 \cdots < x_N)$ we can carry x_2 through all of the other spin-up particles with no change in the amplitudes of the plane waves. Let us call the region $x_1 < x_3 < x_4 \cdots < x_N < x_2$ region q. The only way the periodic boundary conditions may be satisfied is to satisfy periodicity for each plane-wave component independently, again because any other plane-wave component would have a different dependence on the coordinates of the other particles. Thus two typical relations which must be satisfied are

$$(123\cdots N)_2 = e^{ik_2L}(123\cdots N)_q,$$

$$(213\cdots N)_2 = e^{ik_1L}(213\cdots N)_q.$$

The exponential phase factors arise from setting $x_2 = L$ in region q. But we have already argued that every plane-wave amplitude in region q is the same as every plane-wave amplitude in region 1. Thus we may rewrite these relations as

$$\begin{bmatrix} e^{ik_2L}(123\cdots N)_1 \\ e^{ik_1L}(213\cdots N)_1 \end{bmatrix} = \begin{bmatrix} (123\cdots N)_2 \\ (213\cdots N)_2 \end{bmatrix}$$

$$= \begin{bmatrix} 1 + 1/s_{12} & 1/s_{12} \\ -1/s_{12} & 1 - 1/s_{12} \end{bmatrix} \begin{bmatrix} (123\cdots N)_1 \\ (213\cdots N)_1 \end{bmatrix}.$$

We now have a pair of homogeneous equations in the amplitudes $(123 \cdots N)_1$ and $(213 \cdots N)_1$. These equations are inconsistent unless the determinant vanishes, thus

$$\begin{vmatrix} 1 + 1/s_{12} - e^{ik_2L} & 1/s_{12} \\ -1/s_{12} & 1 - 1/s_{12} - e^{ik_1L} \end{vmatrix} = 0.$$

Notice that this determinant vanishes automatically if k_1L and k_2L are integral multiples of 2π. These solutions are the usual all spin-up solutions. Expansion of this determinant yields

$$s_{12} = (e^{ik_1L} - e^{ik_2L})/(1 - e^{ik_2L})(1 - e^{ik_1L})$$
$$= i(k_1 - k_2)/g,$$

which can be put in a more convenient form

$$ik_1/g - \tfrac{1}{2}i \operatorname{ctn} \tfrac{1}{2}k_1L = \tfrac{1}{2}ik_2/g - \tfrac{1}{2}i \operatorname{ctn} \tfrac{1}{2}k_2L,$$

if

$$z_i = \tfrac{1}{2}k_iL \qquad a = 4/gL$$

$$az_1 - \operatorname{ctn} z_1 = az_2 - \operatorname{ctn} z_2.$$

Clearly any pair of velocities may be chosen as the pair with which particles 1 and 2 interact. All of the relations among velocities could then be summarized as

$$az_1 - \operatorname{ctn} z_1 = az_2 - \operatorname{ctn} z_2 = az_3 + \operatorname{ctn} z_3$$
$$= az_N - \operatorname{ctn} z_N.$$

One additional piece of information is necessary to determine the spectrum. This information may be obtained by applying periodic boundary conditions to x_1 as the different particle moves from 0 to L. As we move x_1 from region to region through the various spin-up particles we focus our attention on the amplitude of a given plane wave and notice that this plane-wave amplitude is multiplied by a phase factor for each region change. That phase factor is determined by the velocity of the particle through which we carried x_1. For example

$$(1234\cdots N)_2 = e^{ik_3L}(123\cdots N)_1,$$

$$(123\cdots N)_3 = e^{ik_3L}(123\cdots N)_2 = e^{i(k_3+k_3)L}(123\cdots N)_1,$$

where region 3 is $x_2 < x_3 < x_1 < x_4 \cdots < x_N$. As we carry x_1 from 0 to L we get one phase factor for every k value except the one associated with x_1. Thus in region N $(x_2 < x_3 < x_4 \cdots < x_N < x_1)$

$$(123\cdots N)_N = (123\cdots N)_1 \exp iL \sum_{i=2}^{N} k_i.$$

Periodicity of the wavefunction requires that

$$e^{ik_1L}(123\cdots N)_N = (123\cdots N)_1.$$

Thus

$$\sum k_iL = 2n\pi \cdots n = \text{any integer},$$

or

$$\exp i \sum_{i=1}^{N} k_iL = 1,$$

which is, in terms of the z's, $\sum z_i = n\pi$.

In addition to this law for the allowable values of k, we may also find the ratio of the amplitudes which is dictated by the homogeneous equations. This ratio is

$$(123\cdots N)_1/(213\cdots N)_1 = -(1 - e^{ik_1L})/(1 - e^{ik_2L}).$$

Similar ratios would, of course, be found no matter what pair of velocities we assumed for particles x_1 and x_2.

All of these properties of the periodic solution may be summarized in the following set of rules:

(1) The spectrum is given by selecting N roots of $az - \operatorname{ctn} z = \text{const.}$ subject to the additional constraint that $\sum z_i = n\pi$.

(2) The wavefunction is given by calculating the amplitudes of $N!$ plane waves in each region of space.

We select as the basic amplitude

$$(123\cdots N)_1 = 1 - e^{ik_1L} = -2ie^{\frac{1}{2}ik_1L} \sin \tfrac{1}{2}k_1L$$
$$= -2ie^{iz_1} \sin z_1,$$

where as always region 1 is $x_1 < x_2 < x_3 \cdots < x_N$. The amplitude of any other plane wave in this region is determined by two things: (a) the k associated with particle 1 determines which k is to be used in the amplitude (b) the amplitude is modified by a plus or minus sign according to whether it is an even or odd permutation of the state above.

For example,

$$(q23\cdots 1\cdots N)_1 = -(1 - e^{ik_qL}) = +2ie^{iz_q} \sin z_q.$$

(3) The amplitude of a given plane wave in some other region is calculated by first finding the amplitude of that plane wave in region 1 and multiplying this amplitude by a factor of e^{2iz_q} for each particle that x_1 has passed.

For example in the region

$$x_2 < x_3 < x_4 < x_1 < x_5 \cdots < x_N$$

$$(q234\cdots 1\cdots N) = -(1 - e^{ik_qL})e^{2i(z_2+z_3+z_4)}.$$

IV. GROUND STATE OF THE SYSTEM AT FIXED DENSITY

Now that we have developed this set of rules we may proceed to the calculation of the ground-state energy of our many-fermion system. We want to choose the lowest N roots of the equation

$$az - \text{const} = \text{ctn}\, z,$$

subject to the additional constraint that the sum of these roots is $n\pi$. If N is even, we achieve the lowest energy if the value of the constant is zero. This is easily seen in Fig. 1 which is a sketch of the graphical solution to this transcendental equation, and will be demonstrated numerically in the next section where we calculate the excitation spectrum. The sum condition on the roots is satisfied identically under these conditions because the sum of the roots is zero.

We need only consider the solutions of the above transcendental equation where a is very small, because a is the dimensionless product of the scattering length of the delta function potential divided by the length of the box, which is to be a small number in the infinite length limit.

We can see from Fig. 1 that for small a the roots are separated by an interval which is almost π. If the separation were exactly π we would recover the Fermi energy for N particles. For small values of z, the roots occur very near $z = (n + \frac{1}{2})\pi$, $n =$ any integer. If the number of particles is large enough that $Na\pi$ is much greater than unity, we see that the high values of z occur at integral multiples of π.

It may be easily seen graphically or verified by a repeated substitution process that the sth positive root of our transcendental equation is

$$z_s^+ = s\pi + \text{ctn}^{-1}(sa\pi) \qquad s = 0, 1, \cdots, (\tfrac{1}{2}N - 1)$$

and the sth negative root is

$$z_s^- = -s\pi - \text{ctn}^{-1}(sa\pi) \qquad s = 0, 1, \cdots, (\tfrac{1}{2}N - 1)$$

to order a^2, which is sufficient for our purposes.

In our units, $\hbar = M = 1$, the energy is

$$E = \tfrac{1}{2}\sum k_i^2 = (2/L^2)\sum z_i^2,$$

where the sums run over the occupied states. In the ground state this leads to

$$= \frac{2}{L^2}\left[2\sum_{s=0}^{\frac{1}{2}N-1} s^2\pi^2 + 4\sum_{s=0}^{\frac{1}{2}N-1} s\pi\ \text{ctn}^{-1}(sa\pi) + 2\sum_{s=0}^{\frac{1}{2}N-1}[\text{ctn}^{-1}(sa\pi)]^2\right].$$

The first term in this sum is the energy of a Fermi gas containing $N - 1$ particles, the second term is an energy shift caused by the interaction of the spin down particle with the $N - 1$ spin-up particles, and the third term is negligible to order $1/L$. The total energy is, therefore,

$$E = E(N-1) + \Delta E$$

$$\Delta E = \frac{8}{L^2}\sum_{s=0}^{\frac{1}{2}N-1} s\pi\ \text{ctn}^{-1}\, sa\pi.$$

We convert this sum to an integral by the usual techniques and obtain

$$\Delta E = \frac{8}{a^2L^2\pi}\int_0^{2k_F/a} x\ \text{ctn}^{-1}\, x\, dx,$$

where k_F is the Fermi momentum for the $N - 1$ particles

$$k_F = (N - \tfrac{1}{2})\pi/L.$$

Finally, we obtain

$$\Delta E = \frac{k_F^2}{\pi}\left[\frac{g}{2k_F} + \tan^{-1}\frac{g}{2k_F} - \left(\frac{g}{2k_F}\right)^2\left(\frac{\pi}{2} - \tan^{-1}\frac{g}{2k_F}\right)\right].$$

The first three terms of the energy shift for weak interactions (or high density) are:

$$\Delta E = k_F g/\pi - \tfrac{1}{8}g^2 + g^3/12\pi k_F.$$

These three terms are identical with those obtained by Bethe–Goldstone perturbation theory.[3] Notice that all even powers but the second vanish. The same formula also holds for the attractive case $g < 0$, as is shown in a subsequent paper.

For strong interactions (or low density) the energy shift is $E = \frac{1}{2}k_F^2$, or the energy required to add one particle at the Fermi surface. This result would be anticipated from the work of Girardeau,[4] who showed that particles interacting with infinite strength delta

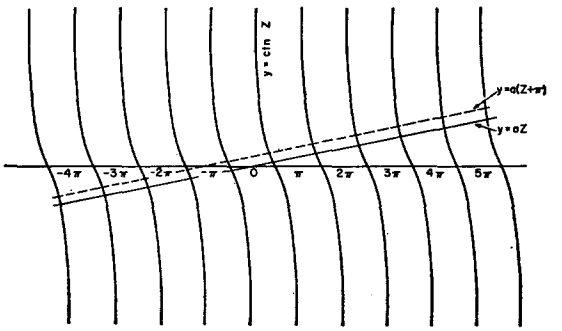

FIG. 1. Sketch of the graphical solution to the equation $az - \text{ctn}\, z = 0$.

[3] B. Day (private communication) (to be published).
[4] M. D. Girardeau, J. Math. Phys. 1, 516 (1963).

function potentials in one dimension have a Fermi-like ground state independent of statistics.

V. EXCITATION SPECTRUM OF THE SYSTEM

There are two distinct ways to excite this system. The first is the familiar way in which a noninteracting Fermi sea is excited viz., leave one of the states of $az = \operatorname{ctn} z$ unoccupied and occupy a higher state. If we characterize the excited states by the total momentum k, where

$$k = (2/L) \sum z_i,$$

the excitation energy of such a state is

$$E_{ex} = k_F k.$$

A more interesting class of states is the class which exhibits collective excitations, or those excitations which depend upon the interactions. These states arise when we consider solutions to $az - \operatorname{ctn} z = \text{const.}$, where the roots occur on the same branches of the cotangent curve, but subject of course to the restriction that $\sum z_i = n\pi$ or $k = (2/L) \sum z_i = 2n\pi/L$. We can calculate the spectrum for these states by first calculating the energy as a function of the constant c which appears in the spectral law and then eliminating c as a function of k. We now imagine graphically solving the equation $az - c = \operatorname{ctn} z$, using the same branches of the cotangent curves which were used in solving for the ground state. In the same manner as before, and to the same order of approximation we have (with $s = 0, 1, \cdots, N/2 - 1$)

$$z_s = s\pi + \operatorname{ctn}^{-1}(sa\pi - c)$$

for all roots $z_s > 0$;

$$z_s = -s\pi - \operatorname{ctn}^{-1}(sa\pi + c)$$

for all roots $z_s < 0$.

Let us first calculate k as a function of c.

$$k = (2/L) \sum z_i$$
$$= (2/L) \sum_{s=0}^{N/2-1} \operatorname{ctn}^{-1}(sa\pi - c) - \operatorname{ctn}^{-1}(sa\pi + c)$$

converting the sum to an integral we have

$$k = \frac{2}{La\pi} \int_0^{2k_F/g} [\operatorname{ctn}^{-1}(x - c) - \operatorname{ctn}^{-1}(x + c)]\, dx,$$

which may be written

$$k = -\frac{g}{2\pi} \int_{2k_F/g-c}^{2k_F/g+c} \tan^{-1} u\, du.$$

This integral may be done in closed form, and would provide a transcendental relationship between c and k. Let us, however, focus our attention on the states of small c (and hence small k) which will be the low-lying states of this system. If we approximate the integral for small c we find

$$k = -(gc/\pi) \tan^{-1}(2k_F/g).$$

This small c approximation is internally consistent because the first state of this type occurs when

$$\sum z_i = \tfrac{1}{2}Lk = \pi = -(gLc_1/2\pi) \tan^{-1}(2k_F/g),$$

or when

$$c_1 = \frac{-2\pi^2}{gL \tan^{-1}(2k_F/g)},$$

which means that the first solution of this type occurs when c is small even when $g \to \infty$.

Notice that in the high-density limit we obtain

$$c_1 = -a\pi.$$

The intercept of the line

$$f(z) = az - c_1$$

occurs when

$$z = c_1/a = -\pi,$$

which means that in this limit the first excited state z's occur at the intersections given by the dotted line in Fig. 1. We shall use this fact later to help describe the wavefunction of these states.

Now we must calculate the energy as a function of c.

$$E = (2/L^2) \sum z_i^2$$

and, substituting for the z's we find

$$= \frac{4}{L^2} \sum_{s=0}^{N/2-1} s^2\pi^2 + \frac{4}{L^2} \sum_{s=0}^{N/2-1} s\pi[\operatorname{ctn}^{-1}(sa\pi + c) + \operatorname{ctn}^{-1}(sa\pi - c)] + O(L^{-1}).$$

Again the first term is the energy for a Fermi gas of $N - 1$ particles. We must now calculate the energy shift as a function of c.

$$\Delta E(c) = \frac{4}{L^2} \sum_{s=0}^{N/2-1} s\pi[\operatorname{ctn}^{-1}(sa\pi + c) + \operatorname{ctn}^{-1}(sa\pi - c)].$$

As before we change the sum to an integral

$$\Delta E(c) = \frac{4}{L^2 a^2 \pi} \int_0^{2k_F/g} [x \operatorname{ctn}^{-1}(x + c) + x \operatorname{ctn}^{-1}(x - c)]\, dx.$$

This integral also can be done in closed form, but the closed form result is difficult to interpret. We use a power series expansion in c to obtain the excitation spectrum in a simpler form which applies where c (and k also) is small. To zeroth order in c we of course obtain the expression to the energy shift which was calculated in the previous section.

It is also easy to see that the first order term in c vanishes. The second order term in c is

$$\Delta E_2(c) = \frac{8c^2}{L^2a^2\pi}\int_0^{2k_F/g}\frac{x^2\,dx}{(1+x^2)^2}$$
$$= \frac{4c^2}{L^2a^2\pi}\left[\tan^{-1}\frac{2k_F}{g} - \frac{2k_F}{g}\Big/\left(1+\frac{4k_F^2}{g^2}\right)\right].$$

Now we eliminate c in favor of the total momentum of the state.

$$\Delta E_2(k) = \frac{k^2\pi}{4}\tan^{-1}\frac{2k_F}{g} - \frac{2k_F}{g}\Big/\left(1+\frac{4k_F^2}{g^2}\right)$$
$$\times\,[\tan^{-1}(2k_F/g)]^{-2}$$

Thus the energy of these excitations is quadratic in the total momentum, which means that we can identify an effective mass for these excitations from the relation $\Delta E = 1/2m^*k^2$. Thus the effective mass of these excitations is

$$m^* = \frac{2}{\pi}\left[\tan^{-1}\frac{2k_F}{g}\right]^2\left[\tan^{-1}\frac{2k_F}{g} - \frac{2k_F}{g}\Big/\left(1+\frac{4k_F^2}{g^2}\right)\right]^{-1}.$$

For weak interactions (high density) $m^* = 1$, the effective mass is thus just the mass of one of the elementary fermions. For strong interactions (low density) the mass becomes infinite and the energy is independent of the total momentum of the state, as would be anticipated because of the Fermi-like nature of the wavefunction in the strong interaction limit.

VI. DISCUSSION OF THE WAVEFUNCTION OF THE SYSTEM

In order to describe the nature of the wavefunction we must return to the rules for the calculation of the wavefunction. The amplitude for the basic plane wave in region 1 is

$$(12\cdots N)_1 = -2ie^{iz_i}\sin z_i.$$

The amplitude for this plane wave in any other region is some phase shift times this amplitude. If we ask for the relative probability that we can associate the wavenumber k_1 with particle 1 in region 1 the answer is

$$|(12\cdots N)_1|^2 = 4\sin^2 z_i.$$

Since the amplitudes in region 1 differ from the coefficients in all other regions by only a phase shift, the probability that we can associate wavenumber k_1 with particle 1 is independent of the region. Thus the relative probability that we can associate k_n with particle 1 is

$$|(n\cdots)|^2 = 4\sin^2 z_n = P(z_n).$$

Notice that this number is of order unity when z_n is near $n\pi/2$ and small when z_n is near $n\pi$.

In the ground state all of the z_n satisfy the relation

$$az_n = \operatorname{ctn} z_n,$$

thus

$$\sin^2 z_n = \frac{1}{1+\operatorname{ctn}^2 z_n} = \frac{1}{1+a^2z_n^2} = \frac{1}{1+4k_n^2/g^2}$$

hence

$$P(k) = g^2/(\tfrac{1}{4}g^2 + k^2).$$

Thus, without attempting the formidable task of a Fourier transformation, we have the rough interpretation that the different particle has relative probability $P(k)$ to occupy any momentum state within the Fermi sea.

The excited states may be shown, by the same line of reasoning, to represent translations of this probability by an amount K. That is the excited state occupation probability is

$$P(k, K) = g^2/[\tfrac{1}{4}g^2 + (k-K)^2].$$

Thus the different particle tries to drop to the center of the Fermi sea, but the interaction makes it advantageous for the particle to distribute itself about zero momentum in momentum space. The normalized distribution would tend to a delta function of k as g tends to zero and becomes uniform when $g \gg 2k_F$. From the calculation of the allowable values of the constant we see that the excited states correspond to giving the different particle some average velocity, and the excitation energy is proportional to the square of that velocity. The effective mass of the particle is, however, increased by the interaction.

VII. PAIR CORRELATIONS IN THE GROUND STATE

As a final example of the calculations which may be made on this exactly soluble problem we consider ground-state pair correlations. The most interesting question is to ask the relative probability to find any one of the spin-up particles in the vicinity of the spin-down particle. We will try to calculate

$$\rho(x_1, x_2) = \int\cdots\int dx_3\cdots dx_N$$
$$\times\,\psi^*(x_1\cdots x_N)\,\psi(x_1\cdots x_N).$$

We choose x_2 arbitrarily, since all of the spin-up particles are indistinguishable.

Let $|345\cdots N|$ denote the Slater determinant

$$\begin{vmatrix} e^{ik_3x_3} & e^{ik_3x_4} & e^{ik_3x_5} \\ e^{ik_4x_3} & e^{ik_4x_4} & \cdot \\ e^{ik_5x_3} & e^{ik_5x_4} & \cdot \end{vmatrix}.$$

We may now write the wavefunction as

$$\Psi = [(12\cdots N)_1 e^{i(k_1x_1+k_2x_2)} + (21\cdots N)_1 e^{i(k_2x_1+k_1x_2)}] \times |345\cdots N| + [(312\cdots N)_1 e^{i(k_3x_1+k_1x_2)} + (12\cdots N)_1 e^{i(k_1x_1+k_3x_2)}] |245\cdots N| + \cdots$$

in the region $x_1 < x_2, x_3; x_4 \cdots x_N \leq x_1 + L$. If we now form $\Psi^*\Psi$ and integrate over all of the x's but x_1 and x_2 each of the Slater determinants are orthogonal in the large volume limit, because they represent Fermi wavefunctions of different energy. Furthermore each of these Slater determinants have the same normalization.

We can simplify our calculation of the pair correlations if we make no attempt to keep track of the normalization of the wavefunctions and choose some convenient normalization after we have the form of the correlation function. If we agree to calculate the correlation function in an unnormalized form we see from the argument above that the entire dependence on x_1 and x_2 may be calculated considering only the sum of the contributions for each pair of k's assigned to particles 1 and 2. A particular elementary contribution would be

$$f_{12}(x_1, x_2) = |(12\cdots N)_1|^2 + |(21\cdots N)_1|^2 + (12\cdots N)_1(21\cdots N)_1^* e^{i(k_1-k_2)(x_1-x_2)} + (21\cdots N)_1(12\cdots N)_1^* e^{-i(k_1-k_2)(x_1-x_2)},$$

which is only a function of $x_1 - x_2$, as expected. Let us now calculate the unnormalized correlation function by putting in the explicit values of the amplitudes obtained from the wavefunction rules. If we let $x = x_1 - x_2$ we obtain

$$f(x) = \sum_{s>t}\sum f_{st} = \sum_{s>t}^{N}\sum [4\sin^2 z_s + 4\sin^2 z_t - 4\, e^{iz_s} e^{-iz_t} \sin z_s \sin z_t\, e^{i(k_s-k_t)x} - 4\, e^{-iz_s} e^{iz_t} \sin z_s \sin z_t\, e^{-i(k_s-k_t)x}],$$

where the sums are understood to be over occupied states of z. This sum may be rearranged so as to read

$$f(x) = 4N \sum_{s=1}^{N} \sin^2 z_s - 4 \left| \sum_{s=1}^{N} e^{iz_s} \sin z_s\, e^{ik_s x} \right|^2.$$

Again we use our large-volume formulas for the z's in the ground state

$$z_s^+ = s\pi + \operatorname{ctn}^{-1} sa\pi, \qquad s = 0, 1, \cdots, N/2 - 1,$$

$$z_s^- = -s\pi - \operatorname{ctn}^{-1} sa\pi, \qquad s = 0, 1, \cdots N/2 - 1.$$

Making this substitution into the first term of f leads to

$$f_1 = 4N \sum_{s=1}^{N} \sin^2 z_s = 8N \sum_{s=0}^{N/2-1} \frac{1}{(sa\pi)^2 + 1} = \frac{8N}{a\pi} \int_0^{2k_F/g} \frac{1}{y^2+1}\, dy = \frac{8N}{a\pi} \tan^{-1} \frac{2k_F}{g}.$$

Now we calculate the second term, making use of the relation

$$k_s = 2z_s/L$$

$$f_2(x) = 4 \left| \sum_{s=0}^{N/2-1} e^{iz_s^+} \sin z_s^+ \exp 2iz_s^+ \frac{x}{L} + \sum_{s=0}^{N/2-1} e^{iz_s^-} \sin z_s^- \exp 2iz_s^- \frac{x}{L} \right|^2,$$

substituting for the z_s

$$= 4 \left| \sum_{s=0}^{N/2-1} \frac{1}{sa\pi - i} \exp 2i \frac{x}{L} (s\pi + \operatorname{ctn}^{-1} sa\pi) - \sum_{s=0}^{N/2-1} \frac{1}{sa\pi + i} \exp -2i \frac{x}{L} (s\pi + \operatorname{ctn}^{-1} sa\pi) \right|^2.$$

The term in the exponential which involves the inverse cotangent is negligible to order $1/L$. We may thus write a single sum

$$f_2(x) = 4 \left| \sum_{s=-N/2+1}^{N/2-1} \frac{1}{sa\pi - i} \exp 2is\pi \frac{x}{L} \right|^2,$$

which may be converted to the integral

$$f_2(x) = \frac{4}{a^2\pi^2} \left| \int_{-2k_F/g}^{2k_F/g} \frac{1}{y - i} e^{\frac{1}{2}igxy}\, dy \right|^2.$$

finally we may write the normalized correlation function

$$\rho(x) = 1 - f_2(x)/f_1 = 1 - [(8k_F/g) \tan^{-1} (2k_F/g)]^{-1} Q^*(x)Q(x),$$

where

$$Q(x) = \int_{-2k_F/g}^{2k_F/g} \frac{1}{y - i} e^{\frac{1}{2}igxy}\, dy.$$

This entire calculation of the ground-state pair correlation function has assumed that we are in region 1 where $x_1 < x_2$ or $x < 0$. If we were to calculate the same function in region 2 where $x > 0$, we would find that we would have the reflection of this function about the point $x = 0$. This is not difficult to show from the rules for calculating the wavefunction in region 2. We must recognize, however, that this explicit form of the correlation func-

tion requires that $x < 0$. This requirement on x implies that any contour integration must be closed so that Im $y < 0$ which excludes the pole at $y = i$.

The function Q may be written in terms of tabulated functions, but these functions are not particularly familiar, so let us discuss first the low- and high-density limits.

For low density ($g \to \infty$), y may be neglected in comparison to i over the entire range of integration and one obtains

$$= 1 - ([8k_F/g \cdot 2k_F/g]^{-1}) \left| i \int_{-2k_F/g}^{2k_F/g} e^{\frac{1}{2}igxy}\, dy \right|^2$$

$$= 1 - (16k_F 2/g^2)^{-1} \, |4i \sin k_F x/gx|^2.$$

$$= 1 - |(\sin k_F x)/k_F x|^2$$

This result again would be anticipated from the work of Girardeau, since this is just the one dimensional analog of the "Fermi hole." In the opposite extreme ($g \to 0$) we may approximate

$$Q = -2i \cdot \int_{2k_F/g}^{\infty} \sin(\tfrac{1}{2}gxy)/y \, dy = 2i \cdot si(k_F x)$$

which leads to

$$\rho = 1 - (g/k_F\pi)[si(k_F x)]^2$$

The complete form of Q in terms of the most generally available tabulated function[5] is

$$Q(x) = i^{-1} e^{\frac{1}{2}gx}[E_1([g/2 - ik_F]x) - E_1([g/2 + ik_F]x)],$$

where

$$E_1(z) = \int_z^{\infty} \frac{e^u}{u}\, du.$$

Figure 2 shows a plot of this correlation function in the two extreme cases.

As one would expect, the stronger the potential the more the ground-state pair correlation deviates from background. As a measure of the depth of the deviation from background we can calculate the value of the pair correlation function where $x = 0$.

$$Q(0) = \int_{-2k_F/g}^{2k_F/g} \frac{1}{y - i}\, dy$$

$$= 2i \tan^{-1} 2k_F/g;$$

thus,

$$\rho(0) = 1 - (g/2k_F) \tan^{-1}(2k_F/g).$$

The width deviation from background may be estimated by calculating the first zero of $Q(x)$. This first zero is found to lie between $k_F x = 1.927^+$ (small-strength limit) and $k_F x = \pi$ (large-strength limit). Thus as the strength of the interaction decreases the deviation from the background becomes shallower and narrower.

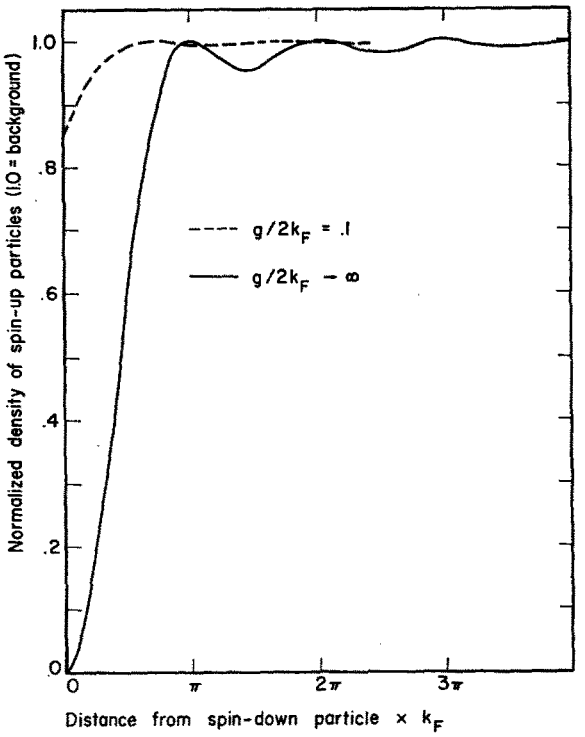

FIG. 2. Normalized ground-state pair correlation functions.

VIII. DISCUSSION OF RESULTS

The introduction of a single spin-down fermion into a Fermi sea of $N - 1$ spin-up fermions has been shown to cause an energy shift which depends upon the interaction strength. It is always true, however, that the total ground-state energy of the N particles lies between the ground-state energies of N and $N - 1$ fermions of the same spin in the same size box. Therefore it is an energetic advantage to have one of the spins reversed. It has been shown to be more of an advantage to reverse the spin of two particles,[6] and in fact the ground state of the system with N particles should have $N/2$ spin-up and $N/2$ spin-down. It is hoped that the results of this paper will provide some sort of a first step towards solving this important problem.

In a subsequent paper we will extend our results to the case of an attractive potential which is considerably more complicated, and also more interesting because of the presence of a bound state.

[5] *Tables of the Exponential Integral for Complex Arguments* (National Bureau of Standards Applied Mathematics Series), (U. S. Government Printing Office, Washington, D. C., 1958), Vol. 51.

[6] E. Lieb and D. Mattis, Phys. Rev. 125, 164 (1962).

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Statistical Ensembles of Complex, Quaternion, and Real Matrices

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Statistical ensembles of complex, quaternion, and real matrices with Gaussian probability distribution, are studied. We determine the over-all eigenvalue distribution in these three cases (in the real case, under the restriction that all eigenvalues are real). We also determine, in the complex case, all the correlation functions of the eigenvalues, as well as their limits when the order N of the matrices becomes infinite. In particular, the limit of the eigenvalue density as $N \to \infty$ is constant over the whole complex plane.

INTRODUCTION

In order to obtain a theoretical description of highly excited regions of heavy-nuclei spectra, several authors[1-6] have developed a theory of statistical matrix ensembles. The energy levels are the eigenvalues of the Hamiltonian H, which is regarded as an Hermitian matrix of very large order N. In the absence of any precise knowledge of H, one assumes a reasonable probability distribution for its matrix elements, from which one deduces statistical properties of its spectrum. An important simplification followed the introduction of unitary instead of Hermitian matrix ensembles.[4] However, the physical origin of the problem—more precisely, the need to interpret part of the spectrum of a matrix as part of the energy spectrum of a physical system—has restricted the attention to matrix ensembles whose spectrum is contained in a one-dimensional line of the complex plane (the real axis for Hermitian, the unit circle for unitary matrices). In the present paper we study the eigenvalue distributions of matrix ensembles for which any point of the complex plane may belong to the spectrum. Apart from the intrinsic interest of the problem,[6] one may hope that the methods and results will provide further insight in the cases of physical interest or suggest as yet lacking applications.

The definition of matrix ensembles consists of two parts:

(1) The definition of an algebraic set of matrices Z. We shall consider: C, complex $N \times N$ matrices; Q, quaternion $N \times N$ matrices; R, real $N \times N$ matrices. The order is that of increasing difficulty. These are the Z's of Dyson's classification (Ref. 5, especially Theorem 7) and they can be characterized as the only irreducible matrix algebras over the real field [Refs. 5, 7 (especially Chap. 3)].

(2) The choice of a measure or probability distribution on Z. Z is a finite-dimensional vector space over the real field. The linear measure $d\mu_L$ which suggests itself naturally, is not suited for a probabilistic interpretation, for the measure of the whole space is infinite. We choose instead

$$d\mu(S) = d\mu_L(S) \exp\left[-(1/4a^2) \operatorname{Tr} S^\dagger S\right] \qquad (0.1)$$

(S generic element of Z, a = real positive constant) which satisfies the two properties:

(i) It is invariant under the adjoint representation of Z_U, where Z_U is the group of unitary matrices in Z. More precisely, for any $U \in Z_U$,

$$d\mu(S) = d\mu(U^\dagger S U).$$

(ii) The matrix elements of S are statistically independent.

These two properties are likely to determine $d\mu(S)$ uniquely.[2] We study the three matrix ensembles thus obtained Z_C, Z_Q, and Z_R in Secs. 1, 2, and 3, respectively, with decreasing success. We obtain for Z_C the over-all eigenvalue distribution and all the correlation functions of n eigenvalues ($1 \leq n \leq N$); for Z_Q the over-all eigenvalue distribution only; for Z_R the over-all eigenvalue distribution in the restrictive case where all eigenvalues are real.

1. COMPLEX MATRICES

Z is the algebra of complex $N \times N$ matrices $S = (S_{ij})$. The linear measure is defined by

$$d\mu_L(S) = \prod_{i,j} dS_{ij}\, dS_{ij}^*, \qquad (1.1)$$

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where $dz\,dz^*$ means $2\,dx\,dy$ if $z = x + iy$, $z^* = x - iy$. $d\mu(S)$ is defined by (0 − 1).

From now on, we take $4a^2 = 1$. We define the eigenvalue distribution $P_N(z_1, \cdots, z_N)$ by

$$\int d\mu(S) = P_N(z_1, \cdots, z_N) \prod_{i=1}^{N} dz_i\, dz_i^*, \qquad (1.2)$$

where z_i $(i = 1, \cdots, N)$ are the eigenvalues of the generic element $S \in Z$.

$\int$ means: for fixed (z_i), integration over all other variables. We now compute P_N. Any $S \in Z$ with distinct eigenvalues (we forget matrices with two equal eigenvalues, which form a set of measure 0) can be diagonalized

$$S = XAX^{-1}, \qquad (1.3)$$

where A is diagonal with $A_{ii} = z_i$, and X is regular and is defined modulo multiplication on the right by any element of the commutator $\mathfrak{A}'$ of A. $\mathfrak{A}'$ consists of all complex diagonal matrices. The correspondence $S \to (A, X \bmod \mathfrak{A}')$ is $1 \to N!$ because there are $N!$ ways to order the eigenvalues.

Infinitesimal variations dA, dX of A, X produce a variation dS of S

$$dS = X(dA + [dR, A])X^{-1}, \qquad (1.4)$$

where $dR = X^{-1}dX$. From (1.4) and the invariance property: $d\mu_L(S) = d\mu_L(XSX^{-1})$ for any regular $X \in Z$, we get

$$d\mu_L(S) = \prod_i dz_i\, dz_i^* \prod_{i \neq j} [dR, A]_{ij}[dR, A]_{ij}^*, \qquad (1.5)$$

$$d\mu_L(S) = \prod_i dz_i\, dz_i^* \prod_{i<j} |z_i - z_j|^4 \prod_{i \neq j} dR_{ij}\, dR_{ij}^*. \qquad (1.6)$$

We substitute (1.6) into (1.2) and get

$$P_N(z_1, \cdots, z_N) = \frac{1}{N!} \prod_{i<j} |z_i - z_j|^4 J, \qquad (1.7)$$

where

$$J = \int \prod_{i \neq j} dR_{ij}\, dR_{ij}^* \exp[-\mathrm{Tr}\, S^\dagger S]. \qquad (1.8)$$

$d\mu_0(X) = \prod_{i,j} dR_{ij}\, dR_{ij}^*$ is the invariant measure on the group $Gl(N, C)$ which we note simply $\mathfrak{G}$ and $\prod_{i \neq j} dR_{ij}\, dR_{ij}^*$ is the quotient measure on $\mathfrak{G}/\mathfrak{A}'$ (which is *not* a group). We need the following

Lemma: Any $X \in \mathfrak{G}$ can be written in one and only one way as

$$X = UYV, \qquad (1.9)$$

where U is unitary $(U \in Z_U)$, Y is triangular $(Y_{ij} = 0$ for $i > j)$, and $Y_{ii} = 1$ $(i = 1, \cdots, N)$. The set of the matrices with these two properties is a unimodular subgroup $\mathfrak{Y}$ of $\mathfrak{G}$. V is diagonal with real positive elements. The set of these matrices is also a subgroup $\mathfrak{V}$ of $\mathfrak{G}$.

(In other words, we have decomposed $\mathfrak{G}$ as the product of three subgroups Z_U, $\mathfrak{Y}$, and $\mathfrak{V}$. None of them is invariant and this decomposition has no simple algebraic property. However, it will provide a useful decomposition of $d\mu_0(X)$.

Proof: Any set X^α $(\alpha = 1, \cdots, N)$ of N linearly independent vectors can be brought by a unitary change of basis into a form where the components X_j^α satisfy $X_j^\alpha = 0$ for $j > \alpha$. We apply this to the column vectors of X and obtain $X = U_1Y_1$ with U_1 unitary and Y_1 triangular. Y_1 can then be written as $Y_1 = U_0YV$ with Y and V as above and U_0 diagonal and unitary. Therefore $X = UYV$ with $U = U_1U_0$. If now $X = UYV = U'Y'V'$, then $B = U'^{-1}U = Y'V'V^{-1}Y^{-1}$ is unitary (left-hand side) and triangular with real positive diagonal elements (right-hand side); therefore $B = 1$, and the decomposition is unique.

We now change the variables in $d\mu_0(X)$ from dR to dU, dY, dV. We start from

$$dR = X^{-1}\,dX = V^{-1}\,dV + V^{-1}Y^{-1}\,dY\,V + V^{-1}Y^{-1}U^{-1}\,dU\,YV. \qquad (1.10)$$

The first term contributes to the real part of the diagonal elements; The second term, to the dR_{ij} with $i < j$. In the third term, $dL = -iU^{-1}dU$ is Hermitian. From $Y \in \mathfrak{Y}$, $Y^{-1} \in \mathfrak{Y}$ it follows that, for $i \geq j$,

$$(Y^{-1}\,dL\,Y)_{ij} = dL_{ij} + (\text{linear combination of } dL_{kl} \text{ with } k - l > i - j). \qquad (1.11)$$

It follows from these remarks that

$$d\mu_0(X) = d\mu_0(U)\, d\mu_0(Y)\, d\mu_0(V), \qquad (1.12)$$

where

$$d\mu_0(U) = \prod_{i>j} dL_{ij}\, dL_{ij}^* \prod_i dL_{ii} = \prod_{i,j} dL_{ij}, \qquad (1.13)$$

$$d\mu_0(Y) = \prod_{i<j} (Y^{-1}\,dY)_{ij}(Y^{-1}\,dY)_{ij}^*, \qquad (1.14)$$

$$d\mu_0(V) = \prod_i (2V_{ii}^{-1}\,dV_{ii}), \qquad (1.15)$$

are the invariant measures on Z_U, $\mathfrak{Y}$, and $\mathfrak{V}$ respectively. We need the quotient measure on $\mathfrak{G}/\mathfrak{A}'$,

$$\prod_{i \neq j} dR_{ij}\, dR_{ij}^* = d\mu_0(\mathfrak{G})/d\mu_0(\mathfrak{A}'). \qquad (1.16)$$

$\mathfrak{A}'$ is the direct product of $\mathfrak{V}$ and the group $\mathfrak{U}_0$ of unitary diagonal matrices, with

$$d\mu_0(\mathfrak{A}') = d\mu_0(\mathfrak{U}_0)\, d\mu_0(\mathfrak{V}). \qquad (1.17)$$

We now come back to (1.8). From (1.3)

$$\operatorname{Tr} S^\dagger S = \operatorname{Tr} A^\dagger H A H^{-1}, \tag{1.18}$$

where H should be $X^\dagger X$. But V commutes with A and therefore disappears, as expected, which enables us to take $H = Y^\dagger Y$. We then get from (1.8), (1.12), (1.16)

$$J \int d\mu_0(\mathfrak{U}_0) = \int \exp\left[-\operatorname{Tr} S^\dagger S\right] d\mu_0(U)\, d\mu_0(Y) \tag{1.19}$$

or

$$J = \frac{\Omega_U}{(2\pi)^N} \int \exp\left[-\operatorname{Tr} S^\dagger S\right] d\mu_0(Y), \tag{1.20}$$

where $(2\pi)^N$ is the volume of $\mathfrak{U}_0$ and $\Omega_U = \int d\mu_0(U)$ is the volume of Z_U. We next perform a last change of variables from Y to H. Any $n \times n$ upper left block Y_n of any $Y \in \mathfrak{Y}$ has determinant 1. This implies that the jacobian of the transformation from $(dY)_{ij}$ to $(Y^{-1}dY)_{ij}$ is 1. Therefore

$$d\mu_0(Y) = \prod_{i<j} dY_{ij}\, dY_{ij}^*. \tag{1.21}$$

H is defined by $H = Y^\dagger Y$ or more explicitly

$$\begin{cases} H_{ij} = Y_{ij} + \sum_{k<i} Y_{ki}^* Y_{kj} & \text{for } i < j, \\ H_{ij} = Y_{ji}^* + \sum_{k<j} Y_{ki}^* Y_{kj} & \text{for } i > j. \end{cases} \tag{1.22}$$

Each $n \times n$ upper left block H_n of H can be defined by $H_n = Y_n^\dagger Y_n$. Therefore $\det Y_n = 1$ determines the diagonal elements of H_n by the condition $\det H_n = 1$. Each diagonal element of H is then defined (by induction) as a polynomial with integer coefficients in the nondiagonal elements.

It follows immediately from (1.22) that the correspondence $Y \to H$ is one to one and that

$$d\mu_0(Y) = \prod_{i<j} dH_{ij}\, dH_{ij}^* = \prod_{i \neq j} dH_{ij}. \tag{1.23}$$

We now perform the integration over H in N steps; each one consists of integrating over the variables of the last row and column of H, and brings back to the original problem for matrices of order smaller by one unit, obtained from the original ones by removing the last row and column. The proof rests on a recursion formula which we now derive:

Let H', A', etc. be the relevant matrices of order n; H, A the matrices of order $n-1$, more precisely the $(n-1) \times (n-1)$ upper left blocks of H', A'. Greek (Latin) indices run from 1 to n $(n-1)$. From $\det H' = 1$, it follows that $H'^{-1}_{\beta\alpha} = \Delta'_{\alpha\beta}$, where $\Delta'_{\alpha\beta}$ is the minor (α, β) of H'. Similarly $H^{-1}_{ij} = \Delta_{ij}$, where Δ_{ij} is the minor (ij) of H. Now let

$$\phi_n = \operatorname{Tr} S'^\dagger S' = \operatorname{Tr} A'^\dagger H' A' H'^{-1} = \sum_{\alpha\beta} H'_{\alpha\beta} z_\alpha^* z_\beta \Delta'_{\alpha\beta}. \tag{1.24}$$

We separate the last row and column; let $e = (e_i)$, $i = 1, \cdots, n-1$, where $e_i = H'_{in}$. Then

$$\phi_n = |z_n|^2 H'_{nn} - z_n \sum_{i,k} e_i z_i^* e_k^* \Delta_{ik} - z_n^* \sum_{i,k} e_i^* z_i e_k \Delta_{ki} + \sum_{i,j,k,l} H_{ij} z_i^* z_j (H'_{nn} \Delta_{ij} - e_i^* e_k \Delta_{ij}^{kl}), \tag{1.25}$$

where Δ_{ij}^{kl} is the minor of H obtained by removing the rows i, k and the columns j, l. From $\det H' = \det H = 1$, we get

$$H'_{nn} = 1 + \sum_{k,l} e_k^* e_k \Delta_{kl}. \tag{1.26}$$

Substituting in (1.26) and using the elementary identity

$$\Delta_{ij}^{kl} = \Delta_{ij}\Delta_{kl} - \Delta_{il}\Delta_{kj}, \tag{1.27}$$

we get, after straightforward algebra,

$$\phi_n = |z_n|^2 + \phi_{n-1} + \langle e^* |\, H^{-1}(A^\dagger - z_n^*) H (A - z_n) H^{-1} \,| e \rangle, \tag{1.28}$$

where

$$\langle e^* |\, B \,| e \rangle = \sum_{k,l} e_k^* B_{lk} e_k. \tag{1.29}$$

We now substitute (1.28) for $n = N$ into (1.20) and get

$$J = \frac{\Omega_U}{(2\pi)^N} \int \exp\left[-|z_N|^2 - \phi_{N-1}\right] \times \prod_{i<j\leq N-1} dH_{ij}\, dH_{ij}^* \int \prod_{i=1}^{N-1} de_i\, de_i^* \times \exp\left[-\langle e^* |\, H^{-1}(A^\dagger - z_N^*) H (A - z_N) H^{-1} \,| e \rangle\right]. \tag{1.30}$$

The last integration is straightforward and gives

$$(2\pi)^{N-1} \left[\prod_1^{N-1} |z_i - z_N|^2\right]^{-1}.$$

The same procedure can be repeated N times and gives

$$J = \Omega_U (2\pi)^{N(N-3)/2} \left[\prod_{i<j} |z_i - z_j|^2\right]^{-1} \times \exp\left[-\sum_{i=1}^N |z_i|^2\right]. \tag{1.31}$$

Ω_U is easily computed.[4] With the normalization

(1.13), we get

$$\Omega_U = (2\pi)^{N(N+1)/2}/1!2!\cdots(N-1)!. \tag{1.32}$$

(1.31), (1.32), and (1.7) then give

$$P_N(z_1, \cdots, z_N) = \frac{(2\pi)^{N(N-1)}}{1!2!\cdots N!} \prod_{i<j} |z_i - z_j|^2 \times \exp\left[-\sum |z_i|^2\right]. \tag{1.33}$$

P_N is normalized according to

$$\int P_N(z_1, \cdots, z_N) \prod_i dz_i\, dz_i^* = \int d\mu(S) = (2\pi)^{N^2}, \tag{1.34}$$

which follows from (0.1) and (1.2) by direct computation. This suggests to define

$$\hat{P}_N(z_1, \cdots, z_N) = [1!2!\cdots N!(2\pi)^N]^{-1} \prod_{i<j} |z_i - z_j|^2 \times \exp\left[-\sum |z_i|^2\right] \tag{1.35}$$

with the normalization

$$\int \hat{P}_N(z_1, \cdots, z_N) \prod dz_i\, dz_i^* = 1. \tag{1.36}$$

We next determine the n-eigenvalue correlation functions which are defined (Ref. 4) by

$$\rho_N(z_1, \cdots, z_n) = \frac{N!}{(N-n)!} \int \hat{P}_N(z_1, \cdots, z_N) \prod_{i=n+1}^{N} dz_i\, dz_i^*, \tag{1.37}$$

and normalized according to

$$\int \rho_N(z_1, \cdots, z_n) \prod_{i=1}^{n} dz_i\, dz_i^* = \frac{N!}{(N-n)!}. \tag{1.38}$$

Now

$$\prod_{i<j} (z_i - z_j) = \det(z_i^{j-1}) = \sum_{\Pi} (-)^{\Pi} z_1^{p_1-1} \cdots z_N^{p_N-1} \tag{1.39}$$

where Π is the permutation $(1, \cdots, N) \to (p_1, \cdots, p_N)$. Each term of the expansion of the right-hand side is multiplied, in P_N, by a similar term in z^*, and integrated over $N - n$ variables $z_i = r_i e^{i\theta_i}$ in $\rho_N(z_1, \cdots, z_n)$. The angular integration gives zero except if every z_i over which one integrates occurs with the same power p_i' as the complex conjugate z_i^*. The subsequent integration on r_i then gives

$$\int_0^\infty d(r^2)(r_i^2)^{p'_i} \exp(-r_i^2) = p_i'!.$$

From this remark and from (1.35), (1.37), $\rho_N(z_1, \cdots, z_N)$ is obtained as follows:

Choose a set of $N - n$ exponents (p_i'), i.e., $N - n$ integers between 0 and $N - 1$, which are to be distributed among the integration variables $z_{n+1}, \cdots, z_N$.

Distribute them among these variables, which gives a factor $(N - n)!$ and cancels the corresponding factor in (1.37).

Integrate over the $N - n$ angles θ_i $(i = n + 1, \cdots, N)$, which gives a factor $(2\pi)^{N-n}$.

Integrate over the $N - n$ variables $|z_i| = r_i$, which gives one factor $p_i'!$ for each p_i' and cancels the corresponding factor in $\hat{P}_N$.

Distribute the remaining set of exponents (p_i) [i.e., the n integers between 0 and $N - 1$ not taken as (p_i')] among $z_1, \cdots, z_n$ and $z_1^*, \cdots, z_n^*$ separately.

Sum over all possible such distributions, after multiplying by the two sign factors which come from the expansion of the original determinants.

Sum over all possible partitions of $(0, \cdots, N - 1)$ into the two families (p_i) and (p_i').

Note that $N!$ in the definition of ρ_N cancels $1/N!$ in the definition of $\hat{P}_N$. We then get

$$\rho_N(z_1, \cdots, z_n) = \frac{1}{(2\pi)^n} \exp\left[-\sum_{i=1}^{n} |z_i|^2\right] \det(D_{ij}), \tag{1.40}$$

where

$$D_{ij} = \sum_{p=0}^{N-1} \frac{(z_i z_j^*)^p}{p!} \quad (i, j = 1, \cdots, n). \tag{1.41}$$

When $N \to \infty$, the correlation functions tend to well-defined limits

$$\rho(z_1, \cdots, z_n) = \frac{1}{(2\pi)^n} \times \exp\left[-\sum_{1}^{n} |z_i|^2\right] \det[\exp(z_i z_j^*)]. \tag{1.42}$$

We now consider in some detail the eigenvalue density in the complex plane

$$\rho_N(z) = \frac{1}{2\pi} \exp[-|z|^2] \sum_{p=0}^{N-1} \frac{|z|^{2p}}{p!}. \tag{1.43}$$

Its limit for $N \to \infty$ is a constant: $\rho(z) = \rho = 1/2\pi$. $\rho_N(z)$ is normalized according to $\int \rho_N(z)\, dz\, dz^* = N$. One verifies directly that each term in the last sum in (1.43) contributes 1 to this integral. $\rho_N(z)$ is invariant by rotation around the origin, as was obvious from the symmetry of the problem. Let $r = |z|$. The last sum in (1.43) is the beginning of the expansion of $\exp r^2$ in powers of r^2. Therefore, for $r^2 \ll N$, $\rho_N(z) \simeq \rho$ and for $r^2 \gg N$, $\rho_N(z) \simeq 0$. More precisely, elementary bounds on the expo-

nential series give

$$1 - 2\pi\rho_N(z) \leq \exp(-r^2)\frac{r^{2N}}{N!}\frac{N+1}{N+1-r^2} \quad \text{for } r^2 \leq N, \tag{1.44}$$

$$2\pi\rho_N(z) \leq \exp(-r^2)\frac{r^{2N}}{N!}\frac{N}{r^2+1-N} \quad \text{for } r^2 \geq N. \tag{1.45}$$

For $r = N^{\frac{1}{2}} \pm u$, $0 \leq u \lesssim 1 \ll N$, the leading term in the right-hand side of (1.44) and (1.45) is $\exp(-2u^2)/2u(2\pi)^{\frac{1}{2}}$. This gives a sharp fall of $\rho_N(z)$ from ρ to 0 when r varies in an interval of order 1 around $N^{\frac{1}{2}}$. As a consequence, the number of eigenvalues in the "tail" of the distribution, defined as

$$\delta N = \int_{|z|>N^{\frac{1}{2}}} \rho_N(z)\, dz\, dz^* \tag{1.46}$$

is proportional to $N^{\frac{1}{2}}$. More precisely $\delta N \simeq (N/2\pi)^{\frac{1}{2}}$ for $N \gg 1$.

Electrostatic Analogy

The electrostatic model introduced by Wigner[8] and Dyson[4] can be extended to the present case. Consider N unit charges in a two-dimensional space, which is taken as the complex plane of the variable z. The positions of the charges are $z_1, \cdots, z_N$. Suppose that the charges move in an harmonic oscillator potential $\frac{1}{2}|z|^2$ centered at the origin. Then the potential energy of the system is

$$U(z_1, \cdots, z_N) = -\sum_{i<j} \log|z_i - z_j| + \frac{1}{2}\sum_i |z_i|^2. \tag{1.47}$$

The probability distribution of the positions $z_1, \cdots, z_N$ when this Coulomb gas is in thermodynamical equilibrium at the temperature T is proportional to $\exp[-\beta U(z_1, \cdots, z_N)]$ (where $\beta = 1/kT$). For $\beta = 2$ this is proportional to P_N.

Therefore the distribution of eigenvalues of a random matrix $S \in Z_C$ is identical with the distribution of the positions of charges of a two-dimensional Coulomb gas in an harmonic oscillator potential, at a temperature corresponding to $\beta = 2$.

2. QUATERNION MATRICES

Z is now the algebra Z_Q of $N \times N$ Q matrices, i.e., matrices with coefficients in the quaternion field Q. Q can be represented as a two-dimensional complex vector space.[9] This representation associates to any $N \times N$ Q matrix a $2N \times 2N$ complex matrix. The image of matrices in Z_Q are characterized by

$$\zeta T = T^*\zeta, \tag{2.1}$$

where * means complex conjugate and ζ is a direct sum of N 2×2 blocks of the form $\left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$. (These matrices are quaternion real in Dyson's notations.[4]) The group Z_U of unitary matrices in Z is characterized by (2.1) and $T^\dagger T = 1$, and satisfies therefore also $T^{\mathrm{T}}\zeta T = \zeta$, where $^{\mathrm{T}}$ means transposed. Z_U is the symptectic group $Sp(N)$. Let $S \in Z_Q$. We first look for eigenvalues of S in Q, i.e., for $\lambda \in Q$ and vectors $v \in Q^N$ such that $Sv = v\lambda$. (The product of a vector $\in Q^N$ by a scalar λ is the product by λ on the right.[9]) Now,

Lemma: If $\lambda \in Q$ is an eigenvalue of S, then $\mu^{-1}\lambda\mu$ is also an eigenvalue of S for any $\mu \neq 0$, $\mu \in Q$. In fact,

$$Sv = v\lambda \quad \text{implies} \quad S(v\mu) = v\mu(\mu^{-1}\lambda\mu). \tag{2.2}$$

Therefore the eigenvalues of S in Q constitute orbits, each of which is the set of quaternions obtained from one $\lambda \in Q$ by the internal automorphisms $\lambda \to \mu^{-1}\lambda\mu$ (which are simply three-dimensional rotations of the imaginary part). Consider now a subspace of Q isomorphic to $\mathbf{C}$. This subspace intersects every orbit in two points which are complex conjugate in $\mathbf{C}$ (this means simply that in the three-dimensional space of purely imaginary quaterernions, we consider the intersection of a sphere with one of its diameters), and these two points determine the orbit completely. Therefore all possible information on the eigenvalues of a Q matrix in Q can be obtained from the eigenvalues in a subspace $\mathbf{C}$ of Q.

From now on we use only the $2N \times 2N$ complex representation of the matrices of Z_Q, and study their (complex) eigenvalues in the ordinary sense. One verifies directly the above mentioned result, namely that due to (2.1), the eigenvalues of any $S \in Z_Q$ are 2×2 complex conjugate. For if $Sv = zv$, $z \in \mathbf{C}$, $v \in \mathbf{C}^{2N}$, then $\zeta Sv = \zeta zv$, or $S(\zeta v^*) = z^*(\zeta v^*)$. Moreover, the eigenvector associated with z^* can be taken to be ζv^*. We shall need the following

Lemma: If $S \in Z_Q$, and if all eigenvalues of S are distinct, then $S = XAX^{-1}$, where $X, A \in Z_Q$, and A is diagonal.

In fact, S can be diagonalized as a complex matrix. One can take A as a direct sum of 2×2

[8] E. P. Wigner, Proc. 4th Can. Math. Cong., Toronto, 1959, p. 174.

[9] C. Chevalley, *Lie Groups* (Princeton University Press, Princeton, New Jersey, 1946).

blocks

$$\begin{pmatrix} z_i & 0 \\ 0 & z_i^* \end{pmatrix}, \qquad (i = 1, \cdots, N).$$

Therefore $A \in Z_Q$. The column vectors of X are the eigenvectors X^α of S. One can take $X^{2n} = \zeta(X^*)^{2n-1}$ $(n = 1, \cdots, N)$, which is equivalent to $X \in Z_Q$.

We now define measures on Z_Q. The linear measure is

$$d\mu_L(S) = \prod_{i,j} dS_{ij}. \tag{2.3}$$

[Note that because of (2.1), the factors in (2.3) are 2×2 complex conjugate.]

$$d\mu(S) = d\mu_L(S) \exp\left[-\tfrac{1}{2} \operatorname{Tr} S^\dagger S\right]. \tag{2.4}$$

The coefficient $\frac{1}{2}$ is intended to achieve greater similarity with the previous case and to compensate for the artificial doubling of the dimension of the matrices.

P_N is defined by (1.2). The first step in its calculation is the same as previously and leads to

$$d\mu_L(S) = \prod_{i=1}^{N} |z_i - z_i^*|^2 \prod_{i<j} |z_i - z_j|^4 |z_i - z_j^*|^4 \times \prod_{i=1}^{N} dz_i\, dz_i^* \prod_{i \neq j} dR_{ij} \tag{2.5}$$

with $dR = X^{-1}dX$, and therefore to

$$P_N(z_1, \cdots, z_N) = \left(\frac{1}{N!2^N}\right) \prod_{i=1}^{N} |z_i - z_i^*|^2 \times \prod_{i<j} |z_i - z_j|^4 |z_i - z_j^*|^4 J, \tag{2.6}$$

where now

$$J = \int \prod_{i \neq j} dR_{ij} \exp\left[-\tfrac{1}{2} \operatorname{Tr} S^\dagger S\right]. \tag{2.7}$$

The factor 2^N in (2.6) comes from the exchanges $z_i \leftrightarrow z_i^*$. $d\mu_0(X) = \prod_{i,j} dR_{ij}$ is the invariant measure on the group $\mathcal{G}$ of regular elements in Z_Q and $\prod_{i \neq j} dR_{ij}$ is the quotient measure on $\mathcal{G}/\mathcal{C}'$ where $\mathcal{C}'$ is the commutator of A in Z_Q. Any $X \in \mathcal{G}$ can be decomposed as previously as a product $X = UYV$ where U is unitary, Y is triangular ($Y_{ij} = 0$ for $i > j$) and satisfies $Y_{ii} = 1$, and V is diagonal with real positive elements. Moreover, it follows from $\zeta X = X^*\zeta$ that

$$B = Y^*V\zeta V^{-1}Y^{-1} = U^{*-1}\zeta U \tag{2.8}$$

is unitary and antisymmetric (right-hand side), and has nonzero elements only in 2×2 blocks along the diagonal (comparison of both sides). From this and the condition $V_{ii} > 0$, it follows easily that $B = \zeta$. Therefore $U \in Z_U (\subset Z_Q)$. It then follows that Y and V belong to Z_Q. In particular,

$$V_{2i-1,2i-1} = V_{2i,2i}$$

and

$$Y_{2i,2i-1} = Y_{2i-1,2i} = 0 \quad (i = 1, \cdots, N).$$

The same argument as previously then leads to

$$J = \frac{\Omega_S}{(2\pi)^N} \int \exp\left[-\frac{1}{2} \operatorname{Tr} S^\dagger S\right] d\mu_0(Y), \tag{2.9}$$

where Ω_S is the volume of the symplectic group and is defined by

$$\Omega_S = \int_{Z_U} d\mu_0(U) = \int \prod_{i \leq j} (iU^T\zeta\, dU)_{ij} \tag{2.10}$$

and

$$d\mu_0(Y) = \prod (Y^{-1}\, dY)_{ij} = \prod dY_{ij}, \tag{2.11}$$

where the product extends over the elements $i < j$, $(i, j) \neq (2k - 1, 2k)$ for $k = 1, \cdots, N$. We next change the integration variables from Y to $H = Y^\dagger Y$. Then

$$d\mu_0(Y) = \prod dH_{ij}, \tag{2.12}$$

where $\prod$ has the same meaning as in (2.11). We integrate over H in N steps as previously. We first derive a recursion formula analogous to (1.28). H', A', etc. now denote matrices of order $2n$, Δ' are the minors of H'. H, A are the $2(n-1) \times 2(n-1)$ upper left blocks of H', A'. Δ are the minors of H. From $H' \in Z_Q$ and $H' = Y'^\dagger Y'$, it follows that the 2×2 diagonal blocks of H' have the form

$$\begin{pmatrix} h_i & 0 \\ 0 & h_i \end{pmatrix}.$$

In particular,

$$H'_{2n-1,2n-1} = H'_{2n,2n} = h_n.$$

Let

$$e = (e_i), \quad e' = (e'_i) \quad [i = 1, \cdots 2(n-1)]$$

where $e_i = H'_{i,2n-1}$ and $e'_i = H'_{i,2n}$. Then

$$e' = \zeta e^*. \tag{2.13}$$

The diagonal elements of H' are defined by the condition that all upper left blocks of H' have determinant one. In particular,

$$h_n = 1 + \sum_{i,j} e_i^* e_i \Delta_{ij}, \tag{2.14}$$

$$h_n = 1 + \sum_{k,l} e_l^{*\prime} e'_k (h_n \Delta_{kl} - \sum_{i,j} e_j^* e_i \Delta_{ij}^{kl}). \tag{2.15}$$

(2.14) defines h_n and (2.14), (2.15) give an identity between e, e', and Δ.

$$\sum_{k,l} (e_l^* e_k - e_l'^* e_k') \Delta_{kl} = \sum_{i,j,k,l} e_l'^* e_k' e_j^* e_i (\Delta_{ij}\Delta_{kl} - \Delta_{ij}^{kl}). \quad (2.16)$$

Now from (2.13) and $H^{-1} \in Z_Q$, it follows easily that

$$\langle e^{*\prime}| H^{-1} |e'\rangle = \langle e^*| H^{-1} |e\rangle, \quad (2.17)$$

$$\langle e^{*\prime}| H^{-1} |e\rangle = -(\langle e^*| H^{-1} |e'\rangle)^*. \quad (2.18)$$

The notation is that of (1.29). From (2.17), (2.18), and $H_{ij}^{-1} = \Delta_{ij}$, it follows that both sides of (2.16) are zero, and (2.16) reduces to

$$\langle e^{*\prime}| H^{-1} |e\rangle = \langle e^*| H^{-1} |e'\rangle = 0. \quad (2.19)$$

Let now

$$\phi_n = \mathrm{Tr}\, A'^{\dagger} H' A' H'^{-1}.$$

We separate the last two rows and columns of the various matrices by applying (1.28) twice.

$$\phi_n = \phi_{n-1} + 2|z_n|^2 + \langle e^*| U |e\rangle + \langle e^{*\prime}| V |e'\rangle, \quad (2.20)$$

where

$$U = H^{-1}(A^{\dagger} - z_n^*) H (A - z_n) H^{-1} \quad (2.21)$$

and

$$V_{ik} = \sum [|z_n|^2 - z_n z_l' - z_n^* z_k'^*][h_n \Delta_{kl} - e_j^* e_i \Delta_{ij}^{kl}] - \sum z_i'^* z_j' H_{ij} [h_n \Delta_{ij}^{kl} - \Delta_{ij}^{ef} e_f^* e_e - (\Delta_{ij} h_n - \Delta_{ij}^{ef} e_f^* e_e)\Delta_{kl}] + (z_i'^* z_n + z_n^* z_j') e_j^* e_i (\Delta_{ij}^{kl} - \Delta_{ij}\Delta_{kl}) \quad (2.22)$$

(summation over all indices e, f, i, j).

In (2.22) some terms have cancelled out because of (2.16), (2.19), and the z_i' $[i = 1, \cdots, 2(n-1)]$ are the $(z_1, z_1^*, z_2, z_2^*, \cdots, z_{n-1}, z_{n-1}^*)$ in that order. We next substitute (2.14) into (2.22). After some straightforward algebra involving repeated use of (2.13), (2.17), (2.19), (1.27) and its analogue for

$$\Delta_{ij}^{ef},$$

the terms of fourth order in e, e' cancel out and we get

$$\phi_n = \phi_{n-1} + 2|z_n|^2 + 2\langle e^*| U |e\rangle. \quad (2.23)$$

The integration over e runs exactly as in the complex case and gives after N successive steps

$$J = \Omega_S (2\pi)^{N(N-2)} \Big[\prod_{i<j\leq N} |z_i - z_j|^2 |z_i - z_j^*|^2\Big]^{-1} \times \exp\Big[-\sum_{i=1}^{N} |z_i|^2\Big]. \quad (2.24)$$

Ω_s is easily computed.[4] With the normalization (2.10), we get

$$\Omega_S = (2\pi)^{N(N+1)}/1!3!\cdots(2N-1)!. \quad (2.25)$$

(2.6), (2.24), and (2.25) give

$$P_N(z_1, \cdots, z_N) = [(2\pi)^{N(2N-1)}/2^N N!1!\cdots(2N-1)!] \times \exp\Big[-\sum_1^N |z_i|^2\Big] \times \prod_{i=1}^{N} |z_i - z_i^*|^2 \prod_{i<j\leq N} |z_i - z_j|^2 |z_i - z_j^*|^2. \quad (2.26)$$

P_N is normalized according to

$$\int P_N(z_1, \cdots, z_N) \prod dz_i\, dz_i^* = (2\pi)^{2N}, \quad (2.27)$$

which follows from (2.4) and (1.2) by direct computation. By analogy with (1.35), we define

$$\hat{P}_N(z_1, \cdots, z_N) = [(4\pi)^N N!1!3!\cdots(2N-1)!]^{-1} \times \exp\Big[-\sum_1^N |z_i|^2\Big] \times \prod_{i=1}^{N} |z_i - z_i^*|^2 \prod_{i<j\leq N} |z_i - z_j|^2 |z_i - z_j^*|^2, \quad (2.28)$$

which is normalized according to (1.36).

The determination of the correlation functions appears to be considerably more difficult than in the complex case, and the electrostatic interpretation of P_N breaks down.

3. REAL MATRICES

Z is now the algebra of real $N \times N$ matrices $S = (S_{ij})$. The linear measure is

$$d\mu_L(S) = \prod_{i,j} dS_{ij}. \quad (3.1)$$

The eigenvalues of S now consist of ν complex-conjugate pairs $(0 \leq 2\nu \leq N)$ and $q = N - 2\nu$ real numbers: $z_{2i} = Z_{2i-1}^*$ for $i = 1, \cdots, \nu$ and z_i real for $i > 2\nu$.

We define $P_N^{\nu}(z_1, \cdots, z_N)$ by

$$\int f\, d\mu(S) = P_N^{\nu}(z_1, \cdots, z_N) \prod_{i=1}^{N} dz_i \quad (3.2)$$

where f has the same meaning as in (1.2).

Any S with distinct eigenvalues can be diagonalized: $S = XAX^{-1}$. A is diagonal with $A_{ii} = z_i$. X is regular. Its first 2ν column vectors X^{α} are 2×2 complex conjugate and the last q are real:

$$X^{2j} = (X^{2j-1})^* \quad \text{for} \quad 1 \leq j \leq \nu$$

and

$$X^j = X^{j*} \quad \text{for} \quad j > 2\nu. \quad (3.3)$$

X is defined modulo multiplication on the right by any element of the group $\mathfrak{W}$ of diagonal matrices W which satisfy:

$$W_{2j,2j} = W^*_{2j-1,2j-1} \quad \text{for} \quad 1 \leq j \leq \nu$$

and

$$W_{jj} = W^*_{jj} \quad \text{for} \quad j > 2\nu.$$

The correspondence $S \to (A, X \bmod \mathfrak{W})$ is $1 \to \nu!(N - 2\nu)!2^\nu$. From (1.4) we get

$$d\mu_L(S) = \prod_i dz_i \prod_{i \neq j} [dR, A]_{ij}, \tag{3.4}$$

where $dR = X^{-1}dX$ or

$$d\mu_L(S) = \prod_i dz_i \prod_{i<j} |z_i - z_j|^2 \prod_{i \neq j} dR_{ij}. \tag{3.5}$$

Therefore

$$P^\nu_N(z_1, \cdots, z_N) = [\nu!(N - 2\nu)!2^\nu]^{-1} \prod_{i<j} |z_i - z_j|^2 J, \tag{3.6}$$

where

$$J = \int \prod_{i \neq j} dR_{ij} \exp [-\mathrm{Tr}\, S^\dagger S]. \tag{3.7}$$

We define a measure on the set $\mathfrak{X}$ of the X which satisfy (3.3) by

$$d\mu_0(X) = \prod_{i,j} dR_{ij}; \tag{3.8}$$

$\mathfrak{X}$ is not a group. However the relation: $X_1 \simeq X_2$ iff $X_1^{-1}X_2 \in \mathfrak{W}$ is an equivalence relation in $\mathfrak{X}$. We pick one element X_0 in each class. Then any $X \in \mathfrak{X}$ can be written as $X = X_0 W$ in one and only one way. Then

$$dR = X^{-1}\, dX = W^{-1}\, dW + W^{-1}X_0^{-1}\, dX_0\, W \tag{3.9}$$

implies

$$d\mu_0(X) = d\mu_0(W) \prod_{i \neq j} dR_{ij}, \tag{3.10}$$

where

$$d\mu_0(W) = \prod_{j=1}^{N} (W^{-1}\, dW)_{jj}$$

is the invariant measure on $\mathfrak{W}$. $\mathfrak{W}$ is the direct product of the subgroup $\mathfrak{U}_0 \subset \mathfrak{W}$ of matrices U_0 which satisfy

$$(U_0)_{2j-1,2j-1} = (U_0)^*_{2j,2j} = e^{i\theta_j} \quad \text{for} \quad 1 \leq j \leq \nu$$

and

$$(U_0)_{jj} = \pm 1 \quad \text{for} \quad j > 2\nu$$

and the subgroup $\mathfrak{V}$ of real positive matrices $V \in \mathfrak{W}$:

$$V_{2j,2j} = V_{2j-1,2j-1} \quad \text{for} \quad 1 \leq j \leq \nu,$$

$$V_{jj} > 0 \quad \text{for} \quad 1 \leq j \leq N.$$

Furthermore,

$$d\mu_0(W) = d\mu_0(V)\, d\mu_0(U_0), \tag{3.1}$$

where

$$d\mu_0(U_0) = \prod_{j=1}^{\nu} d\theta_j, \tag{3.12}$$

$$d\mu_0(V) = \prod_{j=1}^{\nu} 2V^{-1}_{2j,2j}\, dV_{2j,2j} \prod_{j=2\nu+1}^{N} V^{-1}_{jj}\, dV_{jj} \tag{3.13}$$

are the invariant measures on $\mathfrak{U}_0$ and $\mathfrak{V}$.

Note also that the sum over the ± 1 of the $N - 2\nu$ last diagonal elements of $\mathfrak{U}_0$ will result in a factor $2^{N-2\nu}$ in the volume of this group.

We next introduce a representation where only real matrices appear. Let ξ be the unitary matrix

$$\xi = \bigoplus_1^\nu \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \oplus I_{N-2\nu} \tag{3.14}$$

where $\oplus$ means direct sum. Then $X' = X\xi$ is real. Furthermore

$$d\mu_0(X') = \prod_{i,j} (X'^{-1}\, dX')_{ij} = d\mu_0(X). \tag{3.15}$$

X' can be written in one and only one way as $X' = OYV'$ where O, Y, V' are real, O is orthogonal (proper or not), Y is triangular (i.e., $Y_{ij} = 0$ for $i > j$) with $Y_{ii} = 1$, and V' is real > 0 and diagonal. Then it follows from

$$X'^{-1}\, dX' = V'^{-1}\, dV' + V'^{-1}Y^{-1}\, dY\, V' + V'^{-1}Y^{-1}(O^{-1}\, dO)YV' \tag{3.16}$$

and from (3.15) that

$$d\mu_0(X) = d\mu_0(O)\, d\mu_0(Y)\, d\mu_0(V') \tag{3.17}$$

where

$$d\mu_0(O) = \prod_{i<j} (O^{-1}\, dO)_{ij}, \tag{3.18}$$

$$d\mu_0(Y) = \prod_{i<j} (Y^{-1}\, dY)_{ij} = \prod_{i<j} dY_{ij}, \tag{3.19}$$

$$d\mu_0(V') = \prod_i V'^{-1}_{ii}\, dV'_{ii}. \tag{3.20}$$

V' can be decomposed in one and only one way as $V' = VT$ where $V \in \mathfrak{V}$ and

$$T = \bigoplus_1^\nu \begin{pmatrix} t_j & 0 \\ 0 & 1/t_j \end{pmatrix} \oplus I_{N-2\nu} \tag{3.21}$$

with

$$d\mu_0(V') = d\mu_0(V)\, d\mu_0(T), \tag{3.22}$$

where $d\mu_0(V)$ is defined in (3.13) and

$$d\mu_0(T) = \prod_{j=1}^{\nu} dt_j/t_j.$$

We now come back to (3.7). Now $\mathrm{Tr}\ S^\dagger S = \mathrm{Tr}\ A^\dagger H A H^{-1}$, where H should be $X^\dagger X = \xi X'^\dagger X' \xi^\dagger$. However, due to $X' = OYVT$ and the fact that V commutes with both ξ and A, one can take $H = \xi H' \xi^\dagger$, where

$$H' = TY^\dagger YT \tag{3.23}$$

depends only on Y and T. We now introduce in (3.7) an extra integration over $\mathfrak{U}_0$ and make use of (3.10), (3.11), (3.17), and (3.22). We obtain

$$J = \frac{\Omega_0}{(2\pi)^\nu 2^{N-2\nu}} \times \int \exp\left[-\mathrm{Tr}\ S^\dagger S\right] d\mu_0(Y)\, d\mu_0(T), \tag{3.24}$$

where Ω_0 is the volume of the full orthogonal group and $(2\pi)^\nu 2^{N-2\nu}$ is the volume of $\mathfrak{U}_0$. Now it follows from (3.23) that

$$d\mu_0(Y) = \prod_{i<j} dY_{ij} = \prod_{i<j} d(Y^\dagger Y)_{ij} = \prod_{i<j} dH'_{ij}, \tag{3.25}$$

the Jacobian of the last transformation being $(\det T)^{2\nu-1} = 1$. Finally,

$$J = \frac{\Omega_0}{(2\pi)^\nu 2^{N-2\nu}} \times \int \exp\left[-\mathrm{Tr}\ S^\dagger S\right] \prod_{i<j} dH'_{ij} \prod_{j=1}^{\nu} dt_j/t_j. \tag{3.26}$$

It follows from (3.23) that the $2j-1 \times 2j-1$ (or $2j \times 2j$) upper left blocks of H' have determinant t_j^2 (or 1) for $j = 1, \cdots, \nu$ and that the $j \times j$ upper left blocks have determinant 1 for $j \geq 2\nu$. Independent variables are therefore the H'_{ij} with $i < j$, or $i = j = 2k-1$ for $k = 1, \cdots, \nu$. The other diagonal elements of H' are determined in term of them by the previous condition.

We now come back to the original complex representation and express the differential element in (3.26) in terms of H alone. One can replace $\prod dH'_{ij}$ by the corresponding $\prod dH_{ij}$ except perhaps for the first 2×2 blocks along the diagonal.

If $\left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right)$ is the jth such block in H', the corresponding block in H is $\left(\begin{smallmatrix} u & \zeta \\ \zeta^* & \mu \end{smallmatrix}\right)$, where $u = \frac{1}{2}(a+c)$, $\zeta = \frac{1}{2}(a-c) + ib$. From (3.23) it follows that $a = t_j^2 a'$ and $c = t_j^{-2} c'$, where a', c' depend only on Y, as well as b. In particular, for fixed Y:

$$2\frac{dt_j}{t_j} = \frac{da}{a} = -\frac{dc}{c} = \frac{d(a-c)}{a+c}.$$

The contribution of this 2×2 block to the differential element in (3.26) is then easily seen to be $db\, dt_j/t_j = d\zeta\, d\zeta^*/4u$. Therefore

$$J = \frac{\Omega_0}{2^N(2\pi)^\nu} \int \exp\left[-\mathrm{Tr}\ S^\dagger S\right] d\mu(H), \tag{3.27}$$

where

$$d\mu(H) = \prod_{i<j} dH_{ij} \prod_{j=1}^{\nu} (H_{2j,2j})^{-1}\, dH_{2j,2j-1}. \tag{3.28}$$

We can now integrate over the last $N - 2\nu$ rows and columns of H by the same induction procedure as in Sec. 1. We use (1.28) for $n = N$ (z_n real). The integration over the last row and column is then straightforward and gives a factor

$$\exp\left[-|z_N|^2\right] \pi^{(N-1)/2} \left[\prod_{i<N} |z_N - z_i|\right]^{-1}.$$

After $N - 2\nu$ similar steps, we obtain

$$J = \frac{\Omega_0 \pi^{(N-2\nu)(N+2\nu-1)/4}}{2^N(2\pi)^\nu} \times \left[\prod_{2\nu<i<j\leq N} |z_i - z_j| \prod_{l\leq 2\nu<i} |z_l - z_i|\right]^{-1} \times \exp\left[-\sum_{i>2\nu} |z_i|^2\right] F_\nu(z_1, \cdots, z_{2\nu}), \tag{3.29}$$

where $F_\nu(z_1, \cdots, z_{2\nu})$ is the value of the integral $\int \exp\left[-\mathrm{Tr}\ S^\dagger S\right] d\mu(H)$ when S is a $2\nu \times 2\nu$ matrix *without* real eigenvalues for $\nu > 0$, and $F_0 = 1$. Substituting (3.29) into (3.6), we obtain

$$P_N^\nu(z_1, \cdots, z_N) = \frac{\Omega_0 \pi^{(N-2\nu)(N+2\nu-1)/4}}{\nu!(N-2\nu)!(4\pi)^\nu 2^N} \prod_{i<j} |z_i - z_j| \times \exp\left[-\sum_{i>2\nu} |z_i|^2\right] \prod_{i<j\leq 2\nu} |z_i - z_j|\, F_\nu(z_1, \cdots, z_{2\nu}). \tag{3.30}$$

In particular, for $\nu = 0$, all the eigenvalues are real: $z_i = r_i$ ($i = 1, \cdots, N$),

$$P_N^0(r_1, \cdots, r_N) = \frac{\Omega_0 \pi^{N(N-1)/4}}{2^N N!} \prod_{i<j} |r_i - r_j| \times \exp\left[-\sum_{i=1}^{N} r_i^2\right]. \tag{3.31}$$

For $\nu \neq 0$, F_ν cannot be calculated by the previous method. One can obtain a recursion formula analogous to (1.28), though somewhat less simple. However, the integration over the last two rows and columns of H does not lead to elementary functions as previously and the induction procedure breaks down completely.

Therefore we are able to determine P_N explicitly only in the particular case where all eigenvalues

are real. In the general case, we have extracted the dependence of P_N on the real eigenvalues, and the complex eigenvalues still appear in a factor F, for which we have only an intractable integral representation.

CONCLUSION

The results of our investigation are essentially contained in Eqs. (1.35), (1.40), and (1.42) for the complex case; (2.27) for the quaternion case; (3.30) for the real case. They are remarkably simple in the complex case, where, in particular, the eigenvalue density tends to a constant $\rho_N(z) \to \rho = 1/2\pi$ as $N \to \infty$. The quaternion case involves essentially technical problems. In the real case, however, one meets major difficulties which seem to come from the fact that the real field is not algebraically closed. We have considered here only a restricted class of ensembles. One could generalize by keeping the same algebraic set of matrices and defining other measures $d\mu'$ instead of $d\mu$ defined in (0.1). For instance, if $d\mu'(S) = \mathcal{P}(S)d\mu(S)$, where $\mathcal{P}$ is a polynomial in $\mathrm{Tr}\,(S^r)$ $(r = 1, \cdots, N)$ (if $r' > N$, $\mathrm{Tr}\,S^{r'}$ is a polynomial in $\mathrm{Tr}\,S^r$, $r \leq N$), then nothing is changed in the calculation of P_N, because $\mathcal{P}(S)$ depends only on A. However the induction procedure by which we performed the integration on X (or H) seems to be a very specific property of $\exp[-\mathrm{Tr}\,S^\dagger S]$.

One could also consider other algebraic sets of matrices, for instance Dyson's V ensembles (5) with measures analogous to (0.1). Nothing new appears in the complex case where V is identical with Z. In the real case, V is the set of complex symmetric matrices; the calculation of P_N seems to be extremely complicated, and the simplest case of 2×2 matrices is not encouraging. In the quaternion case, we have not reached any conclusion.

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Self-Consistent Approximations in Many-Body Systems*

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Baym's definition of a self-consistent approximation is rephrased in a more diagrammatic way and compared with formulations of the exact many-body problem of Balian, Bloch, and DeDominicis. It is shown that many of the results of these authors are valid for any self-consistent approximation as defined by Baym.

I. INTRODUCTION

A SIGNIFICANT contribution to the theory of approximations was made by Baym[1] who succeeded in defining, within the language of thermal Green's functions,[2] what he termed a self-consistent approximation (henceforth SCA). Essentially, a SCA is one wherein the (approximate) Gibbs potential is stationary with respect to variation of the (approximate) Green's function. Baym showed[1] that a SCA, i.e., one which satisfies his criterion, possess some interesting properties in the equilibrium case: (i) Various common ways to evaluate the partition function from the one particle Green's function all lead to a self-consistent, i.e., the same, result. (ii) In the zero temperature limit a SCA maintains the Hugenholtz–Van Hove theorem. In this note Baym's definition for a SCA is rephrased in a more diagrammatic way (Sec. II). In this way it is shown that the basic expressions that were established, *a la tour de force*, by the group in Saclay[3] are valid for a SCA. Some of these consequences are listed in Sec. III.

II. DIAGRAMMATIC MEANING OF BAYM'S CRITERION

The Gibbs potential, A, is defined through the grand partition function, Z_G, by

$$Z_G = \exp(-\beta A).$$

The exact A can be expanded into infinite number of terms representable by connected diagrams:

$$A - A_0 = \frac{1}{-\beta}\sum_{p=1}^{\infty}(-)^p \int_{\beta>u_1>\cdots u_p>0} du_1 \cdots du_p \times \langle V(u_1)\cdots V(u_p)\rangle_0, \quad (1)$$

A_0 is the Gibbs potential with no interaction. The rules for evaluating the diagrams are given, for example in Ref. 4. As an example of these rules the contribution of the diagram in Fig. 1 to $A-A_0$ is:

$$\sum_{\substack{p_1p_2p_3\\q_1q_2q_3}} \int_{\beta>u_3>u_2>u_1>0} G_0^>(p_1, u_2-u_1)G_0^>(p_2, u_3-u_2) \times G_0^<(q_2, u_2-u_3)G_0^<(q_1, u_1-u_2) \times G_0^>(p_3, u_3-u_1)G_0^<(q_3, u_1-u_3) \times \langle p_1p_3|\, v\,|q_3q_1\rangle\langle p_2q_1|\, v\,|q_2p_1\rangle\langle q_2q_3|\, v\,|p_3p_2\rangle.$$

Note that a directed line from u to u' going up (down) represents $G_0^>(p, u-u')[G_0^<(p, u-u')]$ where $G_0^{><}$ are the free-particle propagators[2]:

$$G_0^<(p, u-u') = f_p^- \exp[\epsilon_p(u-u')],$$
$$G_0^>(p, u-u') = -f_p^+ \exp[\epsilon_p(u-u')],$$

with $f_p^- = 1 - f_p^+ = \{\exp[\beta(\epsilon_p-\mu)]+1\}^{-1}$. All the notation and symbols are standard (cf. Ref. 2).

It is well known[3,5,6] that the exact $A - A_0$ can be expressed as a functional of the exact Green's function G only (apart from a trivial dependence on β)

$$G = G_0 + G_0\Sigma[G]G,$$

Σ being the exact (proper) self-energy. A diagrammatic derivation of this is given by Bloch.[6] Baym's

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[1] G. Baym, Phys. Rev. **127**, 4, 1391 (1962).

[2] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962).

[3] There are a number of publications by Balian, Bloch, and De Dominicis on this subject. In particular we used explicitly the following: R. Balian, C. Bloch, and C. De Dominicis, Nucl. Phys. **25**, 529, (1961), and their articles in: *Lectures on the Many Body Problem*, edited by E. R. Caianiello (Academic Press Inc., New York and London, 1962). These authors are referred to in the text by BBDD.

[4] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, (translated by R. A. Silverman) (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

[5] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 5, 1417 (1960).

[6] C. Bloch, Physica **26**, 62 (1960).

definition of a SCA is: A SCA is one in which the approximate Gibbs potential $(A - A_0)_A$ can be expressed as a functional of an approximate Green's function, G_A

$$G_A = G_0 + G_0\Sigma[G_A]G_A,$$

the functional being the same as for the corresponding exact case. To see the diagrammatic meaning of this we first construct a functional of G_0 through the following self-evident lemma, where G_0 is given by

$$G_0(u, u') = \begin{cases} G_0^{>}(u, u') & \text{for } u > u'; \\ G_0^{<}(u, u') & \text{for } u < u'. \end{cases}$$

Lemma: A necessary and sufficient condition for a set of skeleton diagrams (i.e., diagrams representing $A - A_0$ with no self-energy insertions) to be a functional of G_0 only, rather than of $G_0^{>}$ and $G_0^{<}$, is: Each diagram in the set must appear with all others (when distinct) obtainable from it by placing the interaction in all relative positions.

A set of diagrams with this property will be referred to as t equivalent. For example the totality of t-equivalent family associated with the diagram of Fig. 1 is given in Fig. 2.

Remark: If the replacement of $G_0^{><}$ by G_0 and integrating over the whole range 0 to β implies the repetition of a given skeleton diagram n times, then each member of its t-equivalent family will be repeated n times upon making the corresponding replacement.

The point of all the above is that if we, in an approximation for $A - A_0$, wish to keep a certain skeleton diagram, we must retain all its t equivalents as well. The reason being that only the whole set can be expressed in terms of G_0 only. This is done by multiplying each diagram of the mth order in the interaction by $1/m!$, [The name "t equivalent" stands for "topologically equivalent" diagrams. In Ref. 4, (p. 131), a more restricted meaning is associated with a t-equivalent family. Here, however, we need not concern ourselves with the possibility of repeated diagrams since each diagram is considered separately and hence we have the factor $1/m!$ for a diagram of the mth order in the potential.

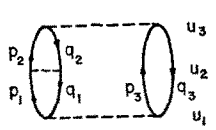

FIG. 1. Diagram referred to in the text.

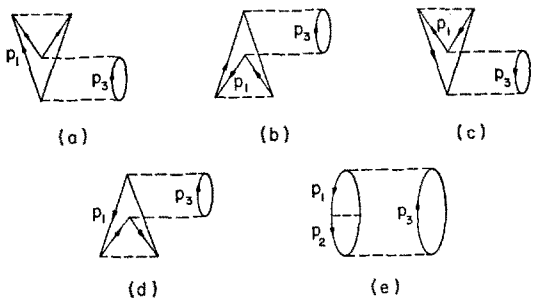

FIG. 2. Diagrams which form a complete t-equivalent family with Fig. 1.

It is convenient to consider together the t-equivalent diagrams in the sense of Ref. 4. In this case, for example, the totals t-equivalent family of Fig. 1 is representable by Fig. 2(a), (b), and (c). The correcting factor now becomes $(m - 1)!/m! = 1/m$. Further simplification is possible by considering together terms in Σ_A (1, 1′) which differ only by the sense of the arrows of the lines attached to the points 1 and 1′. (Remarks pertaining to Hartree–Fock-like terms are omitted here.) For example, Fig. 3 should be considered together with a similar diagram where the line on the top left-hand corner goes up instead of down. With such simplifications the correcting factor becomes $1/2m$; these are implicit in Baym's formalism], replacing all $G_0^{><}$ by G_0 and integrating over the whole range. The approximate self-energy, Σ_A, is dictated by the skeleton diagrams retained in the approximation. For example the diagram of Fig. (1) leads to the terms in Σ_A which are given in Fig. 3. The prescription for evaluating the diagrams for Σ are given, for example, in Ref. 4 and will not be repeated here.

We can now consider composite diagrams, i.e., diagrams with self-energy insertions. Here the prescription is: retain all those and only those diagrams which are built up of our set Σ_A. This defines the approximate Gibbs potential, $(A - A_0)_A$.

To see that the prescription outlined above is equivalent to Baym's definition of SCA we proceed as follows. Consider the set of skeleton diagrams in SCA for $A - A_0$. Replace everywhere $G_0^{><}$ by $G_A^{><}$ the resultant functional is Baym's $\Phi[G_A]$, i.e., it is a "closed" functional with $\delta\Phi[G_A]/\delta G_A = \Sigma_A$. (Note that, by construction, it is a functional of G_A and not of $G_A^{>}$ and $G_A^{<}$ separately.)

$\Phi[G_A]$ contains all[6] the diagrams of $(\log Z_G)_A = -1/\beta(A - A_0)_A$; however each diagram is repeated n_B times where n_B is the number of the proper self-energy terms in the diagram. It can be shown[6] that Luttinger and Ward's[6] expression for the

FIG. 3. One of the self-energy diagrams arising from the diagram of Fig. 1.

logarithm of the partition function [their Eq. (47) which is, in Baym's notation, his Eq. (47)] is obtained upon correcting for overcounting of diagrams. It then easily[6,1] follows that the approximate Gibbs potential is stationary with respect to variation of the approximate Green's function.

We would like to conclude this section with the remark that when the nonequilibrium problem is considered Baym's demand that $G_0(U)$ be a functional of U rather than $G_0(U = 0)$ is a natural extension of the discussion of this section. In either case one requires the functionals Σ and G to depend on the full G_0 of the problem for then, formally, Σ and G are expressible in a sense as a power series in G_0 (This, of course, holds true only for momentum-conserving interactions. In general the expression depends on the potential.) and will follow the latter transformation properties [cf. Baym's Eq. (17)].

III. BBDD FORMULATION

The various remarkable expressions for the Gibbs potential that were obtained by BBDD are valid also in a SCA. To see this one merely notes that BBDD obtained their expression by using the notions of rotated and translated diagrams. A rotated diagram is one obtained from a given diagram by letting the earliest interaction time become the last. For example the diagrams given in Figs. 2(c) and 2(d) are all the rotated diagrams corresponding to Fig. 1. The notion of translated diagrams applies only to composite diagrams; it refers to diagrams obtained from a given diagram by placing the irreducible self-energy parts of a diagram in various relative positions. Clearly for skeleton diagrams the family of rotated diagrams is included in the family of t-equivalent diagrams. In fact it is easy to see that in general a SCA contains automatically the whole family of rotated and translated diagrams if it contains one member thereof.

Since a SCA contains all the rotated and translated diagrams, the techniques developed by BBDD can be applied to it. It then follows, for example, that the time integration can be carried out and the various expansions for the Gibbs potential obtained by BBDD for the exact problem are valid for a SCA. Some of the results of BBDD which are valid for any SCA are listed below. (It is, perhaps, of interest that items 1 through 3 can be formulated under less restrictive conditions then SCA requires.)

(1) The four distinct expansions for the Gibbs potential given, e.g., by Balian[3] are valid for any SCA.

(2) The Gibbs potential factorizes into terms which involve Goldstone-like diagrams, i.e., wherein the Green's function lines of a given momenta go either up or down. In other words for a SCA the so called anomalous diagrams[5] can be eliminated.

(3) Hugenholz–Van Hove theorem is valid for a SCA (e.g., the DeDominicis article in Ref. 3.)

(4) Physical quantities such as average energy, particle number, and entropy can be expressed in terms of the "true" occupation number N_k. N_k being given by $N_k = G_A(k; t, t^+)$.

(5) The Lee–Yang theorem viz:

$$\delta A/\delta N_k = 0, \qquad \delta^2 A/\delta N_k \delta N_{k'} > 0$$

is valid for SCA.

(6) The Landau theory of Fermi liquid is derivable in a SCA. [BBDD do not consider transport coefficients in their formulation of Landau's theory. What is meant here by Landau's theory is the possibility of expressing the Gibbs potential and the physical quantities (viz., entropy, energy, number of particles, and momenta) in terms of a distribution function F_k. The latter has the property of becoming a step function in the limit of zero temperature. The relation between these expressions and Landau's theory is discussed in Ref. 2. Note that BBDD derivation is complicated by the nonuniqueness of F_k however their argument as such can be carried over for a SCA.]

IV. REMARKS AND SUMMARY

The notion of rotated diagrams is associated with the trace character of the Gibbs potential.[3] Retention of families of rotated diagrams in an approximation preserves this property. Retention of translated diagrams in effect enables one to consider $G(k; u, u')$ as a functional of $G^{(0)}(k; u, u')$.

Baym's condition for a SCA is more demanding than an approximation that could be inferred from the above. A SCA implies transformation properties for the self-energy and the Green's function from those obtained for the free-particle Green's function.[1] From the point of view of this note this is traceable to the possibility of replacing in an approximation, the integrals of Eq. 1 by integrals over the whole time range (with a factor $1/p!$, of course). This, in turn, comes from the fact that all $V(u)$ in the equation are the same function. The retention in a SCA of

this property is equivalent to satisfying a necessary condition for the existence of a model Hamiltonian[7] that will reproduce the approximation; however we were unable, so far, to formulate a sufficient condition for this.

To summarize: It was argued in this note that the requirement for a SCA implies that BBDD formalism can be applied; the connection between their approach and Baym's was used to show that a SCA possesses a number of remarkable properties.

[7] Model Hamiltonians which reproduce the well-known approximations were considered by R. H. Kraichnan, J. Math. Phys. 3, 3, 475 (1962).

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Some Recent Developments in Invariant Imbedding with Applications

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(Received 13 August 1964)

A summary of some recent developments in the theory of invariant imbedding is presented. Applications to some simple problems in wave propagation, diffusion theory, and transport theory demonstrate some of the advantages of the new and almost "mechanistic" approach. In addition, a slightly different attack is applied to nonlinear difference equations and to the classical phase-shift problem.

I. INTRODUCTION

A PREVIOUS review[1] of the method of "invariant imbedding" described the subject as it existed in 1959. Since then, considerable progress has been made in understanding the method and in extending its areas of applicability. Some of the development (up to 1961) is briefly sketched in the last chapter of Wing,[2] some has appeared in the various journals, and some is as yet unpublished. The purpose of this new review of the subject is to make some of these developments more readily accessible.

During these past few years the method of invariant imbedding (or the method of invariance) has progressed from a semi-intuitive particle counting technique to a rather straightforward, almost mechanical, analytical device. Indeed it may be thought of as simply a perturbation technique wherein it is the "size" of the system that is being perturbed. In place of the original problem, we consider a *family* of problems generated by a single parameter, the parameter being the "size" of our original problem. The family provides a means of advancing gradually from the solution for one member, usually degenerate, to the solution of the given problem. Most generally this "bridge" between the known and the desired solution takes the form of a differential or integrodifferential equation.

To illustrate the more recent invariant imbedding techniques we begin in Sec. II with a simple problem described by a pair of linear differential equations. These may, if one chooses, be thought of as the mathematical description of a one-dimensional transport process. From such a point of view the earlier "particle counting" technique can be employed, but since that method has been thoroughly described elsewhere,[1,2] we discuss instead several other devices which have nothing to do with the "physics" of the problem. They enable one to derive the invariant imbedding equations directly from the mathematical description of the problem by purely mathematical analysis. One obvious advantage of such a procedure is that the derivation can quite easily be made rigorous.

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† This work was supported by the U. S. Atomic Energy Commission.
[1] R. Bellman, R. Kalaba, and G. M. Wing, J. Math. Phys. 1, 280 (1960).
[2] G. M. Wing, *An Introduction to Transport Theory* (John Wiley & Sons, Inc., New York, 1962). (This book contains an extensive bibliography which we shall refrain from referring to in detail.)

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To summarize: It was argued in this note that the requirement for a SCA implies that BBDD formalism can be applied; the connection between their approach and Baym's was used to show that a SCA possesses a number of remarkable properties.

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In Sec. II we also consider variants of the boundary conditions and briefly extend some of the ideas to higher-order systems.

The techniques of Sec. II are applied in Sec. III to several examples from the theory of wave propagation, diffusion theory, and transport theory. The examples show the considerable unification provided by the new approaches.

The final chapter, involving consideration of the phase shift problem and of difference equations, might have been included as a part of Sec. III. However, the approach is slightly different from that used earlier. Further, the application to the phase shift problem shows clearly how far-reaching the imbedding concept really is.

Since our purpose is to stress the new concepts, ideas, and applications, no effort is made towards presenting a rigorous development of the material. Although occasionally a reference is cited where such a development can be found, we give here only formal mathematical arguments.

Finally, we assume that the reader is fairly familiar with the contents of Ref. 1. For that reason there is no great effort made to describe in detail why one seeks certain functions or what the potential advantages of the invariant imbedding method may be.

II. MATHEMATICAL DEVELOPMENT

A. A Simple System of Linear Differential Equations

We start by considering the system of differential equations

$$\begin{aligned} du(z)/dz &= a(z)u(z) + b(z)v(z), \\ -dv(z)/dz &= c(z)u(z) + d(z)v(z), \quad 0 \leq z \leq x, \end{aligned} \tag{2.1}$$

$$u(0) = 0, \qquad v(x) = 1. \tag{2.2}$$

If, as sometimes happens, we are not really interested in the functions $u(z)$, $v(z)$ in the interior $0 < z < x$ but only in their values at the ends, namely $u(x)$, $v(0)$, we can employ the ideas of invariant imbedding. We begin by considering the family of problems generated by the parameter x, the "size" of our problem. Denoting the solutions to this family of problems by $u(z, x)$, $v(z, x)$ to make clear the x dependence, our goal is to find the quantities $u(x, x)$ and $v(0, x)$.

If one regards the system (2.1) as the mathematical formulation of a transport problem in one dimension, then $u(z, x)$ is the flux of particles to the right at z and $v(z, x)$ is the flux to the left at z due to a steady unit input at x. The condition $u(0, x) = 0$ implies that no particles enter the system at the left end. With this interpretation one can use the "particle counting" technique to obtain a differential equation for the function $R(x) = u(x, x)$, the flux of particles leaving the system at the right end ("reflected" flux), and another differential equation for the function $T(x) = v(0, x)$, the flux leaving the system at the left end ("transmitted" flux). This method, described in great detail in numerous places,[1,2] obtains the "invariant imbedding" equations for $R(x)$ and $T(x)$ by an analysis of the physical transport problem itself rather than from the mathematical formulation (2.1).

However there is a considerable advantage in beginning with (2.1) since such questions as existence and uniqueness can then be dealt with in routine mathematical fashion. Bearing in mind the physical model that (2.1) represents—namely a rod extending from $z = 0$ to $z = x$ experiencing unit flux input at the right end—we consider the material from $z = 0$ to $z = x - \Delta$ as a subrod which experiences a flux input at its right end of strength $v(x - \Delta, x)$. We proceed to relate $R(x)$ and $R(x - \Delta)$.

Rewrite (2.1) in finite difference form as

$$\begin{aligned} u(z, x) &= u(z - \Delta, x) \\ &\quad + \Delta[a(z)u(z, x) + b(z)v(z, x)] + o(\Delta), \\ v(z - \Delta, x) &= v(z, x) \\ &\quad + \Delta[c(z)u(z, x) + d(z)v(z, x)] + o(\Delta). \end{aligned} \tag{2.3}$$

Putting $z = x$, and remembering the boundary conditions, we get

$$\begin{aligned} R(x) &= u(x - \Delta, x) \\ &\quad + \Delta[a(x)R(x) + b(x)] + o(\Delta), \\ v(x - \Delta, x) &= 1 + \Delta[c(x)R(x) + d(x)] + o(\Delta). \end{aligned} \tag{2.4}$$

Now since the system (2.1) is linear, it follows that the flux $u(x - \Delta, x)$ from the subrod due to an input at its right end of strength $v(x - \Delta, x)$ is equal to $v(x - \Delta, x)$ times the flux of such a rod due to a unit input. Thus,

$$\begin{aligned} u(x - \Delta, x) &= v(x - \Delta, x)u(x - \Delta, x - \Delta) \\ &= v(x - \Delta, x)R(x - \Delta). \end{aligned} \tag{2.5}$$

Putting (2.5) in (2.4) and eliminating $v(x - \Delta, x)$ between the two equations gives

$$\begin{aligned} R(x) &= R(x - \Delta)\{1 + \Delta[c(x)R(x) + d(x)] + o(\Delta)\} \\ &\quad + \Delta[a(x)R(x) + b(x)] + o(\Delta), \end{aligned} \tag{2.6}$$

which leads to

$$dR(x)/dx = b(x) + [a(x) + d(x)]R(x) + c(x)R^2(x) \quad (2.7)$$

upon taking the limit as $\Delta \to 0$. Evidently the boundary condition $u(0, x) = 0$ implies that

$$R(0) = 0. \quad (2.8)$$

Equation (2.7) gives directly the value of the reflected flux from the right end due to a unit input without the necessity of finding the fluxes u and v in the interior of the rod. Only the integration of an initial value problem is required. For further discussion, see Refs. 1 and 2.

A moment's reflection concerning the above derivation of (2.7) shows that the physical model served as only a relatively superfluous "crutch." This suggests a completely analytical treatment based on a perturbation of the parameter x, first described in Bellman.[3] We do not give the details of that method here since it in turn soon led to another purely analytical device which is simple, easy to apply, and relatively easy to justify mathematically in a wide variety of circumstances. The method is illustrated by rederiving (2.7). We proceed formally, of course, referring the reader to Bailey[4] for an account of how such matters as existence and uniqueness can be dealt with.

Using subscripts in the customary way to denote differentiation we rewrite (2.1) as

$$\begin{aligned} u_1(z, x) &= a(z)u(z, x) + b(z)v(z, x), \\ -v_1(z, x) &= c(z)u(z, x) + d(z)v(z, x), \end{aligned} \quad (2.9)$$

$$u(0, x) = 0, \qquad v(x, x) = 1. \quad (2.10)$$

Since $R(x) = u(x, x)$, it follows by differentiating that

$$R'(x) = u_1(x, x) + u_2(x, x). \quad (2.11)$$

Now our goal is to express the right side of this equation in terms of known functions and, possibly, R itself. Evidently this can be done for the first term $u_1(x, x)$ by using the first of (2.9) evaluated at $z = x$, remembering the boundary condition $v(x, x) = 1$. We have, namely,

$$u_1(x, x) = a(x)R(x) + b(x). \quad (2.12)$$

As for the second term on the right side of (2.11), we obtain it by noticing that u_2, v_2 satisfy the same differential equations as do u, v but with a slightly different boundary condition at x. For if we differentiate (2.9) and (2.10) with respect to x we get

$$\begin{aligned} u_{21}(z, x) &= a(z)u_2(z, x) + b(z)v_2(z, x), \\ -v_{21}(z, x) &= c(z)u_2(z, x) + d(z)v_2(z, x), \end{aligned} \quad (2.13)$$

$$u_2(0, x) = 0, \qquad v_2(x, x) = -v_1(x, x). \quad (2.14)$$

Our problem (2.9) being linear, it follows that u_2, v_2 are just multiples of u, v. Thus,

$$\begin{aligned} u_2(z, x) &= -v_1(x, x)u(z, x), \\ v_2(z, x) &= -v_1(x, x)v(z, x). \end{aligned} \quad (2.15)$$

In particular,

$$\begin{aligned} u_2(x, x) &= -v_1(x, x)R(x) \\ &= [c(x)R(x) + d(x)]R(x), \end{aligned} \quad (2.16)$$

by (2.9). Using (2.12) and (2.16) in (2.11) gives (2.7) as before.

The differential equation for $T(x) = v(0, x)$ can be obtained in similar straightforward fashion. Just differentiate,

$$T'(x) = v_2(0, x), \quad (2.17)$$

and use (2.15) with $z = 0$, followed by (2.9) with $z = x$. Thus

$$\begin{aligned} T'(x) &= -v_1(x, x)T(x) \\ &= [c(x)R(x) + d(x)]T(x). \end{aligned} \quad (2.18)$$

The initial condition for T is

$$T(0) = 1. \quad (2.19)$$

B. "Input" Prescribed at Both Ends

Of course there is no compelling reason to restrict our attention to the particular boundary conditions (2.2). Obviously we could handle in exactly the same way the boundary conditions $u = 1$ at the left end and $v = 0$ at the right. In that case we would use x to represent the *left* end of the interval instead of the right, and correspondingly we would obtain differential equations for a left-end reflection function and transmission function. And since the differential equations (2.1) are linear, the "output" corresponding to an arbitrary "input" $u = a$ at the left end and $v = b$ at the right is simply some linear combination of the two reflection and two transmission functions. We omit the details.

C. More General Boundary Conditions

A rather different kind of boundary condition for the system (2.1),

$$u(0) = 0, \qquad u(x) = 1, \quad (2.20)$$

[3] R. Bellman and R. Kalaba, Proc. Nat. Acad. Sci. 47, 336 (1961).

[4] P. Bailey, J. Math. & Anal. Appl. 8, 144 (1964).

is of considerable interest. The reason for this is obvious when (2.1) is rewritten in the form

$$d^2u(z)/dz^2 + A(z)\,du(z)/dz + B(z)u(z) = 0. \quad (2.21)$$

Thus we are dealing with a class of problems which arises often in practice. And assuming that only the values of v at the two ends are of interest, we can proceed much as before.

Denote by $u(z, x)$ and $v(z, x)$ the solutions to (2.1) with boundary conditions (2.20). Then manipulations completely analogous to those of Sec. IIA shows that

$$S(x) = v(x, x) \quad (2.22)$$

satisfies the differential equation

$$-S'(x) = c(x) + [a(x) + d(x)]S(x) + b(x)S^2(x). \quad (2.23)$$

Determining the correct initial condition for S presents only a slight difficulty which is soon resolved. In view of the boundary conditions (2.20) for all x it is clear that the derivative du/dz tends to infinity as $x \to 0$. It follows from (2.1), then, that $b(z)v(z)$ must do the same. Consequently the initial condition for S is

$$S(0) = \pm\infty \quad (2.24)$$

according as $b(x)$ is positive or negative near zero.

In the same way one can deal with the function $W(x) = v(0, x)$. In addition one can treat more general boundary conditions, using the linearity of the problem. We leave the details to the interested reader.

D. Larger Systems of Linear Differential Equations

For simplicity we have been considering the case of only two linear differential equations in two dependent variables. We next sketch the case of larger systems in order to illustrate the one essential difference which arises and how it can be dealt with. To emphasize the similarities let us write the system in the form

$$\begin{aligned} dU(z)/dz &= A(z)U(z) + B(z)V(z), \\ -dV(z)/dz &= C(z)U(z) + D(z)V(z), \end{aligned} \quad (2.25)$$

where A, B, C, D are $n \times n$ matrices and U, V are column matrices (vectors) of order n. We take the boundary conditions to be

$$U(0) = 0, \qquad V(x) = V_0. \quad (2.26)$$

It is this last boundary condition which promises trouble. Previously our boundary condition at x involved a single number (it was taken to be the number 1, but obviously any other number different from zero would have been just as satisfactory) whereas now a whole *set* of numbers is needed. More precisely our present boundary condition involves not just one number but a column matrix, namely V_0.

What we must do is to express the solutions of this problem as linear combinations of the solutions to n elementary problems, each of which involves only one nonzero number in its boundary condition. Thus if U^i, V^i are the solutions to (2.25) which satisfy the boundary conditions

$$U^i(0) = 0, \qquad V^i(x) = I^i, \quad (2.27)$$

where I^i is a column matrix whose jth element is 1 and all other elements are zero, then

$$U = HV_0, \quad (2.28)$$

$$V = KV_0, \quad (2.29)$$

where H, K are $n \times n$ matrices with jth column the column of U^i, V^i, respectively.

Denoting the solutions now by $U(z, x)$, $V(z, x)$, $H(z, x)$, $K(z, x)$, if it is the (matrix) function

$$R(x) = U(x, x) \quad (2.30)$$

which is wanted, then in view of (2.28) we need to find

$$r(x) = H(x, x). \quad (2.31)$$

Differentiating,

$$r'(x) = H_1(x, x) + H_2(x, x). \quad (2.32)$$

For $H_1(x, x)$ we use (2.25) (with H, K in place of U, V), put $z = x$ and remember the boundary conditions (2.27), obtaining

$$H_1(x, x) = A(x)r(x) + B(x). \quad (2.33)$$

For $H_2(x, x)$ we notice that U_2^i, V_2^i satisfy (2.25) also but with the second boundary condition

$$V_2^i(x, x) = -V_1^i(x, x). \quad (2.34)$$

Consequently,

$$\begin{aligned} U_2^i(z, x) &= -H(z, x)V_1^i(x, x), \\ V_2^i(z, x) &= -K(z, x)V_1^i(x, x). \end{aligned} \quad (2.35)$$

In particular, putting $z = x$ and remembering the definition of H,

$$\begin{aligned} H_2(x, x) &= -H(x, x)K_1(x, x) \\ &= H(x, x)[C(x)H(x, x) + D(x)K(x, x)], \end{aligned} \quad (2.36)$$

or

$$H_2(x, x) = r(x)[C(x)r(x) + D(x)]. \tag{2.37}$$

Finally, using (2.33) and (2.37) in (2.32) we get

$$r'(x) = B(x) + A(x)r(x) + r(x)D(x) + r(x)C(x)r(x), \tag{2.38}$$

which, incidentally, agrees formally with (2.7).

Other boundary conditions can be dealt with by making the obvious modifications so we omit the details.

E. Discussion

In this section we have developed a "mechanistic" method for obtaining the so-called "invariant imbedding" equations corresponding to a given linear system of differential equations without recourse to physical reasoning. Although the discussion has been a purely formal one, it can all be made perfectly rigorous without any difficulty.

In the next section we apply several of these results to specific problems of physical interest and also show how slight extensions of the ideas can be made so as to handle a wider class of problems.

III. SOME APPLICATIONS TO PHYSICAL PROBLEMS

A. The Wave Equation

We consider the problem of determining the reflection and transmission coefficients $\mathcal{R}$, $\mathcal{J}$ for a plane wave impinging perpendicularly on a slab of nonhomogeneous material sandwiched between two semi-infinite homogeneous media. Explicitly, let the slab occupy the region $0 \leq z \leq x$ and have wavenumber $k(z)$ at the interior point z, and let k_1, k_2 be the respective wavenumbers of the media to the left and right of the slab. We assume that a wave is incident from the right, resulting in a reflected wave in the region $z > x$ and a transmitted wave (only) in the region $z < 0$. Mathematically,

$$\begin{aligned} &\psi''(z) + k^2(z)\psi(z) = 0, && 0 < z < x, \\ &\psi(z) = e^{-ik_2(z-x)} + \mathcal{R}(x)e^{ik_2(z-x)}, && z > x, \\ &\psi(z) = \mathcal{J}(x)e^{-ik_1 z}, && z < 0. \end{aligned} \tag{3.1}$$

The usual requirements of continuity of ψ and ψ' yield

$$\psi(0) = [\mathcal{J}e^{-ik_1 z}]_{z=0}, \tag{3.2}$$

$$\psi'(0) = [d\mathcal{J}e^{-ik_1 z}/dz]_{z=0},$$

$$\psi(x) = [e^{-ik_2(z-x)} + \mathcal{R}e^{ik_2(z-x)}]_{z=x}, \tag{3.3}$$

$$\psi'(x) = [d\,(e^{-ik_2(z-x)} + \mathcal{R}e^{ik_2(z-x)})/dz]_{z=x}.$$

When the unknown coefficients $\mathcal{R}$ and $\mathcal{J}$ are eliminated, these boundary conditions take the form

$$\psi'(0) + ik_1\psi(0) = 0, \tag{3.4}$$

$$\psi'(x) - ik_2\psi(x) = -2ik_2. \tag{3.5}$$

Now make the simple transformation from ψ, ψ' to u, v defined by

$$u = (1/2ik_1)(\psi' + ik_1\psi), \tag{3.6}$$

$$v = -(1/2ik_2)(\psi' - ik_2\psi). \tag{3.7}$$

Then by differentiating and using (3.1) we find that u, v satisfy

$$u'(z) = [1/ik_1(k_1 + k_2)]\{-k_1[k^2(z) + k_1k_2]u(z) - k_2[k^2(z) - k_1^2]v(z)\}, \tag{3.8}$$

$$-v'(z) = [1/ik_2(k_1 + k_2)]\{-k_1[k^2(z) - k_2^2]u(z) - k_2[k^2(z) + k_1k_2]v(z)\},$$

$$u(0) = 0, \qquad v(x) = 1. \tag{3.9}$$

Obviously this system is precisely of the form (2.1), so that if we define [writing now $u(z, x)$ instead of $u(z)$, etc.]

$$R(x) = u(x, x), \tag{3.10}$$

and apply (2.7), we obtain

$$R'(x) = [1/i(k_1 + k_2)]\{k_2k_1^{-1}[-k^2(x) + k_1^2] - 2[k^2(x) + k_1k_2]R(x) + k_1k_2^{-1}[-k^2(x) + k_2^2]R^2(x)\}, \tag{3.11}$$

$$R(0) = 0. \tag{3.12}$$

In order to relate this result to our reflection and transmission coefficients, $\mathcal{R}(x)$ and $\mathcal{J}(x)$, we note from (3.6) and (3.7) that

$$\psi(z, x) = [2/(k_1 + k_2)][k_1u(z, x) + k_2v(z, x)] \tag{3.13}$$

$$\psi'(z, x) = [2ik_1k_2/(k_1 + k_2)][u(z, x) - v(z, x)]. \tag{3.14}$$

Putting $z = x$ and using (3.3) we find that

$$\mathcal{R}(x) = [2k_1/(k_1 + k_2)]R(x) + (k_2 - k_1)/(k_2 + k_1), \tag{3.15}$$

so that from (3.11), finally,

$$\mathcal{R}'(x) = (1/2ik_2)\{[k^2(x) - k_2^2] + 2[k^2(x) + k_2^2]\mathcal{R}(x) + [k^2(x) - k_2^2]\mathcal{R}^2(x)\}, \tag{3.16}$$

and

$$\mathcal{R}(0) = (k_2 - k_1)/(k_2 + k_1). \tag{3.17}$$

An equation for $\mathcal{J}(x)$ may be found similarly using (2.18). We get

$$\mathcal{J}'(x) = (1/2ik_2)\{[k^2(x) + k_2^2] + [k^2(x) + k_2^2]\mathcal{R}(x)\}\mathcal{J}(x), \tag{3.18}$$

$$\mathcal{J}(0) = 2k_2/(k_2 + k_1). \tag{3.19}$$

These results have been derived many times before and in many ways.[5,6] The point we emphasize here is the relative ease of using the results of Sec. II directly.

B. The Diffusion Equation

Let us turn now to a simple problem of diffusion in a slab.

$$D\,\partial^2\theta/\partial z^2 = \partial\theta/\partial t, \qquad 0 \le z \le x, \tag{3.20}$$

$$\theta(0, t) = 0, \qquad \theta(x, t) = 1, \qquad \theta(z, 0) = 0. \tag{3.21}$$

We ask for the flux across the surface $z = x$. This amounts to computing $\partial\theta/\partial z\,|_{z=x}$.

Define the Laplace transform of θ with respect to t:

$$\tilde{\theta}(z, s) = \int_0^\infty \theta(z, t)e^{-st}\,dt. \tag{3.22}$$

Applying the transformation to (3.20) gives

$$D\,\partial^2\tilde{\theta}/\partial z^2 = s\tilde{\theta}, \tag{3.23}$$

$$\tilde{\theta}(0, s) = 0, \qquad \tilde{\theta}(x, s) = 1/s. \tag{3.24}$$

To put (3.23) in a standard form we set

$$\begin{aligned} \tilde{u}(z, s) &= s\tilde{\theta}(z, s), \\ \tilde{v}(z, s) &= s\partial\tilde{\theta}(z, s)/\partial z, \end{aligned} \tag{3.25}$$

and obtain

$$\begin{aligned} \partial\tilde{u}/\partial z &= \tilde{v}, \\ -\partial\tilde{v}/\partial z &= -(s/D)\tilde{u}, \end{aligned} \tag{3.26}$$

$$\tilde{u}(0, s) = 0, \qquad \tilde{u}(x, s) = 1. \tag{3.27}$$

Equations (3.26) are exactly of the form treated in Sec. IIC. Writing $\tilde{v}(z, s, x)$ in place of $\tilde{v}(z, s)$ in order to make clear the x dependence, as usual, and defining

$$\tilde{S}(x, s) \equiv \tilde{v}(x, s, x), \tag{3.28}$$

$$\tilde{S}'(x, s) = s/D - \tilde{S}^2(x, s), \tag{3.29}$$

$$\tilde{S}(0, s) = +\infty. \tag{3.30}$$

The solution of (3.29) is well known:

$$\tilde{S}(x, s) = (s/D)^{\frac{1}{2}} \coth\,[x(s/D)^{\frac{1}{2}}]. \tag{3.31}$$

From (3.25) and (3.28) we get

$$\partial\tilde{\theta}(z, s)/\partial z|_{z=x} = (sD)^{-\frac{1}{2}} \coth\,[x(s/D)^{\frac{1}{2}}], \tag{3.32}$$

the Laplace inverse of which is[7]

$$\frac{\partial\theta}{\partial z}(z, t)|_{z=x} = \frac{1}{x}\,\theta_0\left(\frac{1}{2}, \frac{tD}{x^2}\right), \tag{3.33}$$

where θ_0 is a theta function.

Equation (3.33) has been derived earlier in a quite different manner.[8] It is obvious, of course, that the imbedding method is of no genuine advantage here, since the original problem can be readily handled. It is also clear, however, that our method is applicable in far more difficult cases.

C. The Time-Independent Transport Equation

It was in his work on the transport equation that Ambarzumian[9] employed a technique, subsequently exploited by Chandrasekhar,[10] that stimulated recent interest in the methods of invariant imbedding.

We consider the equation of transport in a slab of finite thickness x, assuming time independence, constant cross section, and isotropic scattering. In standard notation[2] the equation is

$$\mu\frac{\partial I}{\partial z}(z, \mu) + \sigma I(z, \mu) = \frac{\gamma\sigma}{2}\int_{-1}^{1} I(z, \lambda)\,d\lambda, \qquad -1 \le \mu \le 1, \tag{3.34}$$

and the boundary conditions are taken to be

$$I(0, \mu) = 0 \quad \text{for} \quad 0 < \mu \le 1, \tag{3.35}$$

$$I(x, \mu) = f(\mu) \quad \text{for} \quad -1 \le \mu < 0. \tag{3.36}$$

The parameter μ here is the cosine of an angle, so that $\mu > 0$ refers to flux to the right and $\mu < 0$ refers to flux to the left. $f(\mu)$ is the "input" at the right side.

If we write $U(z, \mu)$ for $I(z, \mu)$ when $\mu > 0$ and $V(z, \mu)$ for $I(z, \mu)$ when $\mu < 0$, then this problem (3.34) resembles, at least vaguely, the system (2.25). We can make the resemblance clearer, perhaps, by rewriting the problem as

$$\begin{aligned} \frac{\partial U}{\partial z}(z, \mu) &= \left[-\frac{\sigma}{\mu}\,U(z, \mu) + \frac{\gamma\sigma}{2\mu}\int_0^1 U(z, \lambda)\,d\lambda\right] + \frac{\gamma\sigma}{2\mu}\int_{-1}^{0} V(z, \lambda)\,d\lambda, \\ -\frac{\partial V}{\partial z}(z, \mu) &= -\frac{\gamma\sigma}{2\mu}\int_0^1 U(z, \lambda)\,d\lambda + \left[\frac{\sigma}{\mu}\,V(z, \mu) - \frac{\gamma\sigma}{2\mu}\int_{-1}^{0} V(z, \lambda)\,d\lambda\right], \end{aligned} \tag{3.37}$$

[5] C. MacCallum, "Invariant Imbedding and Wave Propagation in Inhomogeneous Media," Sandia Corporation Res. Rept. 4669 (1961).

[6] R. Bellman and R. Kalaba, J. Math. Mech. 8, 683 (1959).

[7] A. Erdélyi, M. Magnus, F. Oberhettinger, and F. E. Tricomi, *Tables of Integral Transforms* (Bateman Manuscript Project)(McGraw-Hill Book Company, Inc., New York, 1954).

[8] R. Bellman, R. Kalaba, and G. M. Wing, J. Math. Mech., Vol. 9, 933 (1960).

[9] V. A. Ambarzumian, Compt. Rend. (Doklady) de l'Académie des Sciences de l'URSS, 38, 229 (1943).

[10] S. Chandrasekhar, *Radiative Transfer* (Clarendon Press, Oxford, England, 1950).

$$U(0, \mu) = 0, \qquad V(x, \mu) = f(\mu). \tag{3.38}$$

Whereas in the previous problem (2.25), U was for each z in $(0, x)$ a matrix of n elements, in our present problem it represents for each z a function of the continuous variable $\mu > 0$. Where the previous boundary condition for V involved an arbitrary matrix of n elements, our present condition involves an arbitrary function of $\mu < 0$.

One could, if he wished, use the resemblance between the system (2.25) and (3.37) together with the usual analogy between sums and integrals in order to infer the invariant imbedding equation for our present problem from Eq. (2.38). But if one wishes to make his derivation rigorous, it is probably better to use the previous problem as only an analogy.

Thus (2.28) and (2.29) must be replaced by an appropriate representation in terms of integrals. Duhamel's principal leads to

$$U(z, \mu, x) = \int_{-1}^{0} H(z, \mu, \mu', x) f(\mu')\, d\mu' \tag{3.39}$$

in place of (2.28), as expected. Trying to write V in exactly the same fashion in terms of a kernel $K(z, \mu, \mu', x)$ would require K to be not an ordinary function but a *symbolic* one; i.e., K would involve a delta function. This is, of course, only a minor complication which can be dealt with in many ways,[4] but it turns out that (3.39) is all we need here.

Differentiating

$$R(x, \mu) = U(x, \mu, x), \tag{3.40}$$

gives

$$\begin{aligned} R_1(x, \mu) &= U_1(x, \mu, x) + U_3(x, \mu, x) \\ &= -\frac{\sigma}{\mu} R(x, \mu) + \frac{\gamma\sigma}{2\mu} \int_0^1 R(x, \lambda)\, d\lambda \\ &\quad + \frac{\gamma\sigma}{2\mu} \int_{-1}^{0} f(\mu')\, d\mu' + U_3(x, \mu, x), \end{aligned} \tag{3.41}$$

using (3.37) with $z = x$. We get U_3 in terms of R, as usual, by noticing that U_3, V_3 satisfy (3.37) with the last boundary condition replaced by

$$V_3(x, \mu, x) = -V_1(x, \mu, x). \tag{3.42}$$

Duhamel's principal (i.e., linearity) again yields

$$U_3(z, \mu, x) = -\int_{-1}^{0} H(z, \mu, \mu', x) V_1(x, \mu', x)\, d\mu'. \tag{3.43}$$

Using this (with $z = x$) in (3.41) gives

$$\begin{aligned} R_1(x, \mu) &= -\frac{\sigma}{\mu} R(x, \mu) \\ &\quad + \frac{\gamma\sigma}{2\mu} \int_0^1 R(x, \lambda)\, d\lambda + \frac{\gamma\sigma}{2\mu} \int_{-1}^{0} f(\mu')\, d\mu' \\ &\quad + \int_{-1}^{0} H(x, \mu, \mu', x) \left\{ -\frac{\gamma\sigma}{2\mu'} \int_0^1 R(x, \lambda)\, d\lambda \right. \\ &\quad \left. + \left[\frac{\sigma}{\mu'} f(\mu') - \frac{\gamma\sigma}{2\mu'} \int_{-1}^{0} f(\mu'')\, d\mu'' \right] \right\} d\mu'. \end{aligned} \tag{3.44}$$

Finally, in analogy with (2.31), write

$$r(x, \mu, \mu') = 2\pi H(x, \mu, \mu', x). \tag{3.45}$$

(The 2π is just so that our results will agree exactly with those of other writers.) Then by (3.39)

$$\begin{aligned} R(x, \mu) &= \int_{-1}^{0} H(x, \mu, \mu', x) f(\mu')\, d\mu' \\ &= \frac{1}{2\pi} \int_{-1}^{0} r(x, \mu, \mu') f(\mu')\, d\mu', \end{aligned} \tag{3.46}$$

and substituting in (3.44) we get, after some manipulation,

$$\begin{aligned} &\int_{-1}^{0} f(\mu') \left(r_1(x, \mu, \mu') + \sigma\left(\frac{1}{\mu} - \frac{1}{\mu'}\right) r(x, \mu, \mu') \right. \\ &+ \frac{\gamma\sigma\pi}{\mu'} \int_{-1}^{0} r(x, \mu, \mu'')\, d\mu'' - \frac{\gamma\sigma}{2} \int_0^1 r(x, \lambda, \mu') \frac{d\lambda}{\lambda} \\ &\left. - \frac{\gamma\sigma}{4\pi} \int_0^1 r(x, \lambda, \mu') \frac{d\lambda}{\lambda} \int_{-1}^{0} r(x, \mu, \mu'')\, d\mu'' \right) d\mu' = 0. \end{aligned} \tag{3.47}$$

Since this equation must hold for arbitrary functions f, the quantity in parentheses must vanish. For example,

$$\begin{aligned} \frac{\partial r}{\partial x}(x, \mu, \mu') &= -\frac{\sigma\gamma\pi}{\mu'} - \sigma\left(\frac{1}{\mu} - \frac{1}{\mu'}\right) r(x, \mu, \mu') \\ &\quad - \frac{\gamma\sigma}{2\mu'} \int_{-1}^{0} r(x, \mu, \mu'')\, d\mu'' + \frac{\gamma\sigma}{2} \int_0^1 r(x, \lambda, \mu') \frac{d\lambda}{\lambda} \\ &\quad + \frac{\gamma\sigma}{4\pi} \int_0^1 r(x, \lambda, \mu') \frac{d\lambda}{\lambda} \int_{-1}^{0} r(x, \mu, \mu'')\, d\mu''. \end{aligned} \tag{3.48}$$

Evidently also

$$r(0, \mu, \mu') = 0. \tag{3.49}$$

Equation (3.48) was first obtained in quite a different way by Ambarzumian. Whereas we have used purely mathematical arguments concerning the mathematically formulated problem (3.34), he proceeded directly from the physical problem via physical arguments, i.e., "particle counting." Equation (3.48) has been obtained in several different ways,[2,9,10] and has proved valuable for computational purposes.[10,11]

[11] R. Bellman, R. Kalaba, and M. C. Prestrud, *Invariant Imbedding and Radiative Transfer in Slabs of Finite Thickness* (Elsevier Publishing Company, Inc., New York, 1963).

There are, however, several advantages inherent in the kind of derivation we have just given. For one thing, it can be made rigorous.[4] For another, with only added notational complexity it can be extended to cases in which σ is dependent upon x and in which anisotropic scattering is allowed. Finally, this same kind of derivation applies equally well to transport problems in other geometries.

This last observation is quite important. For when the case of transport in a sphere was treated in the above way the resulting invariant imbedding equation contained an extra term which had been overlooked in the previous particle counting derivations. Retrospective analysis of the particle counting method as it had been applied to the sphere and cylinder has revealed the subtle source of error.[12]

D. The Time-Dependent Transport Equation

The fact that the time-dependent transport equation can be handled with only a little additional effort comes as an unexpected bonus. Consider the problem

$$\frac{1}{c}\frac{\partial I}{\partial t}(z,\mu,t) + \mu\frac{\partial I}{\partial z}(z,\mu,t) + \sigma I(z,\mu,t) = \frac{\gamma\sigma}{2}\int_{-1}^{1} I(z,\mu',t)\,d\mu', \tag{3.50}$$

$$I(0,\mu,t) = 0 \quad \text{for} \quad \mu < 0,\ t > 0, \tag{3.51}$$

$$I(x,\mu,t) = f(\mu,t) \quad \text{for} \quad \mu < 0,\ t > 0, \tag{3.52}$$

$$I(z,\mu,0) = 0 \quad \text{for} \quad -1 < \mu < 1,\ 0 < z < x. \tag{3.53}$$

Denoting the Laplace transform of $I(z,\mu,t)$ by $\tilde{I}(z,\mu,s)$, etc., we get

$$\mu\frac{\partial \tilde{I}}{\partial z}(z,\mu,s) + \left(\sigma + \frac{s}{c}\right)\tilde{I}(z,\mu,s) = \frac{\gamma\sigma}{2}\int_{-1}^{1}\tilde{I}(z,\mu',s)\,d\mu', \tag{3.54}$$

$$\tilde{I}(0,\mu,s) = 0 \quad \text{for} \quad \mu > 0, \tag{3.55}$$

$$\tilde{I}(x,\mu,s) = \tilde{f}(\mu,s) \quad \text{for} \quad \mu < 0. \tag{3.56}$$

Comparing with (3.34) and replacing the σ on the left side there by $\sigma + s/c$, shows that the equation satisfied by

$$\tilde{r}(x,\mu,\mu',s) = 2\pi\tilde{H}(x,\mu,\mu',s,x), \tag{3.57}$$

where $\tilde{H}$ is the representation kernel for

$$\tilde{I}(z,\mu,s,x) = \int_{-1}^{0}\tilde{H}(z,\mu,\mu',s,x)\tilde{f}(\mu',s)\,d\mu', \tag{3.58}$$

is

$$\frac{\partial\tilde{r}}{\partial x} = -\frac{\gamma\sigma\pi}{\mu'} - \left(\sigma + \frac{s}{c}\right)\left(\frac{1}{\mu} - \frac{1}{\mu'}\right)\tilde{r} - \frac{\sigma\gamma}{2\mu'}\int_{-1}^{0}\tilde{r}(x,\mu,\mu'',s)\,d\mu'' + \frac{\gamma\sigma}{2}\int_{0}^{1}\tilde{r}(x,\lambda,\mu',s)\frac{d\lambda}{\lambda} + \frac{\gamma\sigma}{4\pi}\int_{0}^{1}\tilde{r}(x,\lambda,\mu',s)\frac{d\lambda}{\lambda}\int_{-1}^{0}\tilde{r}(x,\mu,\mu'',s)\,d\mu''. \tag{3.59}$$

Dividing by s and taking inverse Laplace transforms gives

$$\frac{\partial\rho}{\partial x} + \frac{1}{c}\left(\frac{1}{\mu} - \frac{1}{\mu'}\right)\frac{\partial\rho}{\partial t} = -\frac{\gamma\sigma\pi}{\mu'} - \frac{\gamma\sigma}{2\mu'}\int_{-1}^{0}\rho(x,\mu,\mu'',t)\,d\mu'' + \frac{\gamma\sigma}{2}\int_{0}^{1}\rho(x,\lambda,\mu',t)\frac{d\lambda}{\lambda} - \sigma\left(\frac{1}{\mu} - \frac{1}{\mu'}\right)\rho + \frac{\gamma\sigma}{4\pi}\int_{0}^{t}\int_{0}^{1}\rho(x,\lambda,\mu',t-\tau)\frac{d\lambda}{\lambda} \times \int_{-1}^{0}\frac{\partial\rho}{\partial\tau}(x,\mu,\mu'',\tau)\,d\mu''\,d\tau, \tag{3.60}$$

where

$$\rho(x,\mu,\mu',t) = \int_{0}^{t} r(x,\mu,\mu',\tau)\,d\tau. \tag{3.61}$$

This equation has been the basis of some recent extensive calculations.[13]

IV. FURTHER APPLICATIONS

A. Introduction

In this chapter we apply the ideas of this paper to the study of nonlinear difference equations and to the phase-shift problem of wave mechanics. While the techniques employed still come under the general heading of invariant imbedding, the reader will note a slightly modified point of view. It is for this reason that these examples are put in a new section rather than being included in the previous one.

B. Difference Equations

Consider the system of difference equations

$$u(z+1) - u(z) = f[u(z), v(z), z]$$
$$-v(z+1) + v(z) = g[u(z), v(z), z], \quad \text{for } 0 \le z \le x, \tag{4.1}$$
$$u(0) = 0, \qquad u(x) = y. \tag{4.2}$$

[12] P. Bailey and G. M. Wing, J. Math. Anal. Appl. 8, 170 (1964).

[13] R. Bellman, H. H. Kagiwada, R. Kalaba, and M. C. Prestrud, *Invariant Imbedding and Time-Dependent Transport Processes* (Elsevier Publishing Company, Inc., New York, 1964).

If our interest is in the value of v at the end $z = x$, then we can denote by $u(z, x, y)$, $v(z, x, y)$ the solution to (4.1) and look for a suitable equation for the function

$$S(x, y) = v(x, x, y). \tag{4.3}$$

(The additional parameter y is necessary because our problem this time is *nonlinear*.)

Now $u(z, x + 1, \bar{y})$, $v(z, x + 1, \bar{y})$ are the solution functions to the same system (4.1) but with the last boundary condition

$$u(x + 1, x + 1, \bar{y}) = \bar{y}. \tag{4.4}$$

Hence if we extend the definitions of $u(z, x, y)$, $v(z, x, y)$ slightly by

$$u(x + 1, x, y) = u(x, x, y) + f[u(x, x, y), v(x, x, y), x], \tag{4.5}$$

$$v(x + 1, x, y) = v(x, x, y) - g[u(x, x, y), v(x, x, y), x], \tag{4.6}$$

and assume that the system (4.1) has a unique solution u, v for each x, y, then by choosing

$$\bar{y} = u(x + 1, x, y) \tag{4.7}$$

we shall have succeeded in arranging matters so that actually

$$u(z, x, y) = u(z, x + 1, \bar{y}), \tag{4.8}$$

$$v(z, x, y) = v(z, x + 1, \bar{y}) \quad \text{for all } x, y \text{ and all } z \leq x + 1. \tag{4.9}$$

Putting $z = x + 1$ in (4.9) and using (4.6) and (4.3), gives

$$S(x + 1, \bar{y}) = S(x, y) - g[u(x, x, y), S(x, y), x]. \tag{4.10}$$

Hence from (4.7), (4.5), (4.2), finally,

$$S(x + 1, y + f[y, S(x, y), x]) = S(x, y) - g[y, S(x, y), x]. \tag{4.11}$$

To determine the initial condition for S take $x = 1$. Then from (4.1) it is easy to see that

$$y = f[0, S(0, y), 0]. \tag{4.12}$$

We assume that (4.12) is solvable for $S(0, y)$.

As an example, suppose that the system (4.1) is really linear:

$$f[u(z), v(z), z] = a(z)u(z) + b(z)v(z), \qquad g[u(z), v(z), z] = c(z)u(z) + d(z)v(z). \tag{4.13}$$

Then it must be the case that

$$S(x, y) = ys(x) \tag{4.14}$$

for some s. Hence (4.11) and (4.12) reduce to

$$s(x + 1) = \frac{c(x) + s(x)[1 + d(x)]}{1 + a(x) + b(x)s(x)}, \tag{4.15}$$

$$s(0) = 1/b(0). \tag{4.16}$$

We note in conclusion that the method of this section suggests a way[14] of handling nonlinear differential systems by invariant imbedding.

C. The Phase-Shift Problem

In the last section a slightly different approach was introduced. Results there were obtained by enlarging the domain of the solution of a system of difference equations, obtaining the solution to a new system on an extended interval. The two problems then have identical solutions over their common domains.

We now apply this reasoning to the classical phase-shift problem. Consider the system

$$y''(t) + y(t) = f(t)y(t), \tag{4.17}$$

$$y(0) = \epsilon_0 \cos \theta_0, \qquad y'(0) = \epsilon_0 \sin \theta_0. \tag{4.18}$$

We require

$$\int^{\infty} |f(t)|\, dt < \infty. \tag{4.19}$$

It is known that

$$y(t) = A \cos (t - \alpha) + o(1) \tag{4.20}$$

for large t. The amplitude, A, and the phase shift, α, are clearly dependent upon ϵ_0 and θ_0. We intend to find that relationship.

For any value of $t \geq 0$, say $t = x$, we may write, by proper choice of ϵ and θ,

$$y(x) = \epsilon(x) \cos \theta(x), \qquad y'(x) = \epsilon(x) \sin \theta(x). \tag{4.21}$$

In particular, of course,

$$\epsilon(0) = \epsilon_0, \qquad \theta(0) = \theta_0. \tag{4.22}$$

Now it is well known that the solution to (4.17) satisfies the integral equation

$$y(t) = \epsilon(x) \cos [t - x - \theta(x)] + \int_x^t \sin (t - \tau)f(\tau)y(\tau)\, d\tau. \tag{4.23}$$

[14] R. Bellman, R. Kalaba, and G. M. Wing, Proc. Nat. Acad. Sci. U. S. **46**, 1646 (1960).

Since $y(t)$ is *independent* of x, we have by differentiation

$$0 = \epsilon'(x)\cos[t - x - \theta(x)] + \epsilon(x)[1 + \theta'(x)]\sin[t - x - \theta(x)] - \sin(t - x)f(x)\epsilon(x)\cos\theta(x). \quad (4.24)$$

But (4.24) holds for *all* $t \geq 0$. Therefore,

$$\epsilon'(x) = \epsilon(x)f(x)\sin\theta(x)\cos\theta(x), \qquad \theta'(x) = -1 - f(x)\cos^2\theta(x). \quad (4.25)$$

By integrating (4.25) subject to (4.22) one may find $\epsilon(x)$ and $\theta(x)$.

As yet there is no obvious connection between ϵ and θ and the quantities A and α in (4.20). To find this we rewrite (4.23):

$$y(t) = \epsilon(x)\cos[t - x - \theta(x)] + \int_x^\infty \sin(t - \tau)f(\tau)y(\tau)\,d\tau - \int_t^\infty \sin(t - \tau)f(\tau)y(\tau)\,d\tau. \quad (4.26)$$

(That the integrals converge is a result of (4.19) and the fact that y is bounded.[15]) From (4.26),

$$y(t) = \epsilon(x)\cos[t - x - \theta(x)] + \sin t\int_x^\infty \cos\tau f(\tau)y(\tau)\,d\tau + \cos t\int_x^\infty \sin\tau f(\tau)y(\tau)\,d\tau - \int_t^\infty \sin(t - \tau)f(\tau)y(\tau)\,d\tau, \quad (4.27)$$

which we write as

$$y(t) = A(x)\cos[t - x - \alpha(x)] - \int_t^\infty \sin(t - \tau)f(\tau)y(\tau)\,d\tau. \quad (4.28)$$

But

$$\lim_{t\to\infty}\int_t^\infty \sin(t - \tau)f(\tau)y(\tau)\,d\tau = 0, \quad (4.29)$$

so that (4.28) is exactly in the form (4.20) with

$$A(0) = A, \qquad \alpha(0) = \alpha. \quad (4.30)$$

Differentiating (4.28) with respect to x gives

$$0 = A'(x)\cos[t - x - \alpha(x)] + A(x)[1 + \alpha'(x)]\sin[t - x - \alpha(x)], \quad (4.31)$$

and so

$$A'(x) = 0, \qquad \alpha'(x) = -1. \quad (4.32)$$

Thus, using (4.30),

$$A(x) = A, \qquad \alpha(x) = -x + \alpha. \quad (4.33)$$

Finally subtract (4.28) from (4.27) and let $x \to \infty$. This yields

$$\lim_{x\to\infty}\epsilon(x) = A, \qquad \lim_{x\to\infty}[\theta(x) + x] = \alpha. \quad (4.34)$$

The second equation of (4.33) suggests defining

$$\psi(x) = \theta(x) + x. \quad (4.35)$$

Then the system (4.22) and (4.25) becomes

$$\epsilon'(x) = \tfrac{1}{2}\epsilon(x)f(x)\sin 2[\psi(x) - x], \qquad \psi'(x) = -f(x)\cos^2[\psi(x) - x], \quad (4.36)$$

$$\epsilon(0) = \epsilon_0, \qquad \psi(0) = \theta_0. \quad (4.37)$$

The amplitude A and phase shift α are found by solving (4.36) and evaluating $\epsilon(\infty)$ and $\psi(\infty)$.

The results we have obtained are equivalent to those of Franchetti,[16] derived by him in a somewhat simpler way. The advantage of the present scheme lies in the fact that it is readily generalizable to systems more complicated than (4.17). For a more complete and rigorous analysis, together with a discussion of other differential equations, the reader is referred to Wing,[15] where the imbedding is done from a somewhat different viewpoint.

V. SUMMARY

It has been our intention in this article to describe briefly the evolution of the invariant imbedding method over the last few years and to indicate the unification produced by these developments. No attempt has been made at a complete review of the subject. Examples chosen are only representative and the authors are aware of numerous other applications of the method that have recently been made. In the interest of brevity we have not discussed these nor provided detailed references. Our aim has been to give the interested reader enough insight into the imbedding method to allow him to read existing and forthcoming material with relative ease and understanding. We hope, too, that this paper will lead physicists and applied mathematicians to consider the possibility of applying the method to other classes of problems.

[15] G. M. Wing, J. Math. Anal. Appl. (to be published).

[16] S. Franchetti, Nuovo Cimento 6, 601 (1957).

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Poles in Feynman Diagrams with Several Loops

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A formula is given that extracts the pole contribution to a Feynman diagram having an internal line. The result is more complicated than earlier results for diagrams with only a single loop since the result is not directly expressible as the pole multiplied by a numerator that is the sum of the reduced diagrams. The apparent discrepancy with Cutkosky's formula for the residue of the pole is reconciled. The algebraic techniques employed are in principle applicable to the problem of determining the Landau surface when the diagram has several loops. A derivation of Stokes' formula for Feynman parametric integrals is given.

I. INTRODUCTION

SEVERAL examples have been given in the last few years of formulas that explicitly exhibit the pole contribution to a Feynman diagram.[1-5] These take the form of a rational expression, the denominator is the determinant that vanishes on the Landau surface,[6] and the numerator is the sum of the contributions of all diagrams formed by leaving out one line at a time, each contribution being multiplied by a polynomial. All of these formulas are derived for diagrams with only one loop. In this paper an example is given of this type of formula for a diagram with an internal line.

A large amount of algebra has to be done to get the formula. However, the solution is sufficiently simple that one might hope that a simpler technique to find it could be developed. An auxiliary result of this labor is a systematic method of determining the Landau surface for a diagram with several loops. That is, a necessary and sufficient condition is found for a system of n homogeneous polynomials in n unknowns to have a nontrivial solution. In Sec. II the general conditions under which a diagram has a pole are discussed. The application of Stokes theorem to give a formula explicitly exhibiting the pole is considered. For diagrams without poles the Stokes theorem will not work, but the same algebra will lead to an expression for the Landau surface. Section III contains a particular example of a self-energy diagram in a two-dimensional field theory worked out in detail.

[1] G. Källén and A. S. Wightman, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 1, No. 6 (1958).
[2] L. M. Brown, Nuovo Cimento 22, 178 (1961).
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[5] C. M. Sommerfield (private communication).
[6] L. D. Landau, Nucl. Phys. 13, 181 (1959).

II. GENERAL CONDITIONS FOR POLES AND THE APPLICATION OF STOKES THEOREM

Consider a diagram with n internal lines l loops in a space–time of $a + 1$ dimensions. Its analytic expression will be called F. There are $(a + 1)l$ integrals to be performed if the integral representing F is written down in momentum space. Cutkosky[7] has given a formula for the discontinuity of the function F across any of its cuts. The prescription is to replace propagators by δ functions. If there are more than $(a + 1)l$ internal lines, that is, if

$$n > (a + 1)l,$$

then $(a + 1)l$ of them can be replaced by δ functions and all the integrals can in principle be done, but there will be some propagators left. Thus the discontinuity has a pole and thus F itself has a pole on some sheets.

As an alternative approach to discover the existence of pole we may ask if a formula of the type given in Refs. 1–5 exists. In the following discussion, the usual simplifying assumption that all particles are scalars is made. The expression for a diagram with n internal lines, l loops in $(a + 1)$-dimensional space–time is:

$$F = A \int \cdots \int d^{a+1}k_1 \cdots d^{a+1}k_l \prod_{i=1}^{n} A_i^{-1}, \qquad (1)$$

where $A_i = q_i^2 + m_i^2$, and the momentum q_i of the ith line is to be expressed in terms of the external momenta and the loop momenta k_j. Chisholm's formula[8] permits F to be rewritten as

$$F = A' \int_0^1 \cdots \int_0^1 d\alpha_1 \cdots d\alpha_n \times \frac{\delta(1 - \alpha)(\det \Lambda)^{n-(a+1)(l+1)/2}}{\Delta^{n-(a+1)l/2}}. \qquad (2)$$

[7] R. E. Cutkosky, J. Math. Phys. 1, 429 (1960).
[8] R. Chisholm, Proc. Cambridge Phil. Soc. 48, 300 (1952).

The l-rowed determinant Λ is defined from the expression

$$\sum A_{i\alpha_i} = \Lambda_{\mu\nu}k_\mu k_\nu + 2\sum_\mu k_\mu + \Xi,$$

while Δ is the $(l+1)$-rowed determinant

$$\Lambda = \begin{vmatrix} \Lambda & \Sigma \\ \Sigma & \Xi \end{vmatrix},$$

and $\alpha = \sum \alpha_i$.

In Appendix I a proof is given of a version of Stokes' theorem applicable to integrals over the domain zero to one in n variables α_i subject to the restriction $\alpha = 1$. The elements of Δ and Λ are homogeneous linear functions of the α. Thus Δ and Λ are homogeneous polynomial of degree $l+1$ and l in the α's. The denominator is thus a homogeneous expression of degree $(l+1)[n-(a+1)l/2]$ and the numerator is one of degree

$$l[n-(a+1)(l+1)/2].$$

To apply Stokes' theorem a set of functions F_a $(a = 1, 2, \cdots, n)$ is required with $\sum F_i = 0$ and

$$\frac{\partial F_i}{\partial \alpha_i} = \frac{(\det \Lambda)^{n-(a+1)(l+1)/2}}{(\Delta)^{n-l(a+1)/2}}. \tag{3}$$

The problem may be restricted to be a completely algebraic one by looking for F_a of the form, $F_a = N_a/(\Delta)^{n-l(a+1)/2-1}$ where N_a is a polynomial in the α's. If this is substituted in (3), the equation for N_i becomes

$$\Delta\,\partial N_i/\partial\alpha_i - [n - l(a+1)/2 - 1]N_i\,\partial\Delta/\partial\alpha_i = (\det\Lambda)^{n-(a+1)(l+1)/2}. \tag{4}$$

If a set of functions P_i such that

$$P_i\,\partial\Delta/\partial\alpha_i = (\det\Lambda)^{n-(a+1)(l+1)/2}, \tag{5}$$

and

$$\partial P_i/\partial\alpha_i = 0, \tag{5a}$$

then a satisfactory set of N_i is given by

$$N_i = (P\alpha_i - P_i\alpha)/[n - l(a+1)/2 - 1], \tag{6}$$

where $P = \sum P_i$, and the degree of P must be

$$r = l[(n-1) - (l+1)(a+1)/2]. \tag{7}$$

That the N_i are a solution of (4) may be verified by substitution of (6) into (4). Conversely, if a solution of (4) exists it may be put in the form (6). The equations (5) and (5a) are to be regarded as linear equations for the coefficients of the n polynomials P_i. A homogeneous polynomial of degree r in n variables has $\binom{n+r-1}{r}$ coefficients. Thus there are $n\binom{n+r-1}{r}$ unknowns in (5) and, since the right-hand side has degree $r+l$, there are $\binom{n+r+l-1}{r+l}$ linear equations in (5). There are $\binom{n+r-2}{n-1}$ further equation in (5a). For a solution there should be as many unknowns as equations, that is

$$n\frac{(n+r-1)!}{r!(n-1)!} \geq \frac{(n+r+l-1)!}{(r+l)!(n-1)!} + \frac{(n+r-2)!}{(r-1)!(n-1)!}. \tag{8}$$

Roughly speaking, a large l must be compensated by a large n.

Since the system of equations (5) and (5a) are linear, there are some restrictions on the coefficients for the equations to be soluble. The coefficients are of course the masses and invariant energies. If the equations $\partial\Delta/\partial\alpha_1 = 0$ have a simultaneous solution, that is for values of the invariants on the Landau surface, then Eqs. (5) and (5a) will not have solutions unless (det Λ) vanishes. Thus the condition on the coefficients that a solution should not exist (vanishing of a determinant) is the equation of the Landau surface.

To extract a pole contribution it is necessary to satisfy (7) and (8) simultaneously. From (7) it follows that r is an increasing function of n and (8) is easier to satisfy for large r. Thus if a diagram has a pole, increasing the number of internal lines without adding loops retains the pole. Actually, the order increases. This is in accord with the earlier result that $n > l(a+1)$. The interesting numbers are the smallest pair (n, r) for each value of l that satisfy (7) and (8). For example, for $l = 1$ (7) and (8) become

$$r = n - 1 - (a+1), \tag{7'}$$

$$n\frac{(n+r-1)!}{r!(n-1)!} \geq \frac{(n+r)!}{r!(n-1)!} + \frac{(n+r-2)!}{(r-1)!(n-1)!}. \tag{8'}$$

These are both satisfied for $r=0$ and $n=1+(a+1)$. The same as $n = 1 + l(a+1)$ with $l = 1$. For $l = 2$, (7) and (8) become after some simplification

$$r = 2(n-1) - 3(a+1), \tag{7''}$$

$$(n-1) \geq (n+r+1)(n+r-1)/(r+1)(r+2). \tag{8''}$$

The simplest case that works is $a + 1 = 2$, $r = 2$, and $n = 5$, which again satisfies the $n = 1 + l(a+1)$ requirement. The example, $a = 1$, $r = 2$, $n = 5$, is worked out in detail in the next section, that is, the polynomials P_i are solved for. Although it is not obvious that (7) and (8) are equivalent to $n = 1 +$

$l(a + 1)$, the two results are identical for the simple cases checked so far. It seems reasonable then that whenever a pole exists, Stokes' theorem is applicable in principle.

III. AN EXAMPLE

As an illustration of the use of Stokes' theorem the graph of Fig. 1 is considered in (1 + 1)-dimensional space–time.

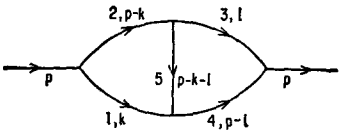

FIG. 1. A graph whose analytic expression contains a pole in a two-dimensional field theory.

The contribution from this graph is

$$I = \iint \frac{d^2k\, d^2l}{[k^2 + m^2][(P - k)^2 + m^2][l^2 + m^2][(P - l)^2 + m^2][(P - k - l)^2 + m^2]}. \tag{9}$$

The masses of all five internal particles have been chosen all equal to m for simplicity.

The quantities $\det \Lambda$ and Δ are found in this case to be

$$\det \Lambda = (\alpha_1 + \alpha_2)(\alpha_3 + \alpha_4) + \alpha_5(\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4)$$

$$\begin{aligned}\Delta = {} & m^2(\alpha_1^2\alpha_3 + \alpha_1^2\alpha_4 + \alpha_5 + \alpha_1\alpha_3^2 + \alpha_1\alpha_4^2 \\ & + \alpha_1\alpha_5^2 + \alpha_2^2 + 3 + \alpha_2^2\alpha_4 + \alpha_2^2\alpha_5 + \alpha_2\alpha_3^2 + \alpha_2\alpha_4^2 \\ & + \alpha_2\alpha_5^2 + \alpha_3^2\alpha_5 + \alpha_3\alpha_5^2 + \alpha_4^2\alpha_5 + \alpha_4\alpha_5^2) \\ & + (P^2 + 2m^2)(\alpha_1\alpha_2\alpha_3 + \alpha_1\alpha_2\alpha_4 + \alpha_1\alpha_2\alpha_5 + \alpha_1\alpha_3\alpha_4 \\ & + \alpha_2\alpha_3\alpha_4 + \alpha_3\alpha_4\alpha_5) + (P^2 + 3m^2)(\alpha_1\alpha_3\alpha_5 + \alpha_2\alpha_4\alpha_5) \\ & + 3m^2(\alpha_1\alpha_4\alpha_5 + \alpha_2\alpha_3\alpha_5).\end{aligned}$$

The degree of the P_i's is $r = 2$. So that in this case the P_i's are of the form: $P_i = a_{ijk}\alpha_j\alpha_k$. For each i, a_{ijk} forms a symmetric 5×5 matrix in j and k to give 15 independent elements. Then for all i there are 75 elements.

Since the mass have been chosen equal, there exists some symmetry in $(\det \Delta)^2$ and $\partial\Delta/\partial\alpha_i$ that may be exploited to simplify the calculation somewhat. (See Appendix II for $\partial\Delta/\partial\alpha_i$.) Any permutation of the α_i's which leaves $(\det \Delta)^2$ and $\partial\Delta/\partial\alpha_i$ invariant must also leave the P_i's invariant. When all such possible symmetries are taken into account, the P_i's are of the form given in Appendix III.

When the coefficients of $\alpha_i\alpha_j\alpha_k\alpha_l$ are set equal in Eq. (5), 70 equations for the 21 unknowns which appear in the P_i's are found.

However, only 17 of these 70 equations turn out to be independent. These are listed in Appendix III. Also, there is one more condition, that of Eq. (5a). This produces the requirement that

$$(2A + F + G + H + U)\left(\sum_{i=1}^{4}\alpha_i\right) + (4I + 2Q)\alpha_i = 0,$$

which yields the equations

$$2A + F + G + H + U = 0$$

and $2I + Q = 0$.

The 19 equations thus found are self-consistent. Since there are 21 unknowns, two arbitrary constants remain in the solutions which do not affect the value of the integral. The solutions are listed in Appendix IV.

The formula of Appendix I can now be applied and the integral (9) becomes the sum of five integrals,

$$I = 4\pi^2 \sum_{i=1}^{5} I_i \tag{10}$$

where

$$I_i = \int_0^1 \cdots \int_0^1 \prod_{j\neq i}^{5} d\alpha_j\, \delta\left(1 - \sum_{j\neq i}^{5}\alpha_j\right)\left(\frac{P_i}{D^2}\right)_{\alpha_i=0}. \tag{11}$$

Upon permuting the integration variables in I_1, I_2, I_3, and I_4, it can be shown that these four integrals are equal.

It was found to be impossible to interpret the five integrals as the expressions of the five four-line graphs shown in Fig. 2. In the case of the single loop, the correspondence is possible since the numerator is very simple, $\det \Lambda = \alpha$. But in this case, the numerators of the integrands cannot be made equal to those of the four-line graphs although there are two free parameters in the solution. The denominators are, however, equal.

Since the integral I is independent of the choice

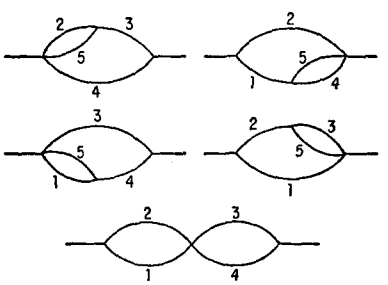

FIG. 2. The five possible contractions of Fig. 1.

of B and C, the choice of $B = C = 0$ immediately reveals a singularity at $P^2 = -3m^2$. Since on the physical sheet the propagator has only a pole at $P^2 = -m^2$ and a cut starting at $P^2 = -4m^2$, the singularity at $P^2 = -3m^2$ must be on an unphysical sheet.

The existence and position of this singularity can also be easily seen from Cutkosky's recipe for finding the residues of poles. If in integral (9) the change of variables:

$$x = (P - k)^2, \quad y = k^2, \quad z = l^2, \quad w = (P - l)^2,$$

or

$$k_1 = \frac{P_1(y - x + P^2)}{2P^2} + \frac{P_0[(y - x + P^2)^2 - 4Py]^{\frac{1}{2}}}{2P^2},$$

$$k_0 = \frac{P_0(y - x + P^2)}{2P^2} + \frac{P_1[(y - x + P^2) - 4Py]^{\frac{1}{2}}}{2P^2},$$

$$l_1 = \frac{P_1(z - w + P^2)}{2P^2} + \frac{P_0[(z - w + P^2) - 4P^2z]^{\frac{1}{2}}}{2P^2},$$

$$l_0 = \frac{P_0(z - w + P^2)}{2P^2} + \frac{P_1[(z - w + P^2) - 4P^2z]^{\frac{1}{2}}}{2P^2},$$

is made; then the pole occurs at $(P-k-l)^2+m^2=0$. Upon making the transformation and putting $x=y=z=w=-m^2$, the pole at $P^2 = -3m^2$ appears.

The numerator of Eq. (11) should reduce to the above expression at $p^2 = -3m^2$, so that although the residue of the pole is not expressed as the sum of other diagrams in an obvious manner, the numerator of (11) does have this correct value at the pole.

APPENDIX I: PROOF OF A STOKES THEOREM

The following notation is introduced to simplify the ensuing discussion:

$$\int F = \int_0^1 dx_1 \int_0^1 dx_2 \cdots \int_0^1 dx_n \times \delta(1 - x_1 - x_2 - \cdots - x_n) F(x_1, x_2, \cdots, x_n),$$

$$\int_{ij\cdots k} F = \int_0^1 dx_1 \int_0^1 dx_2 \cdots \int_0^1 dx_n \times \delta(1 - x_1 - x_2 - \cdots - x_n) \times F(x_1, x_2, \cdots, x_n)\,\delta(x_i)\,\delta(x_j) \cdots \delta(x_k).$$

Lemma I:

$$I = \int \left(\frac{\partial F}{\partial x_i} - \frac{\partial F}{\partial x_j}\right) = \int_j F - \int_i F. \qquad \text{(A1)}$$

Proof: The proof is carried out for $i = 1$ and $j = 2$ to avoid notational difficulties. First, the integral with respect to x_n is carried out using the factor $\delta(1 - x_1 - x_2 - \cdots - x_n)$. The total derivatives are then given by

$$\frac{dF}{dx_a} = \frac{\partial F}{\partial x_a} - \frac{\partial F}{\partial x_n}, \qquad a \neq n,$$

so that

$$\frac{\partial F}{\partial x_1} - \frac{\partial F}{\partial x_2} = \frac{dF}{dx_1} - \frac{dF}{dx_2}.$$

Now the two total derivatives may be integrated easily, the first over x_1 and the second over x_2. The integrals over the variables $x_3, x_4, \cdots, x_{n-1}$ are identical, the only difference being in the integrals over x_1 and x_2. To symbolize this the notation $\int_\xi$ will be used to represent the integrals over $x_3, x_4, \cdots, x_{n-1}$ with appropriate limits, and the number $\xi = x_3 + x_4 + \cdots + x_{n-1}$.

$$I = \int_\xi \left\{ \int_0^{1-\xi} dx_2 \int_0^{1-\xi-x_2} \frac{dF}{dx_1}\, dx_1 - \int_0^{1-\xi} dx_1 \int_0^{1-\xi-x_1} \frac{dF}{dx_2}\, dx_2 \right\}.$$

After integration and substitution of the limits of integration

$$I = \int_\xi \left\{ \int_0^{1-\xi} dx_2 \,[F(1 - \xi - x_2, x_2, x_3, \cdots, x_{n-1}, 0) - F(0, x_2, x_3, \cdots, x_{n-1}, 1 - \xi - x_2)] - \int_0^{1-\xi} dx_1 \,[F(x_1, 1 - \xi - x_1, x_3, \cdots, x_{n-1}, 0) - F(x_1, 0, x_3, \cdots, x_{n-1}, 1 - \xi - x_1)] \right\}.$$

The first term in the integral over x_1 and x_2 cancel each other out identically which can be seen by making the substitution $\eta = x_2$ in the x_2 integral and $\eta = 1 - \xi - x_1$ in the second. Thus I is given by

$$I = \int_\xi \left\{ \int_0^{1-\xi} dx_1\, F(x_1, 0, x_3, \cdots, x_{n-1}, 1 - \xi - x_1) - \int_0^{1-\xi} dx_2\, F(0, x_2, x_3, \cdots, x_{n-1}, 1 - \xi - x_2) \right\},$$

but this is just the required answer if the δ functions on the right-hand side of (A1) are used to do two integrals. The specialization to 1, 2, and n is not necessary but saves some notation. If there are only two variables x_1 and x_2 the proof is trivial.

Lemma II: If $F_{ab} = -F_{ba}$ and $F_a = \sum_{b=1}^m F_{ab}$ $(a, b = 1, 2, \cdots, m)$, then

$$\sum_{a=1}^m F_a = 0. \qquad \text{(A2)}$$

Proof:

$$\begin{aligned}\sum F_a &= \sum\sum F_{ab} \\ &= \sum_{a>b} (F_{ab} + F_{ba}) \\ &= \sum 0 = 0.\end{aligned}$$

Lemma III: Given a set of functions F_a such that $\sum F_a = 0$, there is at least one set of functions F_{ab} with $F_{ab} = -F_{ba}$ such that

$$F_a = \sum_b F_{ab}.$$

Proof: Write the functions F_{ab} as an m by m matrix a suitable choice is

$$\begin{bmatrix} 0 & 0 & \cdots & 0 & F_1 \\ 0 & 0 & \cdots & 0 & F_2 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & F_{n-1} \\ -F_1 & -F_2 & \cdots & -F_{n-1} & 0 \end{bmatrix}.$$

Theorem: If $\sum F_a = 0$ then

$$I = \int \sum \frac{\partial F_a}{\partial x_a} = -\sum_a \int_a F_a. \qquad \text{(A3)}$$

Since $\sum F_a = 0$, Lemma III may be applied to determine a set of functions F_{ab}. The integrand of the left-hand side of (A3) is modified by the following sequence of steps:

$$\begin{aligned}\sum_a \partial F_a/\partial x_a &= \sum_a \sum_b \partial F_{ab}/\partial x_a \\ &= \sum_a \sum_b \partial F_{ba}/\partial x_b \\ &= -\sum_a \sum_b \partial F_{ab}/\partial x_b \\ &= \tfrac{1}{2} \sum_a \sum_b (\partial F_{ab}/\partial x_a - \partial F_{ab}/\partial x_b).\end{aligned}$$

Thus we have

$$I = \tfrac{1}{2} \sum_a \sum_b \int (\partial F_{ab}/\partial x_a - \partial F_{ab}/\partial x_b),$$

Lemma I may be applied to integrate this, and finally some substitutions and the properties of the functions F_{ab} to complete the proof:

$$\begin{aligned}I &= \tfrac{1}{2} \sum_a \sum_b \left\{ \int_b F_{ab} - \int_a F_{ab} \right\} \\ &= \sum_a \sum_b \left\{ \int_b F_{ab} - \int_b F_{ba} \right\} \\ &= \sum_a \sum_b \int_b F_{ab} \\ &= -\sum_b \int_b F_b.\end{aligned}$$

APPENDIX II

$$\begin{aligned}\partial\Delta/\partial\alpha_1 &= m^2(\alpha_3^2 + \alpha_4^2 + \alpha_5^2) + 2m^2\alpha_1\alpha_3 + 2m^2\alpha_1\alpha_4 \\ &\quad + 2m^2\alpha_1\alpha_5 + (P^2 + 2m^2)\alpha_2\alpha_3 + (P^2 + 2m^2)\alpha_2\alpha_4 \\ &\quad + (P^2 + 2m^2)\alpha_2\alpha_5 + (P^2 + 2m^2)\alpha_3\alpha_4 \\ &\quad + (P^2 + 3m^2)\alpha_3\alpha_5 + 3m^2\alpha_4\alpha_5, \\ \partial\Delta/\partial\alpha_2 &= m^2(\alpha_3^2 + \alpha_4^2 + \alpha_5^2) + (P^2 + 2m^2)\alpha_1\alpha_3 \\ &\quad + (P^2 + 2m^2)\alpha_1\alpha_4 + (P^2 + 2m^2)\alpha_1\alpha_5 \\ &\quad + 2m^2\alpha_2\alpha_3 + 2m^2\alpha_2\alpha_4 + 2m^2\alpha_2\alpha_5 + (P^2 + 2m^2)\alpha_3\alpha_4 \\ &\quad + 3m^2\alpha_3\alpha_5 + (P^2 + 3m^2)\alpha_4\alpha_5, \\ \partial\Delta/\partial\alpha_3 &= m^2(\alpha_1^2 + \alpha_2^2 + \alpha_5^2) + (P^2 + 2m^2)\alpha_1\alpha_2 \\ &\quad + 2m^2\alpha_1\alpha_3 + (P^2 + 2m^2)\alpha_1\alpha_4 \\ &\quad + (P^2 + 3m^2)\alpha_1\alpha_5 + 2m^2\alpha_2\alpha_3 + (P^2 + 2m^2)\alpha_2\alpha_4 \\ &\quad + 3m^2\alpha_2\alpha_5 + 2m^2\alpha_3\alpha_5 + (P^2 + 2m^2)\alpha_4\alpha_5, \\ \partial\Delta/\partial\alpha_4 &= m^2(\alpha_1^2 + \alpha_2^2 + \alpha_5^2) + (P^2 + 2m^2)\alpha_1\alpha_2 \\ &\quad + (P^2 + 2m^2)\alpha_1\alpha_3 + 2m^2\alpha_1\alpha_4 + 3m^2\alpha_1\alpha_5 \\ &\quad + (P^2 + 2m^3)\alpha_2\alpha_3 + 2m^2\alpha_2\alpha_4 + (P^2 + 3m^2)\alpha_2\alpha_5 \\ &\quad + (P^2 + 2m^2)\alpha_3\alpha_5 + 2m^2\alpha_4\alpha_5, \\ \partial\Delta/\partial\alpha_5 &= m^2(\alpha_1^2 + \alpha_2^2 + \alpha_3^2 + \alpha_4^2) + (P^2 + 2m^2)\alpha_1\alpha_2 \\ &\quad + (P^2 + 3m^2)\alpha_1\alpha_3 + 3m^2\alpha_1\alpha_4 + 2m^2\alpha_1\alpha_5 \\ &\quad + 3m^2\alpha_2\alpha_3 + (P^2 + 3m^2)\alpha_2\alpha_4 + 2m^2\alpha_2\alpha_5 \\ &\quad + (P^2 + 2m^2)\alpha_3\alpha_4 + 2m^2\alpha_3\alpha_5 + 2m^2\alpha_4\alpha_5.\end{aligned}$$

APPENDIX III

$$\begin{aligned}P_1 &= A\alpha_1^2 + B\alpha_2^2 + C\alpha_3^2 + D\alpha_4^2 + E\alpha_5^2 + F\alpha_1\alpha_2 \\ &\quad + G\alpha_1\alpha_3 + H\alpha_1\alpha_4 + I\alpha_1\alpha_5 + J\alpha_2\alpha_3 + K\alpha_2\alpha_4 \\ &\quad + L\alpha_2\alpha_5 + M\alpha_3\alpha_4 + N\alpha_3\alpha_5 + O\alpha_4\alpha_5, \\ P_2 &= B\alpha_1^2 + A\alpha_2^2 + D\alpha_3^2 + C\alpha_4^2 + E\alpha_5^2 + F\alpha_1\alpha_2 \\ &\quad + K\alpha_1\alpha_3 + J\alpha_1\alpha_4 + L\alpha_1\alpha_5 + H\alpha_2\alpha_3 + G\alpha_2\alpha_4 \\ &\quad + I\alpha_2\alpha_5 + M\alpha_3\alpha_4 + O\alpha_3\alpha_5 + N\alpha_4\alpha_5, \\ P_3 &= C\alpha_1^2 + D\alpha_2^2 + A\alpha_3^2 + B\alpha_4^2 + E\alpha_5^2 + M\alpha_1\alpha_2 \\ &\quad + G\alpha_1\alpha_3 + J\alpha_1\alpha_4 + N\alpha_1\alpha_5 + H\alpha_2\alpha_3 + K\alpha_2\alpha_4 \\ &\quad + O\alpha_2\alpha_5 + F\alpha_3\alpha_4 + I\alpha_3\alpha_5 + L\alpha_4\alpha_5, \\ P_4 &= D\alpha_1^2 + C\alpha_2^2 + B\alpha_3^2 + A\alpha_1^2 + E\alpha_5^2 + M\alpha_1\alpha_2 \\ &\quad + K\alpha_1\alpha_3 + H\alpha_1\alpha_4 + O\alpha_1\alpha_5 + J\alpha_2\alpha_3 + G\alpha_2\alpha_4 \\ &\quad + N\alpha_2\alpha_5 + F\alpha_3\alpha_4 + N\alpha_3\alpha_5 + I\alpha_4\alpha_5, \\ P_5 &= P^2(\alpha_1^2 + \alpha_2^2 + \alpha_3^2 + \alpha_4^2) + Q\alpha_5^2 + R\alpha_1\alpha_2 \\ &\quad + S\alpha_1\alpha_3 + T\alpha_1\alpha_4 + U\alpha_2\alpha_5 + T\alpha_2\alpha_3 + S\alpha_2\alpha_4 \\ &\quad + U\alpha_2\alpha_5 + R\alpha_3\alpha_4 + U\alpha_3\alpha_5 + U\alpha_4\alpha_5.\end{aligned}$$

APPENDIX IV

The coefficients from which the equations come are listed on the left.

$$\alpha_1^4 : C + D + P = 0,$$

$$\alpha_1^3\alpha_2 : 2M + R = 0,$$

$$\alpha_1^3\alpha_4 : 2m^2A + (P^2 + 2m^2)B + P^2C + m^2(H + J + P + T) = 0,$$

$$\alpha_1^3\alpha_5 : 2m^2A + (P^2 + 2m^2)B + (P^2 + m^2)C + m^2D + m^2(N + O + U) = 0,$$

$$\alpha_5^4 : E = 0,$$

$$\alpha_1^2\alpha_3^2 : 2m^2(A + B) + 4m^2G + 2(P^2 + 2m^2)K + 2m^2P + (P^2 + 3m^2)S = 1,$$

$$\alpha_1^2\alpha_4^2 : 2m^2(A + B) + 4m^2H + 2(P^2 + 2m^2)J + 2m^2P + 3m^2T = 1,$$

$$\alpha_1^2\alpha_5^2 : m^2(A + B + C + D) + 2m^2I + (P^2 + 2m^2)L + (P^2 + 3m^2)N + 3m^2O + m^2Q + 2m^2U = 1,$$

$$\alpha_1^2\alpha_2\alpha_4 : (P^2 + 2m^2)A + 2m^2B + P^2C + (P^2 + 4m^2)F + m^2G + (P^2 + 2m^2)H + (P^2 + 2m^2)J + m^2K + (P^2 + 4m^2)M + (P^2 + m^2)P + 3m^2R + m^2S + (P^2 + 2m^2)T = 0,$$

$$\alpha_1^2\alpha_2\alpha_5 : (P^2 + 2m^2)A + 2m^2B + m^2C + (P^2 + m^2)D + (P^2 + 4m^2)F + (P^2 + 2m^2)M + (P^2 + 3m^2)(N + O + U) = 0,$$

$$\alpha_1^2\alpha_2\alpha_3 : (P^2 + 2m^2)A + 2m^2B + P^2D + (P^2 + 4m^2)F + (P^2 + 2m^2)G + m^2H + m^2J + (P^2 + 2m^2)K + P^2M + m^2P + (P^2 + m^2)R + (P^2 + 2m^2)S + m^2T = 0,$$

$$\alpha_1^2\alpha_4\alpha_5 : 3m^2A + (P^2 + 3m^2)B + P^2C + 5m^2H + 3m^2I + (2P^2 + 5m^2)J + (P^2 + 3m^2)L + (P^2 + 2m^2)N + 2m^2(O + T) + 4m^2U = 2,$$

$$\alpha_1\alpha_2\alpha_3\alpha_5 : (P^2 + 6m^2)F + (P^2 + 5m^2)G + (2P^2 + 5m^2)H + 3(P^2 + 2m^2)I + 5m^2J + (P^2 + 5m^2)K + (P^2 + 6m^2)L + P^2M + (P^2 + 4m^2)(N + O) + 2m^2(S + T) + 2P^2 + 8m^2U = 4,$$

$$\alpha_1\alpha_2\alpha_5^2 : 2m^2F + 2(P^2 + 2m^2)I + 4m^2L + 2m^2M + 6m^2N + 2(P^2 + 3m^2)O + (P^2 + 2m^2)Q + 4m^2U = 2,$$

$$\alpha_1\alpha_3\alpha_5^2 : 2m^2G + 2(P^2 + 3m^2)I + 2m^2K + 6m^2L + 4m^2N + 2(P^2 + 2m^2)O + (P^2 + 3m^2)Q + 4m^2 = 2,$$

$$\alpha_1\alpha_4\alpha_5^2 : 2m^2H + 6m^2I + 2m^2J + 2(P^2 + 3m^2)L + 2(P^2 + 2m^2)N + 4m^2O + 3m^2Q + 4m^2U = 2,$$

$$\alpha_1\alpha_5^3 : I + L + N + O + 2Q = 0.$$

APPENDIX V

$$3m^2A = (P^2 + 5m^2)B - (P^2 + 2m^2)C + (P^2 + 2m^2)/(3P^2 + 9m^2),$$

$$B = B,$$

$$C = C,$$

$$m^2D = (P^2 + 4m^2)B - (P^2 + 2m^2)C + (P^2 + 2m^2)/(3P^3 + 9m^2),$$

$$E = 0,$$

$$3m^2F = (P^2 + 8m^2)B + 2(P^2 - m^2)C - [2(P^2 - m^2)/(3P^2 + 9m^2)],$$

$$3m^3G = (P^2 + 5m^2)B + 2(P^2 + 2m^2)C + (P^2 + 11m^2)/(3P^2 + 9m^2),$$

$$3m^2H = (4P^2 + 17m^2)B - 4(P^2 + 2m^2)C + [4(P^2 + 5m^2)/(3P^2 + 9m^2)],$$

$$3I = 8B - 2C + 11/(3P^2 + 9m^2),$$

$$J = B + 2C + 1/(3P^2 + 9m^2),$$

$$m^2K = (P^2 + 5m^2)B = 2m^2C + 4m^2/(3P^2 + 9m^2),$$

$$L = 4B - 2C + 4/(3P^2 + 9m^2),$$

$$m^2M = (P^2 + 4m^2)B - 2m^2C + (P^2 + 4m^2)/(3P^2 + 9m^2).$$

$$N = 2C + 1/(3P^2 + 9m^2),$$

$$O = 4B - 2C + 6/(3P^2 + 9m^2),$$

$$m^2P = -(P^2 + 4m^2)B + (P^2 + 2m^2)C - (P^2 + 4m^2)/(3P^2 + 4m^2),$$

$$3Q = -16B + 4C - 22/(3P^2 + 9m^2),$$

$$m^2R = -2(P^2 + 4m^2)B + 4m^2C - 2(P^2 + 4m^2)/(3P^2 + 9m^2),$$

$$m^2S = -2(P^2 + 4m^2)B - 5m^2/(3P^2 + 9m^2),$$

$$m^2T = -2(P^2 + 4m^2)B - (P^2 + 5m^2)/(3P^2 + 9m^2),$$

$$3m^2U = -8(P^2 + 5m^2)B + 2(2P^2 + 5m^2)C - (5P^2 + 37m^2)/(3P^2 + 9m^2).$$

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Construction of the Charge Operator for Higher Symmetry Schemes*

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(Received 18 September 1964)

The problem of the construction of an additively conserved operator with integral eigenvalues, to be identified with the electric charge is solved in complete generality for the groups locally isomorphic to $U(1) \otimes SU(n)$. It is found that the representations fall into classes on which different charge operators may be defined. Several results previously obtained for particular classes of representations are found here as special cases. We specialize the results to $N = 4$ and discuss several models presently in the literature.

I. INTRODUCTION

SYMMETRIES for the strongly interacting particles beyond that of the familiar eightfold way of Gell-Mann and Ne'eman[1] have been proposed by many authors. In particular we might mention models based on $U(3)$,[2] W_3,[3] $SU(4)$,[4-7] and $Sp(6)$.[8] Experience with these theories has indicated that the requirement that there exist an additively conserved quantum number with integral eigenvalues, to be identified with the electric charge provides limitations on the types of models which can be considered and it is of interest to determine the general form which these limitations take. Discussion of this question has been initiated by Hagen and Macfarlane[9] who show how to construct an operator which satisfies the above criteria for the plurality zero representations of $SU(n)$. Okubo, Marshak, and Ryan[10] have proposed a solution which involves considering $U(3)$ rather than $U(1) \otimes SU(3)$.[11] In the present work, we discuss the groups locally isomorphic to $U(1) \otimes SU(n)$ using a different method and with greater generality than Ref. (9), and construct valid charge operators for a much wider class of representations. In particular the results of Hagen and Macfarlane for plurality zero representations are obtained as a special case.

It is clear that the most general form for the charge operator is a linear combination of the diagonal generators of the Lie algebra. That is,

$$Q = \sum_{i=1}^{n-1} \gamma_i Y^{(i)} + \gamma_b B, \tag{1}$$

where the $Y^{(i)}$ are particular combinations of the diagonal generators of the Lie algebra of $SU(n)$ defined previously[5] and B is the generator of the

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$$m^2P = -(P^2 + 4m^2)B + (P^2 + 2m^2)C - (P^2 + 4m^2)/(3P^2 + 4m^2),$$

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$U(1)$ transformations which we explicitly identify with the baryon gauge group. Since the eigenvalues of B are integral it is clear that for the purposes of finding all possible γ_i and γ_b we may require $0 \leq \gamma_b < 1$. In particular, the case $\gamma_b = 0$ is conveniently treated separately from $\gamma_b \neq 0$.

If all the states of a particular representation $\mathbf{L}$ of the algebra of $U(1) \otimes SU(n)$ have integral charge then, since the adjoint representation is always contained at least once[12] in the decomposition $\mathbf{L} \otimes \mathbf{L}^\dagger$ we must have integral charges for the adjoint representation as well. This follows from the fact that weights are combined linearly with integral coefficients in the decomposition of a direct product and, from (1), so is Q. However, the nonzero weights of the adjoint representation are the roots of the Lie algebra and since for any representation the roots are differences of weights, we see that all the states of a representation have integral charge if and only if the highest weight of that representation and the simple roots of the algebra[13] have integral charge. It is the latter two requirements that we study.

In the next section, we obtain conditions for the charges of an arbitrary representation to be integral, first for the case $\gamma_b = 0$ and then for $0 < \gamma_b < 1$. In Sec. III we consider some specific models for the charge operator. In the Appendix we consider the problem of finding all homomorphisms of $R \otimes SU(n)$ defined by

$$R \otimes SU(n)/\Delta_i = F_i, \tag{2}$$

where Δ_i is a discrete normal subgroup of $R \otimes SU(n)$, and show that this problem is equivalent to that solved in Sec. II. The main results of the paper are Eqs. (12)–(14) and (17) which allow one to determine all possible γ's of Eq. (1).

II. THE CHARGE OPERATOR

An irreducible representation $\mathbf{L}$, of $SU(n)$ is uniquely specified by giving the $n - 1$ components of its highest weight, L. This highest weight[14] can be decomposed uniquely as the sum

$$L = \sum_{i=1}^{n-1} \beta_i L^{(i)}, \tag{3}$$

where β_i are nonnegative integers and the $L^{(i)}$ are the fundamental weights. These are the highest weights of the $n - 1$ fundamental representations $\mathbf{L}^{(i)}$ which are the representations induced on completely antisymmetric tensors of rank i. $\mathbf{L}^{(1)}$, in particular, is the defining representation of $n \times n$ unitary unimodular matrices. In terms of the $Y^{(i)}$ the highest weights $L^{(i)}$ take the form

$$\begin{aligned} L^{(1)} &= 1/2, 1/3, 1/4, \cdots, 1/n \\ L^{(2)} &= 0, 2/3, 2/4, \cdots, 2/n \\ L^{(3)} &= 0, 0, 3/4, \cdots, 3/n \\ &\vdots \\ L^{(n-1)} &= 0, 0, 0, \cdots, (n-1)/n. \end{aligned} \tag{4}$$

We also need an explicit expression for the $n - 1$ simple roots of $SU(n)$ considered as weights for the adjoint representation. The simple roots are sufficient since any root (and hence any nonzero weight of the adjoint representation) may be written as the sum of simple roots with integral coefficients. If we call the simple roots $l^{(i)}$ then we have

$$\begin{aligned} l^{(1)} &= 1, 0, 0, \cdots, 0 \\ l^{(2)} &= -\tfrac{1}{2}, 1, 0, \cdots, 0 \\ &\vdots \\ l^{(i)} &= 0, 0, \cdots, -i/(i-1), 1, \cdots, 0 \\ l^{(n-1)} &= 0, 0, \cdots, -(n-2)/(n-1), 1. \end{aligned} \tag{5}$$

Corresponding to (3) and (4) we have the charge of the highest weight of the representation L specified by $\{\beta_1, \beta_2, \cdots, \beta_{n-1}\}$ is

$$\begin{aligned} Q^L = \gamma_1\beta_1/2 + \gamma_2(\beta_1 + 2\beta_2)/3 + \cdots + \gamma_{n-1} \\ \times (\beta_1 + 2\beta_2 + \cdots + [n-1]\beta_{n-1})/n + \gamma_b B, \end{aligned} \tag{6}$$

while for the ith simple weight of (5)

$$Q^i = \gamma_i - (i-1)/i\gamma_{i-1} + \gamma_b B. \tag{7}$$

In accordance with the remarks made in the introduction for the charges of *all* the states of $\mathbf{L}$ to be integral it is necessary and sufficient for the left-hand sides of Eqs. (6) and (7) to be integral.

Let us rewrite Eq. (6) by introducing a new parameter, λ_i, defined by

$$\begin{aligned} \beta_i &= \lambda_i - \lambda_{i+1} \quad i = 1, 2, \cdots, n-2 \\ \beta_{n-1} &= \lambda_{n-1}. \end{aligned} \tag{8}$$

The λ_i are thus the parameters which give the number of columns in the ith row of the Young diagram describing the tensor character of $\mathbf{L}$.

Some simple manipulation then yields

[12] J. Ginibre, J. Math. Phys. 4, 720 (1963).

[13] E. B. Dynkin, "The Structure of Semi Simple Algebras," A. M. S. Trans. Series 1, Vol. 9 (1962).

[14] We define the relation $>$ for weights by saying that a weight is positive if its *last* nonvanishing component is > 0. This simplifies the formulas.

$$Q^L = \lambda_1\gamma_1 + (\lambda_1 + \lambda_2)(\gamma_2 - \tfrac{1}{2}\gamma_1) + \cdots + (\lambda_1 + \lambda_2 + \cdots + \lambda_{n-1}) \times \left(\gamma_{n-1} - \frac{n-2}{n-1}\gamma_{n-2}\right) - \gamma_{n-1}\frac{n-1}{n}\sum_{i=1}^{n-1}\lambda_i + \gamma_b B. \quad (9)$$

Thus considering (7), it is necessary that

$$I \equiv \gamma_{n-1}\frac{n-1}{n}\sum_{i=1}^{n-1}\lambda_i + \gamma_b B \quad (10)$$

be an integer for the charges of **L** to be integers.

Let us first consider $\gamma_b = 0$. Then we may clearly distinguish various possibilities by considering the cases

$$\sum_{i=1}^{n-1}\lambda_i = 0 \bmod \frac{n}{\kappa}, \quad (11)$$

where κ runs through the divisors of n. We remark that the quantity $\sum_{i=1}^{n-1}\lambda_i \bmod (n)$ is the plurality of the representation **L** as defined by Hagen and Macfarlane[9] and is conserved when reducing the Clebsch–Gordan series of an inner product. Thus if a representation **L**, given by a set of λ_i, satisfies (11) for a given κ so will all inner products of **L** times itself and **L** times the adjoint representation [since the adjoint representation satisfies (11) for $\kappa = 1$]. But this is just what is required if **L** is to have integral charges (i.e., all representations in the above-mentioned class should have integral charges as well). Thus if we call representations of class κ those which satisfy (11) then we can find a proper charge operator for all representations of this class (for $\gamma_b = 0$) by solving (7) and (10) for the allowed γ_i. Conversely, an integral charge operator for a particular representation of class κ must also be integral for all other representations of this class. We will later see that representations of class κ are actually representations of different, locally isomorphic, groups.

Suppose we fix our attention on representations of class κ. Then from (10) we immediately have

$$\gamma_{n-1} = r_{n-1}/(n-1), \quad (12)$$

where r_{n-1} is an integer such that

$$r_{n-1} = 0 \bmod \kappa. \quad (13)$$

Then from (7) we obtain the complete solution

$$\gamma_i = i^{-1}\sum_{j=1}^{n-1} r_j \Big/ i \quad (14a)$$

where

$$r_j = 0 \bmod j+1 \qquad j < n-1. \quad (14b)$$

The set (13), (14), and (15) are the most general solution to the problem of constructing the charge operator for γ_b an integer.

Now let us take γ_b not an integer. It is immediately clear that if a solution for the charge operator exists it cannot be for a theory in which we may assign baryon number arbitrarily to representations of $SU(n)$. That is if $\mathbf{L}_B$ is a representation with integer charges for noninteger γ_b then $\mathbf{L}_{B+1}$ cannot have integer charges. Thus the class of representations which admit a solution for a given charge operator are not representations of a group which has $U(1)$ as a direct product factor. Because of the ambiguities involved with the automorphisms of the Abelian group $U(1)$ it is quite complicated to repeat the arguments of the first part of this section here although this may be done. Instead we shall make use of the results of the Appendix to obtain the formula, analogous to (11), which expresses the class of representations on which we should define the charge operator. This is

$$\sum \lambda_i + b = 0 \bmod (n/\kappa). \quad (15)$$

As in (11), κ runs through the divisors of n and we have defined b to be the baryon number.

Now all the arguments establishing (7) and (9) as necessary and sufficient conditions for the representation $\mathbf{L}_B$ to have integer charges are still valid since the adjoint representation with $B = 0$ is contained in the inner product of $\mathbf{L}_B$ with its conjugate. Consider (15) with $b = 0$ which yields all the representations of class κ of Eq. (11). Since the charge operator is to be integral for all representations of class κ of (15), we see that for $b = 0$ it must be an integral charge operator for all representations of calss κ of (11) as well, thus the γ_i are given by (14). So for $b \neq 0$ we have only to satisfy

$$(r_{n-1}/n)\sum \lambda_i - \gamma_b b = \text{integer}, \quad (16)$$

where $r_{n-1} = 0 \bmod \kappa_1$ and λ_i and b satisfy (15). The solution to this is clearly

$$\gamma_b = -r_{n-1}/n \quad (17)$$

and we thus have the complete solution to the case where $\gamma_b \neq 0$ for the class κ defined by (15).

III. DISCUSSION

We have obtained the most general possibilities for constructing a charge operator with integer eigenvalues in Sec. II. In general we found that it was consistent to ask that the charge operator be defined on a class κ given by (11) or (15) correspond-

ing to representations of $U(1) \otimes SU(n)/Z_{n/\kappa}$ and $U^{(\kappa)}(n)$. [See (A12) and (A15).] For a class κ, the coefficients γ_i and γ_b are determined by (12)–(14) and γ_b = integer for $U(1) \otimes SU(n)/Z_{n/\kappa}$, and (12)–(14) and (17) for $U^{(\kappa)}(n)$. It is interesting that there is a one-to-one correspondence between the charge operators defined for γ_b = integer and those for γ_b not an integer.

Let us consider $\gamma_b = 0$, $r_{n-1} = 1$, $r_{i\neq n-1} = 0$. Then we have

$$\gamma_l = 1/l \tag{18}$$

which is precisely the solution of Hagen and Macfarlane[9] for plurality zero representations of $SU(n)$. If we consider the solution for $\gamma_b \neq 0$ corresponding to this we get [in addition to (18)] from (17),

$$\gamma_b = 1/n. \tag{19}$$

This is the generalization to $U(n)$ of the proposal of Okubo, Marshak, and Ryan[10] for $U(3)$.

Several models for $n = 4$ have been proposed recently. In particular, in Ref. (5) we have (18) and hence a model based on $U(1) \otimes SU(4)/Z_4$. In models (1) and (2) of Amati, Bacry, Nuyts, and Prentki,[7] (19) obtains so this model is more correctly described as based on $U(4)$. For their model (3) and (4)

$$Q = y^{(1)} + \tfrac{1}{2}y^{(2)} - \tfrac{2}{3}y^{(3)} + \tfrac{1}{2}B \tag{20}$$

which follows from

$$r_3 = -2, \qquad r_2 = 3, \qquad r_1 = 0.$$

Since $r_3 = 0$ mod (2), this model accommodates integral charges for all representations of $U^{(2)}(4)$. Thus the limitation imposed by a fundamental quartet for this model [which effectively restricts it to representations of $U(4)$] is, perhaps, too confining.

Although the choice of the charge operator within a class κ, i.e., the choice of the r_i, is independent of group theory, the division of representations into these classes, which are distinguished by the charge operator they admit, is quite interesting. To reverse the statement, a choice of charge operator picks out a maximal class κ and thus defines the particular full Lie group which is relevant to the theory being considered. Groups of the type $U^{(\kappa)}(n)$ are particularly interesting since here we have definite relations (15) between the baryon number b and the possible $SU(n)$ representations.

It should be emphasized that, although the values $\gamma_1 = 1$, $\gamma_2 = \frac{1}{2}$ are well established by experiment, if the higher symmetries proposed are meaningful then we are allowed any γ_3 consistent with the restrictions found in Sec. II and we should consider all their implications to determine which choice is actually realized.

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APPENDIX: LOCAL ISOMORPHISMS OF $U(1) \otimes SU(n)$

In this appendix we consider the significance of the classes of representations (11) and (15). It is well known that to a given Lie algebra there corresponds several, locally isomorphic, Lie groups. To a semisimple Lie algebra there corresponds a unique, simply connected Lie group G the universal covering group. All other Lie groups with the same algebra are obtained as factor groups of G.

$$F_i = G/\Delta_i, \tag{A1}$$

where Δ_i is a discrete normal subgroup of G and thus is a subgroup of its center, Z. The universal covering group for our problem is $R \otimes SU(n)$ where R is the additive group of the real numbers.[15]

The discrete central normal subgroups of $R \otimes SU(n)$ fall into two distinct classes:

(1) Those whose generators are products of the identity of one of them times a generator of a central normal subgroup of the other.

(2) Those whose generators are products of nontrivial generators of the central normal subgroups of each of them.

We first consider groups Δ_i of the type (1) as defined above. Since we wish to have integral baryon number we take one of the generating elements of Δ_i to be $(2\pi, 1)$ which defines the homomorphism

$$R \otimes SU(n) \to U(1) \otimes SU(n).$$

The other generator will be of the form $(0, \omega_i)$. Thus $U(1)$ is always a direct factor of the resulting group and we can ignore it in the following. We emphasize however that this implies that the baryon number B is unrelated to any other quantum number in this scheme.

The center Z_n of $SU(n)$ is a discrete group isomorphic to the multiplicative group of the nth roots of unity and we may denote it as the collection,

$$(\omega_1, \omega_2, \cdots, \omega_n) = Z_n. \tag{A3}$$

[15] See L. Michel, Istanbul Summer School (1962) (to be published).

It is clear that any element ω_i, except one for which i is a divisor of n may be taken as a generator for this group. The distinct subgroups of Z_n are given by

$$Z_{n/\kappa},\ Z_{n/\lambda},\ \cdots,$$

where n/κ, n/λ, $\cdots$, are integers. The group $Z_{n/\kappa}$ is composed of elements

$$[(\omega_1)^\kappa = \omega_\kappa, \omega_{2\kappa} \cdots \omega_{(n/\kappa)\cdot\kappa} = \omega_n = 1] = Z_{n/\kappa} \quad \text{(A4)}$$

and the remarks concerning generating elements of (3) also apply here.

In the defining representation $\mathbf{L}^{(1)}$ it is clear that the elements ω_i are represented by

$$L^{(1)}: \omega_i \to \epsilon_i \mathbf{1}, \quad \text{(A5)}$$

where $\epsilon_i = e^{2\pi i i/n}$. Moreover, from the definition of $L^{(l)}$ as the totally antisymetric projection of $L^{(1)} \otimes L^{(1)} \cdots L^{(1)}$ l times, in this representation we have

$$L^{(l)}: \omega_i \to (\epsilon_i)^l l = \epsilon_{li} \mathbf{1}, \quad \text{(A6)}$$

where subscripts on epsilons are always meant to be taken modulo n. Now in the representation whose highest weight is given by

$$L: [\beta_1, \beta_2, \cdots, \beta_{n-1}] \quad \text{(A7)}$$

of Eq. (2) we clearly have, using (A6),

$$L: \omega_i \to (\epsilon_i)^{\beta_1}(\epsilon_i)^{2\beta_2} \cdots (\epsilon_i)^{(n-1)\beta_{n-1}} \mathbf{1}, \quad \text{(A8)}$$

or

$$L: \omega_i \to \epsilon_{i[\beta_1 + 2\beta_2 + \cdots + (n-1)\beta_n]} \mathbf{1}. \quad \text{(A9)}$$

In order that all the elements of $Z_{n/\kappa}$ be represented by the identity it is clearly necessary and sufficient that any generator of $Z_{n/\kappa}$ be represented by the identity, or, using (4)

$$\kappa(\beta_1 + 2\beta_2 + \cdots + n - 1\beta_n) = 0 \bmod n. \quad \text{(A10)}$$

In virtue of the fact that κ is a divisor of n we obtain that a representation of $SU(n)$ is a representation of $SU(n)/Z_{n/\kappa}$ if the components of the highest weights of the representation satisfy

$$\sum_{i=1}^{n-1} i\beta_i = 0 \bmod \frac{n}{\kappa}. \quad \text{(A11)}$$

In terms of the λ_i(11) becomes

$$\sum_{i=1}^{n-1} \lambda_i = 0 \bmod \frac{n}{\kappa}. \quad \text{(A12)}$$

which is identical to (11) defining the class, κ, of representations.

Now let us consider homomorphisms of type (2), those for which a generating element of Δ_i contains generators of discrete subgroups of both R and $SU(n)$. In order to obtain these homomorphisms we must consider the structure of R, the additive group of the reals in more detail. The discrete subgroups of this group are generated by α_0 where α_0 is arbitrary. For different α_0 we generate isomorphic groups. A representation of R is given by $e^{i\alpha b}$ and denoted b where b is a fixed number. Now consider the generating element

$$(2\pi/n, \omega_\kappa), \quad \text{(A13)}$$

which generates a discrete subgroup of $R \times SU(n)$, and the representation defined by the mapping

$$(\alpha, \theta) \to e^{i\alpha b}\mathbf{L}(\theta) \quad \text{(A14)}$$

of the same group where we multiply the matrix $\mathbf{L}$ by the factor $e^{i\alpha b}$. Then using (9) for the representative of ω_i in the representation L we clearly see we must have

$$\sum_{i=1}^{n-1} i\beta_i + b = 0 \bmod \frac{n}{\kappa} \quad \text{(A15a)}$$

$$b = \text{integer} \quad \text{(A15b)}$$

in order that the generating element (21) be mapped into unity in this representation. Thus we may identify b with the baryon number since it is integral. (A15a) is recognized as defining a class of representations just as did (A12). Using the λ_i this equation becomes (15) which we now see is the correct generalization of (11) for the case where we wish to include the baryon number in a nontrivial way.

For the case $\kappa = 1$ (A15a) defines representations of $U(n)$. When $\kappa \neq 1$ we write $U^{(\kappa)}(n)$ to distinguish the group defined by (15). Since (23) yields a relation between b and the β_i we see we are not free to assign baryon number arbitrarily to the representation $\mathbf{L}$ of $SU(n)$. Such restrictions are well known in the Sakata model based on $U(3)$ and if we wish to use the baryon number in our definition of charge we must accept them.

We might mention that there are no other nonisomorphic solutions to the mapping problem (1) with the generating element (13) other than (15).

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Transformation Having Applications in Quantum Mechanics

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By properly ordering functions of noncommuting operators, a one-to-one transformation between operator functions and corresponding functions of commuting algebraic variables can be made. With this transformation, boson operator equations such as the Schrödinger equation can be converted to differential equations for the transformed functions, the resulting equations containing solely commuting variables. Once the solution to the transformed equation is obtained, the inverse transformation may be applied to yield the solution to the original operator equation. The method is extended to include angular momentum operators.

1. INTRODUCTION

THE general solution for the time evolution of a quantum state is

$$|\psi(t)\rangle = U_{tt_0}\,|\psi(t_0)\rangle, \tag{1.1}$$

where U_{tt_0} is the unitary transformation satisfying the Schrödinger equation

$$i\hbar\,\partial U_{tt_0}/\partial t = \mathfrak{IC}(t)U_{tt_0} \tag{1.2}$$

subject to the initial condition $U_{t_0t_0} = 1$. Formally, U_{tt_0} may be written as

$$U_{tt_0} = P\left\{\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}\mathfrak{IC}(t')\,dt'\right]\right\}, \tag{1.3}$$

where P is the time-ordering operator. If the exponential is expanded and the time ordering is performed, one obtains

$$U_{tt_0} = 1 - \frac{i}{\hbar}\int_{t_0}^{t}\mathfrak{IC}(t')\,dt' + \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}dt''\times\int_{t_0}^{t''}dt'\mathfrak{IC}(t')\mathfrak{IC}(t'') + \cdots, \tag{1.4}$$

the standard time-dependent perturbation relation.

There is another method of solution which is particularly effective for the solution of operator differential equations which involve operators obeying commutator (as opposed to anticommutator) relations. This method, which is described here, also involves an ordering procedure, but an ordering of operators rather than a time ordering. Once the ordering has been performed, a unique correspondence can be made between the operator function and an equivalent function of commuting variables. The operator differential equation is then transformed into an equivalent algebraic variable differential equation and can be solved by conventional methods. Once the solution is obtained, it can be transformed back to give the operator function which is the solution to the original operator differential equation.

2. PRELIMINARY DEFINITIONS

Let us consider a function of noncommuting operators. For simplicity, we shall consider functions of the boson annihilation and creation operators a_i and $a_i^\dagger$—the extension to other conjugate operators such as p and q is straightforward. We consider then a general function $f(a_i^\dagger, a_i)$ of the set of operators obeying the commutation relation

$$[a_i, a_j^\dagger] = \delta_{ij}. \tag{2.1}$$

We define the ordered or *normal form* of any function $f(a_i^\dagger, a_i)$ of the $a_i^\dagger$ and a_i operators as the form in which all creation operators appear to the left of all annihilation operators. Given any function $f(a_i^\dagger, a_i)$, we use the commutation relations to move annihilation operators to the right and creation operators to the left to obtain its normal form $f^{(n)}(a_i^\dagger, a_i)$. In general, we can write the normal form of any function as

$$f^{(n)}(a_i^\dagger, a_i) = \sum c_{n_1,n_2\cdots n_k m_1 m_2\cdots m_j} a_1^{\dagger n_1} a_2^{\dagger n_2}\cdots a_k^{\dagger n_k} a_1^{m_1} a_2^{m_2}\cdots a_j^{m_j}. \tag{2.2}$$

Here the coefficients of the expansion may be functions of the time or other parameters. Except for the inconsequential ordering among the sequence of creation operators or among the sequence of annihilation operators, every function has a unique normal form. Moreover, since the commutation relations have been used to put f in normal form,

$$f^{(n)} = f, \tag{2.3}$$

in that both represent the same over-all operation.

Let us now define a transformation T which transforms a function $f(a_i^\dagger, a_i)$ of the operators $a_i^\dagger$ and a_i to a function of new *commuting* algebraic variables $\bar{a}_i^\dagger$ and $\bar{a}_i$ in the following way: the function $f(a_i^\dagger, a_i)$ is first put into normal form and then the substitution of the variable $\bar{a}_i^\dagger$ as made for the operator $a_i^\dagger$ and the variable $\bar{a}_i$ for the operator a_i. Symbolically, if

$$\bar{f}(\bar{a}_i^\dagger, \bar{a}_i) = T\{f(a_i^\dagger, a_i)\}, \tag{2.4a}$$

then

$$\bar{f}(\bar{a}_i^\dagger, \bar{a}_i) = f^{(n)}(\bar{a}_i^\dagger, \bar{a}_i). \tag{2.4b}$$

In passing we should note that from (2.2)

$$T\{\partial f/\partial t\} = \partial T\{f\}/\partial t, \tag{2.5}$$

a relation which is of importance later.

Since each function has a unique normal form, the T transformation results in a one-to-one correspondence between a function of the algebraic commuting variables $\bar{a}_i^\dagger$ and $\bar{a}_i$ and a function of the operators $a_i^\dagger$ and a_i. We have thus mapped the space of operator functions onto the space of algebraic variable functions in a unique way.

Next we must consider the inverse transformation T^{-1} applied to a function $f(\bar{a}_i^\dagger, \bar{a}_i)$ of the algebraic variables $\bar{a}_i^\dagger$, $\bar{a}_i$. We first define the normal ordering symbol, $\mathfrak{N}$, which when applied to a function of the operators $a_i^\dagger$ and a_i serves to reorder the expression without regard to the commutation relations in such a way that all annihilation operators appear to the right of all creation operators. Thus, for example,

$$\mathfrak{N}\{(a_1 a_1^\dagger a_2^\dagger a_2\} = a_1^\dagger a_2^\dagger a_1 a_2$$

and

$$\mathfrak{N}\{(a_i + \partial/\partial a_1^\dagger) a_2 a_1^\dagger\} = a_1^\dagger a_1 a_2 + a_2.$$

In general,

$$\mathfrak{N}\{f(a_i^\dagger, a_i)\} \neq f(a_i^\dagger, a_i);$$

the exception arises when $f(a_i^\dagger, a_i)$ is in normal form. Then

$$\mathfrak{N}\{f^{(n)}(a_i^\dagger, a_i)\} \equiv f^{(n)}(a_i^\dagger, a_i). \tag{2.6}$$

Using the normal ordering symbol, we can write the inverse transformation relation as

$$T^{-1}\{\bar{f}(\bar{a}_i^\dagger, \bar{a}_i)\} = \mathfrak{N}\{\bar{f}(a_i^\dagger, a_i)\}. \tag{2.7}$$

That is, the inverse transformation converts a function of the commuting variables $\bar{a}_i^\dagger$ and $\bar{a}_i$ into the same function of the operators $a_i^\dagger$ and a_i with the condition that all annihilation operators operate to the right—the resulting operator function being in normal form. Let us give some illustrations to clarify this operation. For example,

$$T^{-1}\{\bar{a}_i \bar{a}_i^{\dagger 2} \bar{a}_i \bar{a}_i^\dagger\} = a_i^\dagger a_i^{\dagger 2} a_i a_i.$$

Again, since the barred variables commute, we see

$$\begin{aligned} T^{-1}\{(\bar{a}_1 + \partial/\partial \bar{a}_1^\dagger)\bar{a}_2 \bar{a}_1^{\dagger 2}\} &= T^{-1}\{\bar{a}_1 \bar{a}_2 \bar{a}_1^{\dagger 2} + 2\bar{a}_2 \bar{a}_1^\dagger\} \\ &= a_1^{\dagger 2} a_2 a_1 + 2a_1^\dagger a_2. \end{aligned}$$

Using (2.4a), (2.4b), (2.7), (2.6), and (2.3) we see that

$$\begin{aligned} T^{-1}T\{f(a_i^\dagger, a_i)\} &= T^{-1}f^{(n)}(\bar{a}_i^\dagger, \bar{a}_i) = \{f^{(n)}(a_i^\dagger, a_i)\} \\ &= \mathfrak{N}f^{(n)}(a_i^\dagger, a_i) = f(a_i^\dagger, a_i). \end{aligned}$$

Thus

$$T^{-1}T = 1. \tag{2.8}$$

We need the relations which allow us to transform the product of two functions of operators,

$$\begin{aligned} h(a_i^\dagger, a_i) &= f(a_i^\dagger, a_i) g(a_i^\dagger, a_i) \\ &= f^{(n)}(a_i^\dagger, a_i) g^{(n)}(a_i^\dagger, a_i), \end{aligned} \tag{2.9}$$

the latter equality resulting from (2.3), since from (2.4) the transformation of $h(a_i^\dagger, a_i)$ results in

$$\bar{h}(\bar{a}_i^\dagger, \bar{a}_i) = h^{(n)}(\bar{a}_i^\dagger, \bar{a}_i). \tag{2.10}$$

We must explore the technique of putting products of functions in normal form. To do this, we note that to put $a_i f^{(n)}(a_i^\dagger, a_i)$ in normal form we may use the familiar relation

$$a_i f^{(n)}(a_i^\dagger, a_i) = f^{(n)}(a_i^\dagger, a_i) a_i + \partial f^{(n)}(a_i^\dagger, a_i)/\partial a_i^\dagger. \tag{2.11}$$

The right-hand side is in normal form as indicated by positional ordering. We may write this same relation using the normal ordering symbol as

$$[a_i f^{(n)}(a_i^\dagger, a_i)]^{(n)} = \mathfrak{N}\{(a_i + \partial/\partial a_i^\dagger) f^{(n)}(a_i^\dagger, a_i)\}$$

and, in general, for any function of annihilation operators,

$$[g(a_i) f^{(n)}(a_i^\dagger, a_i)]^{(n)} = \mathfrak{N}\{g(a_i + \partial/\partial a_i^\dagger) f^{(n)}(a_i^\dagger, a_i)\}.$$

Indeed, if we have a function of $a_i^\dagger$ and a_i in normal form, we find

$$\begin{aligned} &[g^{(n)}(a_i^\dagger, a_i) f^{(n)}(a_i^\dagger, a_i)]^{(n)} \\ &\quad = \mathfrak{N}\{g^{(n)}(a_i^\dagger, a_i + \partial/\partial a_i^\dagger) f^{(n)}(a_i^\dagger, a_i)\}. \end{aligned} \tag{2.12}$$

As an example, we see

$$\begin{aligned} [(a_1^\dagger a_1)(a_1^\dagger + a_1)]^{(n)} &= \mathfrak{N}\{a_1^\dagger (a_1 + \partial/\partial a_1^\dagger)(a_1^\dagger + a_1)\} \\ &= \mathfrak{N}\{a_1^\dagger a_1 a_1^\dagger + a_1^\dagger a_1^2 + a_1^\dagger\} = a_1^{\dagger 2} a_1 + a_1^\dagger a_1^2 + a_1^\dagger. \end{aligned}$$

By using the Hermitian equivalent to (2.11),

$$f^{(n)}(a_i^\dagger, a_i)a_i^\dagger = a_i^\dagger f^{(n)}(a_i^\dagger, a_i) + \partial f^{(n)}(a_i^\dagger, a_i)/\partial a_i,$$

we can show in the same fashion

$$[g^{(n)}(a_i^\dagger, a_i)f^{(n)}(a_i^\dagger, a_i)]^{(n)} = \mathfrak{N}\{g^{(n)}(a_i^\dagger, a_i)f^{(n)}(a_i^\dagger + \overleftarrow{\partial}/\partial a_i, a_i)\}. \quad (2.13)$$

The operation of differentiation is applied to the function on the left. Using these two relations together with (2.10), we find

$$T\{g(a_i^\dagger, a_i)f(a_i^\dagger, a_i)\} = g^{(n)}(\bar{a}_i^\dagger, \bar{a}_i + \partial/\partial\bar{a}_i^\dagger)f^{(n)}(\bar{a}_i^\dagger, \bar{a}_i) \quad (2.14)$$

or

$$T\{g(a_i^\dagger, a_i)f(a_i^\dagger, a_i)\} = f^{(n)}(\bar{a}_i^\dagger + \partial/\partial\bar{a}_i, \bar{a}_i)g^{(n)}(\bar{a}_i^\dagger, \bar{a}_i). \quad (2.15)$$

Here the normal ordering symbol has been removed since once the transformation to the algebraic variables $\bar{a}_i^\dagger$ and $\bar{a}_i$ has been made, the ordering is immaterial. No matter how this function is written, it is the transformation of the normal ordered form of the operator function.

In view of the relations (2.4), we may rewrite (2.14) and (2.15) as

$$T\{g(a_i^\dagger, a_i)f(a_i^\dagger, a_i)\} = g^{(n)}(\bar{a}_i^\dagger, \bar{a}_i + \partial/\partial\bar{a}_i^\dagger)T\{f(a_i^\dagger, a_i)\} \quad (2.16)$$

and

$$T\{g(a_i^\dagger, a_i)f(a_i^\dagger, a_i)\} = f^{(n)}(\bar{a}_i^\dagger + \partial/\partial\bar{a}_i)T\{g(a_i^\dagger, a_i)\}. \quad (2.17)$$

3. APPLICATION TO THE SOLUTION OF SCHRÖDINGER'S EQUATION

Let us consider the solution to the Schrödinger equation for the unitary transformation, $U(t, t_0)$

$$i\hbar\,\partial U/\partial t = \mathfrak{K}(a_i^\dagger, a_i, t)U, \quad (3.1)$$

where $\mathfrak{K}$ is solely a function of the boson operators a_i and $a_i^\dagger$ but may depend on time. Let us apply the T transformation to both sides of the equation. Using (2.5) and (2.16) we obtain

$$i\hbar\,\partial\bar{U}/\partial t = \mathfrak{K}^{(n)}(\bar{a}_i^\dagger, \bar{a}_i + \partial/\partial\bar{a}_i^\dagger, t)\bar{U}, \quad (3.2)$$

where we have let $\bar{U}(\bar{a}_i^\dagger, \bar{a}_i, t) = T\{U(a_i^\dagger, a_i, t)\}$. Equation (3.2) is a differential equation in ordinary function space. Once having obtained the solution for $\bar{U}$, for which we can employ the standard methods for solving partial differential equations, we can apply the inverse transformation T^{-1} to determine the desired unitary transformation involving the noncommuting operators a_i and $a_i^\dagger$. Thus, from (2.7),

$$U(a_i^\dagger, a_i, t) = T^{-1}\{\bar{U}(\bar{a}_i^\dagger, \bar{a}_i, t)\} = \mathfrak{N}\{\bar{U}(a_i^\dagger, a_i, t)\}. \quad (3.3)$$

An example may serve to clarify the procedure. Consider an harmonic oscillator with a time-dependent forcing term. The Hamiltonian is of the form

$$\mathfrak{K} = \hbar\omega a^\dagger a + \hbar e(t)(a^\dagger + a) \quad (3.4)$$

and we wish to find the unitary transformation such that

$$|\psi(t)\rangle = U_{tt_0}\,|\psi(t_0)\rangle. \quad (3.5)$$

For simplicity we work in the interaction picture where

$$U_{tt_0} = e^{-(i/\hbar)a^\dagger a(t-t_0)}V_{tt_0}. \quad (3.6)$$

The operator V_{tt_0} satisfies the equation

$$i\hbar\,\partial V_{tt_0}/\partial t = \mathfrak{K}_I V_{tt_0}, \quad (3.7)$$

where

$$\mathfrak{K}_I = \hbar e(t)(a^\dagger e^{i\omega t} + ae^{-i\omega t}). \quad (3.8)$$

Applying the T transformation to both sides of (3.7) we have

$$i\,\partial\bar{V}/\partial t = e(t)[\bar{a}^\dagger e^{i\omega t} + \bar{a}e^{-i\omega t} + (\partial/\partial\bar{a}^\dagger)e^{-i\omega t}]\bar{V}, \quad (3.9)$$

with the initial condition $\bar{V}(t = t_0) = 1$ since we demand $U_{t_0t_0} = 1$. The equation is easily solved by assuming a solution

$$\bar{V} = e^{S(\bar{a}^\dagger, \bar{a}, t)}. \quad (3.10)$$

With this substitution (3.9) becomes

$$i\,\partial S/\partial t = e(t)[\bar{a}^\dagger e^{i\omega t} + \bar{a}e^{-i\omega t} + (\partial S/\partial\bar{a}^\dagger)e^{-i\omega t}]. \quad (3.11)$$

We now determine S by demanding a functional form which gives algebraically equivalent terms on both sides of (3.11). In this case, the form of S is quite simple, namely:

$$S = A(t) + B(t)\bar{a}^\dagger + C(t)\bar{a}. \quad (3.12)$$

The initial condition implies $A(t_0) = B(t_0) = C(t_0) = 0$. By equating coefficients of similar terms on both sides of (3.11) we readily obtain solutions for A, B, and C, to give

$$\bar{V} = \exp\left[-iF(t)\bar{a}^\dagger - iF^*(t)\bar{a} - \int_{t_0}^{t} e(t')F(t')e^{-i\omega t'}\,dt'\right], \quad (3.13)$$

where

$$F(t) = \int_{t_0}^{t} e(t')e^{i\omega t'}\,dt'. \quad (3.14)$$

By applying the inverse transformation T^{-1} we

obtain

$$V_{t,t_0} = \mathfrak{N}\left\{\exp\left[-iF(t)\bar{a}^\dagger - iF^*(t)\bar{a} - \int_{t_0}^{t} e(t')F(t')e^{-i\omega t'}\,dt'\right]\right\}$$
$$= \exp\left[-iF(t)a^\dagger\right]\exp\left[-iF^*(t)a\right] \times \exp\left[-\int_{t_0}^{t} e(t')F(t')e^{-i\omega t'}\,dt'\right]. \quad (3.15)$$

Equation (3.6) then gives the entire unitary transformation, U_{tt_0}.

The T transformation may also be employed to determine the time evolution of the density operator. We may apply it to the operator equation

$$i\hbar\,\partial\rho/\partial t = \mathfrak{K}\rho - \rho\mathfrak{K}, \quad (3.16)$$

whence by making use of (2.16) and (2.17) we obtain

$$i\hbar\,\partial\bar{\rho}/\partial t = \left[\mathfrak{K}^{(n)}\left(\bar{a}^\dagger, \bar{a} + \frac{\partial}{\partial\bar{a}^\dagger}, t\right) - \mathfrak{K}^{(n)}\left(\bar{a}^\dagger + \frac{\partial}{\partial\bar{a}}, \bar{a}, t\right)\right]\bar{\rho} \quad (3.17)$$

as the differential equation obeyed by the transformed function $\bar{\rho} = T\{\rho\}$. This equation is slightly more complicated than (3.2) only because the initial condition on $\bar{\rho}$ is more complicated.

The same techniques may be employed to obtain solutions in antinormal form in which all annihilation operators appear to the left of all creation operators in each term. There are times when such solutions are useful.

4. THE TREATMENT OF ANGULAR MOMENTUM OR SPIN

The T-transformation technique as has been developed so far is applicable only to problems involving solely operators whose commutator is a "c" number or at least whose commutator itself commutes with its components. Thus it can not be applied directly to problems involving angular momentum or spin operators. There is, however, a standard transformation which converts angular momentum operators to boson creation and anihilation operators. For each particle we define boson operators b_i, $b_i^\dagger$, c_i, $c_i^\dagger$ such that

$$[b_i, b_i^\dagger] = [c_i, c_i^\dagger] = \delta_{ij}, \quad [b_i, b_j] = [c_i, c_j] = [b_i, c_j] = [b_i, c_i^\dagger] = 0. \quad (4.1)$$

We then define the components of the angular momentum of the ith particle in the (1), (2), and (3) directions as[1]

$$J_{i1} = \tfrac{1}{2}[c_i^\dagger b_i + b_i^\dagger c_i],$$
$$J_{i2} = \tfrac{1}{2}i[c_i^\dagger b_i - b_i^\dagger c_i], \quad (4.2)$$
$$J_{i3} = \tfrac{1}{2}[b_i^\dagger b_i - c_i^\dagger c_i],$$

and its magnitude as

$$\bar{J}_i^2 = S_i[S_i + 1], \quad (4.3)$$

where

$$S_i = \tfrac{1}{2}[b_i^\dagger b_i + c_i^\dagger c_i]. \quad (4.4)$$

One finds the eigenvalues of $\bar{J}_i^2$ are $j_i(j_i + 1)$ where

$$j_i = 0, \tfrac{1}{2}, 1, \cdots, \tfrac{1}{2}n, \cdots,$$

and those of J_{i3} are m_i.

The representation of a state $|j_i, m_i\rangle$ of the ith particle in terms of the b_i and c_i states is

$$|j_i, m_i\rangle = [(j_i + m_i)!(j_i - m_i)!]^{-\frac{1}{2}} b_i^{\dagger(j_i+m_i)} c_i^{\dagger(j_i-m_i)}\,|00\rangle$$
$$= |(j_i + m_i)(j_i - m_i)\rangle. \quad (4.5)$$

Here, and in what follows, we adopt the convention that the first number labeling the bc eigenstate signifies the occupation number of the b variables while the second, that of the c variables.

We are always concerned with a small subspace of the entire Hilbert space of the bc system, namely that for a given j value where m takes on values $m = -j, -j + 1, \cdots, j - 1, j$. Within this subspace, the familiar angular momentum commutation relations are obeyed. Moreover this is a closed subspace since no operations involving angular momentum operators can transform a state within the subspace to a state outside it.

For spin-$\frac{1}{2}$ particles where $j = \frac{1}{2}$, this is a particularly simple subspace consisting of two eigenvectors, one for $j = \frac{1}{2}$, $m = +\frac{1}{2}$:

$$|+\rangle = |10\rangle,$$

and the other for $j = \frac{1}{2}$, $m = -\frac{1}{2}$:

$$|-\rangle = |01\rangle.$$

We see that for the allowed states in the general case

$$b_i^k c_i^l\,|(j_i + m_i)(j_i - m_i)\rangle = 0 \quad \text{if} \quad (k + l) > 2j.$$

Thus any normally ordered product containing more than $2j$ annihilation operators of the same particle gives zero independently of whether the operators refer to the b or c system. This feature often allows considerable simplification in the solution of angular momentum problems posed in these variables.

Once the change to the bc boson variables has been made, the transformation technique of the

[1] See A. Messiah, *Quantum Mechanics* (Interscience Publishers, Inc., New York, 1962), Vol. II, Chap. 13.

previous section may be used. As an example, Appendix A presents the solution to the problem of a single spin in an rf magnetic field.

One might inquire as to the applicability of this general transformation technique in problems involving fermion operators. Indeed, one can develop a parallel formalism to transform fermion operator equations into differential equations in algebraic variables. If many particles are involved, such a transformed equation is, if anything, more difficult of solution than the original operator equation.

Note added in proof: It has been pointed out to one of us (W.H.L.) by J. R. Klauder that results similar to those reported here are known in field theory. See J. L. Anderson, Phys. Rev. **94**, 703 (1954); N. N. Bogoliubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields* (Interscience Publishers, New York, 1959), p. 486.

APPENDIX A: SEMICLASSICAL TREATMENT OF A SPIN IN A MAGNETIC FIELD

Consider a particle with spin in a magnetic field

$$\mathbf{H} = [H_1 \cos \omega t, H_1 \sin \omega t, H_0]. \tag{A1}$$

The Hamiltonian is

$$\mathcal{H} = \tfrac{1}{2}\gamma\hbar[H_0\sigma_z + H_1\sigma_x \cos \omega t + H_1\sigma_y \sin \omega t]. \tag{A2}$$

Using the boson transformation of (4.2) and letting $\gamma H_0 = \omega_0$ we have

$$\mathcal{H} = \tfrac{1}{2}\hbar\omega_0(b^\dagger b - c^\dagger c) + \tfrac{1}{2}\hbar\gamma H_1(b^\dagger c e^{-i\omega t} + c^\dagger b e^{i\omega t}). \tag{A3}$$

We now proceed to solve

$$i\hbar\, \partial U/\partial t = \mathcal{H}U \tag{A4}$$

using the T transformation. The transformed equation is, from (3.2),

$$i\frac{\partial \bar{U}}{\partial t} = \left[\frac{\omega_0}{2}\left(\bar{b}^\dagger\bar{b} + \bar{b}^\dagger\frac{\partial}{\partial \bar{b}^\dagger} - \bar{c}^\dagger\bar{c} - \bar{c}^\dagger\frac{\partial}{\partial \bar{c}^\dagger}\right) + \frac{\gamma H_1}{2} \times \left(\bar{b}^\dagger\bar{c}e^{-i\omega t} + \bar{b}^\dagger\frac{\partial}{\partial \bar{c}^\dagger}e^{-i\omega t} + \bar{c}^\dagger\bar{b}e^{i\omega t} + \bar{c}^\dagger\frac{\partial}{\partial \bar{b}^\dagger}e^{i\omega t}\right)\right]\bar{U}, \tag{A5}$$

where $\bar{U} = T\{U\}$. We make the substitution

$$\bar{U} = e^S \tag{A6}$$

and find (A5) becomes

$$i\frac{\partial S}{\partial t} = \frac{\omega_0}{2}\left(\bar{b}^\dagger\bar{b} + \bar{b}^\dagger\frac{\partial S}{\partial \bar{b}^\dagger} - \bar{c}^\dagger\bar{c} - \bar{c}^\dagger\frac{\partial S}{\partial \bar{c}^\dagger}\right) + \frac{\gamma H_1}{2}\left(\bar{b}^\dagger\bar{c}e^{-i\omega t} + \bar{b}^\dagger\frac{\partial S}{\partial \bar{c}^\dagger}e^{-i\omega t} + \bar{c}^\dagger\bar{b}e^{i\omega t} + \bar{c}^\dagger\frac{\partial S}{\partial \bar{b}^\dagger}e^{i\omega t}\right). \tag{A7}$$

The solution for S is of the form

$$S = (A-1)\bar{b}^\dagger\bar{b} + (B-1)\bar{c}^\dagger\bar{c} + D\bar{b}^\dagger\bar{c} + E\bar{c}^\dagger\bar{b}. \tag{A8}$$

The coefficients of (A8) may be found by equating the coefficients of similar terms in (A7). The resulting differential equations are

$$\begin{aligned} i\,\partial A/\partial t &= \tfrac{1}{2}\omega_0 A + \tfrac{1}{2}\gamma H_1 e^{-i\omega t}E, \\ i\,\partial B/\partial t &= -\tfrac{1}{2}\omega_0 B + \tfrac{1}{2}\gamma H_1 e^{i\omega t}D, \\ i\,\partial D/\partial t &= \tfrac{1}{2}\omega_0 D + \tfrac{1}{2}\gamma H_1 e^{-i\omega t}B, \\ i\,\partial E/\partial t &= -\tfrac{1}{2}\omega_0 E + \tfrac{1}{2}\gamma H_1 e^{i\omega t}A. \end{aligned} \tag{A9}$$

The initial conditions result from the demand that U be unity at $t = 0$, thus $S = 0$ at $t = 0$ or

$$A(0) = B(0) = 1; \qquad D(0) = E(0) = 0. \tag{A10}$$

The equations (A9) may easily be solved to give

$$\begin{aligned} A &= B^* = (\gamma H_1 e^{-i(\omega/2)t}/W)\sin(\tfrac{1}{2}Wt + \phi), \\ D &= -E^* = (i\gamma H_1 e^{-i(\omega/2)t}/W)\sin\tfrac{1}{2}Wt, \end{aligned} \tag{A11}$$

where $W^2 = (\gamma H_1)^2 + (\omega - \omega_0)^2$; $\tan\phi = i - W/(\omega - \omega_0)$. Thus, upon taking the inverse transformation, we find

$$U = \mathfrak{N}\{\exp[(A-1)\bar{b}^\dagger\bar{b} + (B-1)\bar{c}^\dagger\bar{c} + D\bar{b}^\dagger\bar{c} + E\bar{c}^\dagger\bar{b}\}. \tag{A12}$$

As yet, we have not made any restriction on the spin of the particle. If the particle has spin $\frac{1}{2}$, (A12) may be simplified by recognizing that in a power series expansion of the exponential all terms having more than one ($2j = 1$) annihilation operator gives zero when applied to one of the possible spin states. Thus for a spin-$\frac{1}{2}$ particle in a magnetic field, we obtain for the time evolution operator

$$U = 1 + (A-1)b^\dagger b + (B-1)c^\dagger c + Db^\dagger c + Ec^\dagger b. \tag{A13}$$

Here positioned ordering eliminates the need for the normal ordering symbol.

To obtain a somewhat more familiar result than (A13) may appear, we may compute the probability that after a time t the spin is in the lower state assuming that initially it started in the upper state. That is, we ask for the value of

$$|\langle -|\,U\,|+\rangle|^2 = |\langle 01|\,U\,|10\rangle|^2 = |E|^2 = \frac{(\gamma H_1)^2}{(\gamma H_1)^2 + (\omega-\omega_0)^2}\sin^2\{\tfrac{1}{2}[(\gamma H_1)^2 + (\omega-\omega_0)^2]^{\frac{1}{2}}t\}.$$

Isoperimetric Problem with Application to the Figure of Cells

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Biological applications suggest the following geometrical problem. Consider n three-dimensional cells, touching or not, and assume that the free energy of their figure is the sum $H = A + \alpha B$ of the area A of the cell walls adjacent to the ambient fluid plus an adjustable constant $0 \leq \alpha \leq 2$ times the area B of the walls separating two cells. Given the partial volumes of the cells, the problem is to describe the shape of the (optimal) figure that renders H as small as possible; the analogous problem for *two-dimensional* cells is the subject of this paper. Geometrical proofs of the following features of optimal two-dimensional figures are presented below: (a) the edges bounding the cells are circular arcs; (b) at an inside corner, three edges meet at angles $2\pi/3$; (c) at an outside corner, three edges meet with outside angle $2\cos^{-1}\alpha/2$; (d) pressures can be ascribed to the cells so that the pressure drop across an edge is proportional to its curvature; (e) bubbles appear at each inside corner as α passes $3^{1/2}$. All these facts have three-dimensional analogues with similar proofs.

1. INTRODUCTION

THE shape of soap bubbles can be predicted by solving an isoperimetric problem[1,2]; this comes about by fixing the partial volumes of the bubbles and assuming that the free energy is proportional to surface area. It is then a geometrical problem to find the figure that makes this energy as small as possible; see, for instance, Kelvin.[2] A fascinating application of this idea is to the equilibrium figure of a small number of cells. Thompson (Ref. 3, p. 631) found the predicted figures in good agreement with the actual shapes in a wide class of cases; see also Steinberg[4] for the application of such ideas to explain the ability of cells of several species to sort themselves out.

Surface tension is commonly thought to be produced by attraction and repulsion between the molecules of a cell wall and those of the fluid on either side of it. For the soap-bubble problem, it is natural to assume like forces throughout the figure, but this need not be so for the biological case since the ambient fluid is not the same as the fluid inside the cells. The simplest expression for the free energy of a figure of several cells of the same species that accounts for this anomaly is $H = A + \alpha B$, A being the total area of the walls adjacent to the ambient fluid and B the total area of the internal walls; the adjustable factor α permits us to deal with the inside and outside walls on a different footing. Under the condition that the number and volumes of the cells be constant, the mathematical problem is to find the figure of n cells that makes the energy H as small as possible; the discussion below is confined to *two-dimensional* figures, though most of the results have three-dimensional analogs.

Given $\alpha < 0$, $H = -\infty$, while for $\alpha \geq 2$ an optimal figure is n nonoverlapping discs; accordingly the interesting case is $0 \leq \alpha < 2$.

Given $0 < \alpha < 2$, the edges separating the cells, bubbles, and unbounded region of an n-cell optimal figure are circular (Sec. 3) filling out a connected graph (Sec. 6); at each corner of this graph three edges meet (Secs. 4 and 5); at an inside corner three calls meet at angles $\frac{2}{3}\pi$ (Sec. 4), while at an outside corner two cells meet a bubble or the unbounded region at an outside angle of $2\cos^{-1}\frac{1}{2}\alpha$ (Sec. 5). Quantities playing the role of cell pressures are proved to exist and the pressure drop across an edge is found to be proportional to its curvature (Sec. 7). Bubbles are discussed in Sec. 8; especially it is found that three-sided bubbles must be produced at each inside corner as α passes $3^{\frac{1}{2}}$. Section 9 is devoted to minimal energy as a function of surface tension. Section 10 contains examples and a remark on change of phase. Section 11 lists the corresponding facts for three-dimensional figures.

2. OPTIMAL FIGURES

A *figure* is a plane graph with n_0 corners, joined by n_1 piecewise smooth simple *edges* dividing the plane into n_2 bounded regions and a single unbounded region. The *outside* of the figure is the unbounded region together with some (or none) of the bounded regions (*bubbles*), subject to the condition that no two outside regions be adjacent across

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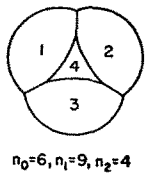

FIG. 1. A typical figure with six vertices, nine edges, and four regions.

an edge; the *inside* of the figure is made up of the other bounded regions (cells). An edge or corner is *outside* or *inside* according as it meets the outside or not. A possible figure is shown in Fig. 1; 1, 2, 3, are cells, and 4 is either a a cell or a bubble.

Given a figure of n cells with areas v_1, v_2, etc., let A and B denote the sum of the lengths of its outside and inside edges, define the (free) energy of the figure to be $H = A + \alpha B$, and let h be the *infimum* of the energies of such figures: $h = h(\alpha, v_1, v_2, \cdots, v_n) = a + \alpha b = \inf H$, thinking of α as the ratio of the surface tensions of the inside and outside edges. The basic physical assumption is that the natural configuration of cells is such as to make the energy of the figure as small as possible ($= h$); the basic mathematical assumption is that an optimal figure or perhaps several optimal figures actually exist.

Note that $\alpha < 0$ leads to $h \equiv -\infty$, while for $\alpha = 0$ an optimal figure is a disc divided at pleasure into cells with $h = 2\pi(R_1^2 + R_2^2 + \cdots)^{\frac{1}{2}}$, $(v = \pi R^2)$, and for $\alpha \geq 2$ it is n nonoverlapping discs with $h = 2\pi(R_1 + R_2 + \cdots)$. Because of this, *the condition $0 < \alpha < 2$ is to be understood below.*

3. EDGES ARE CIRCULAR

Theorem: Each edge of an optimal figure is a circular arc (of curvature ≥ 0).

Proof: Choose a point (not a corner) of an edge γ and draw about it a little disc Δ whose perimeter cuts γ at just two points but does not meet the other edges (Fig. 2). Now draw the (dotted) circular arc γ_1 joining these two points and cutting the area of the disc in the same proportion as γ does, and let γ_2 be the rest of the (dotted) full circle containing γ_1. According to the classical isoperimetric inequality (Ref. 1, p. 97), $\gamma \cap \Delta$ is longer than γ_1 unless it coincides with γ_1, because the circle $\gamma_1 + \gamma_2$ encloses the same area as the simple closed curve $\gamma \cap \Delta + \gamma_2$. Since the figure is optimal, $\gamma \cap \Delta = \gamma_1$, and since a locally circular arc is circular in the large, the proof is complete.

4. INSIDE CORNERS

Theorem: At an inside corner of an optimal figure three cells are adjacent along three edges meeting at angles of $2\pi/3$.

Proof: At an inside corner ≥ 3 edges meet (Sec. 2), so it is enough to prove that the angle between adjacent edges is $\geq \frac{2}{3}\pi$; for then exactly three edges must meet, and if they did not separate three distinct cells, one edge could be suppressed, diminishing the energy.

Suppose two adjacent edges meet an angle $0 < \theta \frac{2}{3}\pi$ (the case $\theta = 0$ is left to the reader). Draw a little circle γ of radius δ centered at the corner as in Fig. 3, showing the two edges, the three adjacent cells (1, 2, 3), the little circle γ, and (dotted) modified edges of curvature O meeting at angles $2\pi/3$ and separating modified cells 1*, 2*, 3*. Note that 1*, 2*, 3* do not have the same areas as 1, 2, 3; this is ignored for the moment. Up to an error of magnitude $O(\delta^2)$, the total length of the portions of the unmodified edges inside γ is just 2δ, so their contribution to the energy of the unmodified figure is $j = 2\alpha\delta + O(\delta^2)$ while the contribution of the dotted edges to the energy of the modified figure is

$$i = \alpha\delta(\sin \tfrac{1}{3}\pi)^{-1}[\sin(\tfrac{1}{3}\pi - \tfrac{1}{2}\theta) + 2\sin\tfrac{1}{2}\theta].$$

Now the coefficient of $\alpha\delta/\sin\frac{1}{3}\pi$ in the difference $i - j$ is

$$f(\theta) = \sin(\tfrac{1}{3}\pi - \tfrac{1}{2}\theta) + 2\sin\tfrac{1}{2}\theta - 2\sin\tfrac{1}{3}\pi;$$

this vanishes at $\theta = \frac{2}{3}\pi$ and its slope is negative for $0 \leq \theta < \frac{2}{3}\pi$, so the modification diminishes the energy for small δ, contradicting the fact that the figure was optimal. The proof is now complete except that the area imbalance due to the modification has to be undone. Consider for this purpose a portion of an edge of length 1 (say) and of curvature k and bow it out or in, keeping it circular and making a small change ϵ in the areas on each side of it;

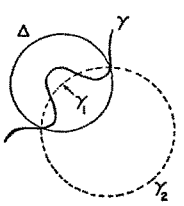

FIG. 2. Edge adjustment for the proof of circularity.

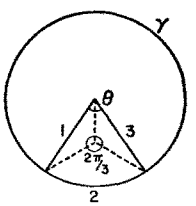

FIG. 3. Angle adjustment for the proof that inside angles equal $2\pi/3$.

its length changes by $\pm\epsilon k + O(\epsilon^2)$ according as the bowing is out or in as a simple geometrical argument proves. Now it is clear that since the area imbalance of the modified figure is $O(\delta^2)$ this can be adjusted by small bowings of edges at the expense of a change of $O(\delta^2)$ in its energy. But such a change is negligible compared to $\alpha\delta(\sin \frac{1}{3}\pi)^{-1}(i - j)$ for small δ, so the proof is complete.

5. OUTSIDE CORNERS

Theorem: At an outside corner of an optimal figure 2 cells meet the outside, and the two outside edges meet the outward pointing prolongation of the inside edge at angles of $\cos^{-1} \frac{1}{2}\alpha$; in particular, the edges of an outside region all bulge toward the outside, and at each corner (outside or inside) three edges meet.

Proof: $\cos^{-1} \frac{1}{2}\alpha$ can be guessed by balancing forces at the corner, but this is not a mathematical proof. Suppose two outside edges meet at an outside corner at an angle $0 < \theta < 2 \cos^{-1} \frac{1}{2}\alpha$ (the case $\theta = 0$ is left to the reader as before). Draw a little circle of radius δ centered at the corner. Draw also (dotted) modified edges meeting at angle $2 \cos^{-1} \frac{1}{2}\alpha$ as in Fig. 4. Proceeding as in Sec. 4, correct the area imbalance and compute the change in energy: this change is

$$\delta(\sin \cos^{-1} \tfrac{1}{2}\alpha)^{-1}[\alpha \sin (\cos^{-1} \tfrac{1}{2}\alpha - \tfrac{1}{2}\theta) + 2 \sin \tfrac{1}{2}\theta] - 2\alpha\delta + O(\delta^2),$$

and the coefficient of δ vanishes at $\theta = 2 \cos^{-1} \frac{1}{2}\alpha$, is negative at $\theta = 0$, and has positive slope between, i.e., the modification diminishes the energy if δ is small enough, against the fact that the figure was optimal. Now distinguish two cases, according as two outside edges (1, 2) meet ≥ 1 inside edges (3) as in Fig. 5(a), or ≥ 4 outside edges meet at the corner as in Fig. 5(b). For the case of Fig. 5(a), the method used above shows that the angles $\widehat{23}$ and $\widehat{31}$ *adjacent* to the outside are both $\geq \pi - \cos^{-1} \frac{1}{2}\alpha$, and by the argument of Sec. 4 all the other *inside* angles are $\geq \frac{2}{3}\pi$. But such additional angles cannot be fitted in, so there is just one inside edge, and this edge separates two distinct cells, for otherwise it could be suppressed with an improvement

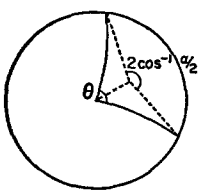

FIG. 4. Angle adjustment for the proof that outside angles equal $2 \cos^{-1} \frac{1}{2}\alpha$.

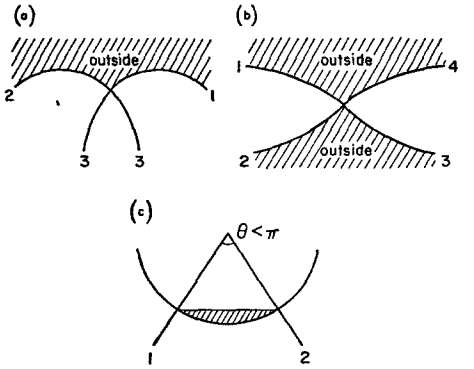

FIG. 5. *A priori* possibilities for cell arrangements at an outside corner.

in energy. Now the outside angle is (exactly) $2 \cos^{-1} \frac{1}{2}\alpha$, and the two adjacent angles are (exactly) $\pi - \cos^{-1} \frac{1}{2}\alpha$; therefore the inside edge bisects the angle between the outside edges, and the proof is complete in this case. As to the other possible situation at an outside corner, Figure 5(b), since $\cos^{-1} \frac{1}{2}\alpha > 0$, the arc from 1 to 2 plus the arc from 3 to 4 is less than 2π, and supposing $\theta =$ the arc from 1 to $2 < \pi$, the energy can be improved by drawing a little disc of radius δ about the corner as in Fig. 5(c), erasing the edges between 1 and 2 inside the disc, adding the straight edge of the shaded part (disconnecting the graph, but no matter), and picking up the infinitesimal area imbalance as usual; the actual improvement is

$$\geq 2\delta(1 - \sin \tfrac{1}{2}\theta) + O(\delta^2).$$

6. CONNECTEDNESS

Theorem: The graph of an optimal figure is connected.

Proof: Otherwise the edges fall into ≥ 2 connected parts and such a connected part (subfigure) lies in an open region Δ (cell, bubble, or unbounded region). Regard this subfigure as *floating* Δ and move it without changing its shape until it just touches the boundary of Δ. Contact along an arc is impossible since that would diminish the energy ($\alpha < 2$), while contact at a single point (new corner) violates Sec. 4 or Sec. 5 since four edges cannot meet at a corner. The proof is now complete.

Bubbles, cells, and the unbounded region are simply connected; this is just another statement of the absence of floating subfigures.

Theorem: A subfigure of an optimal figure not meeting the boundary of the unbounded region is bordered by ≥ 3 bounded regions.

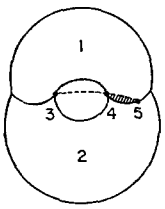

FIG. 6. Construction for the proof that a subfigure is bordered by at least three regions.

Proof: Otherwise it floats (impossible), or is suspended by a single edge (also impossible), or it is suspended by two edges in the union of two cells (1, 2) as in Fig. 6. Draw the (dotted) circular arc γ connecting the suspension points (3, 4) with a movable point 5, slide the subfigure rigidly along γ until it touches 5, slide the shaded area along γ until it touches 3, and erase γ. This can be done without touching the boundary of 1 + 2 if 5 is close enough to 4; moreover, the areas of 1 and 2 and the total energy are unchanged, so the new figure is optimal. But this violates the fact that edges are circular (Sec. 2) unless the two suspending edges (and so also γ) lie on a single circle, in which case it is permissible to slide the subfigure along this circle until it just touches the boundary of 1 + 2; the proof is then completed as for floating subfigures.

7. PRESSURES

An optimal figure of n cells with areas $v = (v_1, v_2, \cdots)$ is *stable* if to each $u = (u_1, u_2, \cdots)$ in a small neighborhood of v corresponds an optimal figure with n cells, cell areas u, and the same graph, with corners and edges close to those of the original figure. Given such a stable figure it makes sense to *label* its cells 1, 2, *etc.* and to speak of the associated *pressures* $p_1 = \partial h/\partial v_1$, $p_2 = \partial h/\partial v_2$, etc.; we assert that

Theorem: Pressures exist and if the pressure p_0 of the outside regions is declared to be $\equiv 0$ and if the curvature k of an edge is declared to be positive or negative according as the edge bulges out from or in towards the spectator, then the pressure drop across an edge is αk or k according as the edge is inside or outside. Also $\frac{1}{2}h = p_1v_1 + p_2v_2 + \cdots$.

Proof: Consider an outside edge of a stable figure

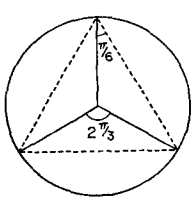

FIG. 7. Construction for the proof that bubbles are present if $\alpha > 3^{\frac{1}{2}}$.

FIG. 8. The two-cell figure.

separating a cell (1) from an outside region (0) and bow it a little out or in, keeping it circular and changing the area of cell 1 by a small amount ϵ. Counting the curvature k of the edge as positive, the change in its length is $\pm\epsilon k + O(\epsilon^2)$, according as the edge is bowed out or in (this fact was used already in Sec. 4), and since the optimal energy $h(v_1 \pm \epsilon, v_2, \cdots)$ cannot exceed the energy of the modified figure, one finds

$$h(u \pm \epsilon, v_2, \cdots) \leq h(u, v_2, \cdots) \pm \epsilon k + O(\epsilon^2)$$
$$(u = v_1).$$

Because the figure was stable, this bound holds in a small neighborhood of $u = v_1$, and it follows that $p_1 = \partial h/\partial v_1$ exists. Once the existence of the pressures of the cells bordering the outside is proved, one can proceed across inside edges establishing the existence of the pressures of inside cells and verifying the pressure drops αk in exactly the same fashion; moreover the formula $\frac{1}{2}h = p_1v_1 + p_2v_2 + \cdots$ follows at once from the hact that h is a homogeneous function of degree $\frac{1}{2}$, i.e.,

$$h(tv_1, tv_2, \cdots) = t^{\frac{1}{2}}h(v_1, v_2, \cdots) \qquad (t > 0).$$

One deduces the following rules.

(1) At an inside corner, the curvatures k_{12}, k_{23}, k_{31} of the three edges, as viewed during a counterclockwise circuit, add up to 0: $k_{12} + k_{23} + k_{31} = 0$; especially, 2 edges have the same (unsigned) curvature if, and only if the other edge is straight.

(2) At an outside corner, the curvatures k_{10}, k_{02}, k_{21} of the edges, as viewed during a counter clockwise circuit passing from cell 1 to the outside (0) to cell 2 and back to cell 1, satisfy $k_{10}+k_{02}+\alpha k_{21}=0$; especially, the outside edges have the same (unsigned) curvature if and only if the inside edge is straight.

8. BUBBLES

Theorem: An optimal figure has no inside corners if $\alpha > 3^{\frac{1}{2}}$; this means that bubbles must be present for $\alpha > 3^{\frac{1}{2}}$ if the figure contains $\geq$ three cells.

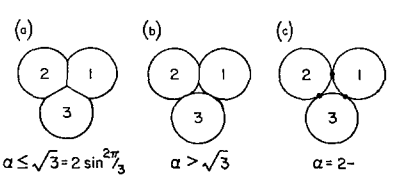

FIG. 9. The three-cell figure (trefoil) at several values of α.

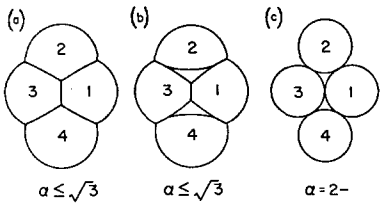

FIG. 10. One of the possible four-cell figures ("switchback") at several values of α.

Proof: Consider an inside corner, draw about it a small circle of radius δ, and introduce a (dotted) triangular bubble as in Fig. 7. Up to an error of $O(\delta^2)$ including the area imbalance, the energy is diminished by

$$3\alpha\delta - 3\delta \sin \tfrac{2}{3}\pi/\sin \tfrac{1}{6}\pi = 3\delta(\alpha - 3^{\frac{1}{2}}),$$

and this is positive unless $\alpha \leq 3^{\frac{1}{2}}$, as desired.

Theorem: Bubbles have ≥ 3 sides. A bubble of m sides cannot occur unless $\alpha > 2 \sin \pi/m$.

Proof: Because the sides of a bubble bend inwards, $m \geq 3$. During a counterclockwise circuit, a unit vector tangent to a bubble rotates through the angle 2π; this angle is the sum of m positive jumps $\pi - 2 \cos^{-1} \frac{1}{2}\alpha$ coming from the corners and m negative angles coming from the edges, and so $2\pi < m(\pi - 2 \cos^{-1} \frac{1}{2}\alpha)$, or, what is the same,

$$0 > \cos^{-1} \tfrac{1}{2}\alpha - \tfrac{1}{2}\pi + \pi/m = -\sin^{-1} \tfrac{1}{2}\alpha + \pi/m.$$

Combining the two preceding items, one finds for $n \geq 3$, that *bubbles must be present for* $\alpha > 3^{\frac{1}{2}}$ *and three-sided bubbles cannot be present for* $\alpha < 3$. A natural conjecture is that all bubbles are three-sided, and the fact that shrinking a $\geq$ four-sided bubble to a point leads to an inside corner at which $\geq$ four cells meet tends to support this idea. But catastrophic geometrical changes could occur to avoid this, and the proof escapes us. Be that as it may, as α decreases a bubble either disappears or develops more sides according to the rule $m > \pi/\sin^{-1} \frac{1}{2}\alpha$.

9. ENERGY AS A FUNCTION OF SURFACE TENSION

Given $n \geq 1$ and $v_1, v_2, \cdots$, consider $h = a + \alpha b$ as a function of $0 \leq \alpha \leq 2$ alone and let us prove

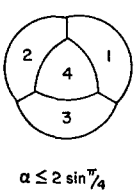

FIG. 11. The 4-flower.

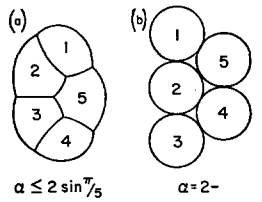

FIG. 12. The five-cell "switchback."

Theorem: That b is decreasing and h is continuous, increasing, and concave, with one-sided slopes:

$$b(\alpha+) = h^+(\alpha) \leq b(\alpha) \leq h^-(\alpha) = b(\alpha-);$$

in particular, $h^+ = h^- = b(\alpha\pm) = b(\alpha)$, i.e., h is differentiable, except perhaps at a countable number of corners.

Note that $b(\alpha)$ is the sum of the lengths of inside edges of *an* optimal figure and so is ambiguous if several optimal figures exist; thus, $h^+(\alpha) = b(\alpha+)$ means that as $\beta \downarrow \alpha$, each possible value of $b(\beta)$ is close to $h^+(\alpha)$. A similar ambiguity is present in $a(\alpha)$.

Proof: $H = a(\beta) + \alpha b(\beta)$ is the energy of an admissible figure; as such it cannot be smaller than $h(\alpha)$, so

$$h(\beta) = a(\beta) + \alpha b(\beta) + (\beta - \alpha)b(\beta) \geq h(\alpha) + (\beta - \alpha)b(\beta),$$

and using this bound both for $\alpha < \beta$ and $\alpha > \beta$, one finds

$$b(\beta) \leq [h(\beta) - h(\alpha)]/[\beta - \alpha] \leq b(\alpha), \qquad (\alpha < \beta),$$

or, what is the same,

$$b(\alpha + \epsilon) \leq [h(\alpha + \epsilon) - h(\alpha)]/\epsilon \leq b(\alpha) \leq [h(\alpha) - h(\alpha - \epsilon)]/\epsilon \leq b(\alpha - \epsilon), \qquad (\epsilon > 0),$$

from which the stated facts are evident.

Actual formulas for $n = 2$ or 3 show that h has no corners (see Sec. 10). Corners probably correspond to drastic geometrical changes of the optimal figure (see Secs. 7, 8, and 10). Berger[5] pointed out that if g is the (concave downwards) lower envelope of the set R of the points (A, B) [A (B) denotes the sum of the outside (inside) edges] corresponding to all admissible figures (optimal or not), then h and g are related according to the reciprocal rules

$$h(\alpha) = \inf_{\beta \geq 0} [g(\beta) + \alpha\beta], \qquad g(\beta) = \sup_{\alpha \geq 0} [h(\alpha) - \alpha\beta],$$

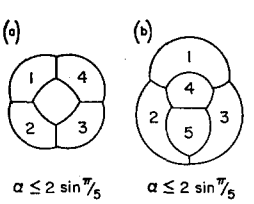

FIG. 13. Two possible 5-flowers.

[5] C. Berger (private communication).

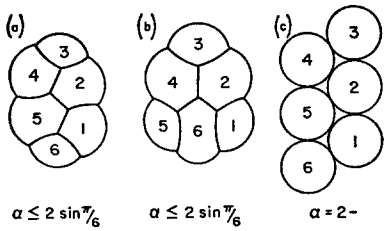

FIG. 14. Two different six-cell "switchbacks" and a six-figure at $\alpha = 2^-$.

connected with the transformation between Gibbs and Helmholz free energies in statistical mechanics. A corner of the graph of h produces a straight segment of the envelope g, and since a point of contact between R and its envelope corresponds to an optimal figure, a corner of the graph of h indicates the existence of ≥ 2 optimal figures.

10. EXAMPLES

Consider an optimal figure of n cells each of area π and note from Sec. 8 that bubbles cannot be present for $\alpha \leq 2 \sin \pi/n$. Of the possible figures for $\alpha = 0+$ (no bubbles) and $n \leq 6$, most can be seen to be nonoptimal on the basis of information at hand (for example, according to Sec. 6, a figure with two outside corners cannot be optimal for $n \geq 3$); the surviving figures are indicated in Figs. 8–16.

Brief comments on the figures follow.

Geometrical considerations provide us with simple formulas for h for $n = 2, 3$ assuming that Fig. 8 and the trefoil (Fig. 9) with identical outside cells and radial edges are optimal. Letting $\theta = \cos^{-1} \frac{1}{2}\alpha$, we have:

$$n = 2 : h = 4[\pi(\pi - \theta + \tfrac{1}{2}\alpha \sin \theta)]^{\frac{1}{2}},$$

$$n = 3 : h = 6\left[\pi\left(\frac{5\pi}{6} - \theta\right) + \frac{\alpha}{2}\left(\sin \theta + \frac{\alpha}{2(3)^{\frac{1}{2}}}\right)\right]^{\frac{1}{2}} \qquad (\alpha \leq 3^{\frac{1}{2}})$$

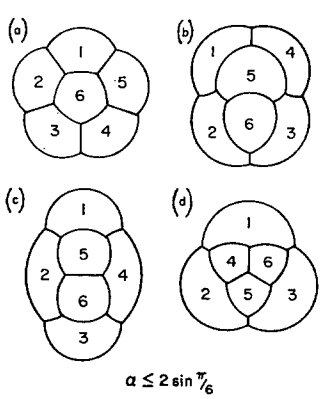

FIG. 15. Four different 6-flowers.

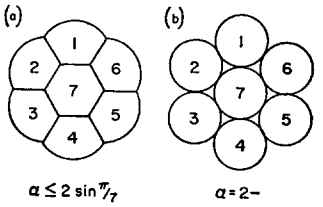

FIG. 16. The 7-flower at several values of α.

$$= 6[\pi(\pi - 2\theta + \alpha \sin \theta)]^{\frac{1}{2}} \qquad (\alpha > 3^{\frac{1}{2}});$$

note that h (trefoil) does not have a corner at $\alpha = 3^{\frac{1}{2}}$. Energies can also be computed for $n = 4, 5, 6$ for the best flowers (Figs. 11, 13a, 15a) under the same assumption as for the trefoil, with the result that the best of the figures 10(12) is better than the best 4(5)-flower of Fig. 11(13a) near $\alpha = 0$; this is proved by checking that the energy of a pie is smaller than that of the best flower (false for $n = 6$) and then using the method of Sec. 4 (see Fig. 3) to deform the pie into a figure 10(12) with smaller energy. Because of this, it is plausible that Fig. 10(12) is optimal for all $0 < \alpha \leq 2$, but this is not proved. On the other hand as α approaches 2 from below, an optimal figure probably tends smoothly to n nonoverlapping discs. Of the six-celled figures, only the figures 14(a) and (b) have the proper inside corners (possible bubbles) for this to happen with as much touching between cells as possible (smallest energy), so if some flowerlike figure such as Fig. 15(d) is optimal near $\alpha = 0$ (as seems possible, for large n if not for $n = 6$) then the optimal figure undergoes some geometrical catastrophe (phase change) at one (or several) critical points $\alpha = \beta$ $(0 < \beta < 2)$; probably such a phase change is accompanied by a corner of the optimal energy curve. For $n = 7$, the flower (Fig. 16) bursts symmetrically at $\alpha = 2$ into seven nonoverlapping discs; for large n and α near 0, the optimal figure is probably quite elaborate, but after a few phase changes it should begin to look like interlocked 7-flowers with bubbles, making an approximately hexagonal pattern.

11. THREE-DIMENSIONAL FIGURES

Most of the discussion can be adapted to the three-dimensional case with small technical changes: cell walls are now spherical, 4(3) regions meet at each corner (edge) with specified inclinations, the walls form a connected surface (no floating subfigures), tetrahedral bubbles appear at each inside corner as α approaches 2 from below, pressures can be defined as before, and the pressure drop across a cell wall is proportional to its curvature; the discussion of h as a function of surface tension is identical.

Calculation of Certain Phase-Space Integrals

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(Received 18 September 1964)

We give the result of an approximate calculation of the phase-space integral
$$\Omega_n(Q) = \int \delta_4(Q - \textstyle\sum_i k_i) \prod_i \delta(k_i^2 - \mu_i^2)\vartheta(k_{i0})f_i(k_{iT})\, d_4k_i,$$
which appears when one takes into account the fact that only a part of the kinematically allowed phase-space is accessible to particles produced in high-energy collisions, because of the observed smallness of their transverse momenta.

1. INTRODUCTION

IF one considers a set of secondaries produced in a high-energy collision, one finds that only a part of the kinematically allowed phase-space is accessible to them, due to the limitations imposed by the dynamics of the interaction on the transverse momenta of the particles. It is an attractive hypothesis, compatible with the present experimental evidence,[1-4] that the limitation of transverse momenta to small values is the only strong constraint imposed by the dynamics on the collision amplitude. In other words, it is tempting to suppose that within the accessible, limited region of the phase space the usual statistical assumption approximately holds, namely that the dimension of the phase-space volume corresponding to a given physical situation essentially determines the probability of the realization of this situation in the collision process.[5] It is obvious that if one attempts to reformulate the Fermi statistical theory so as to take into account the smallness of the transverse momenta of particles, one is faced with the necessity of calculating the phase-space integrals of the type[6]

$$\Omega_n(Q) = \int \delta_4(Q - \sum_i k_i) \times \prod_i \delta(k_i^2 - \mu_i^2)\vartheta(k_{i0})f_i(k_{iT})\, d_4\, k_i, \qquad (1)$$

where k_{iT} is the transverse momentum of the ith secondary and the cutoff function $f_i(k_{iT})$ is nonvanishing for small k_{iT} only. [Subscripts L and T denote the longitudinal and the transverse component of a vector with respect to an *a priori* chosen privileged direction in momentum space (in practice, the direction of motion of the incident particle).] To discriminate between the consequences of the "amputation" of the phase space and some new dynamical effects one has to be able to calculate effectively the integrals $\Omega_n(Q)$ of the type (1). Such a calculation has been outlined in Ref. 4. In this paper we give the result of a complete calculation. The approximation method used is described shortly in Sec. 2. Section 3 contains the approximate formula for $\Omega_n(Q)$, in the form which can easily be used in computer calculations.

2. THE METHOD OF CALCULATION

In order to calculate $\Omega_n(Q)$ it is convenient to use the method proposed by Lurcat and Mazur,[7] which gives $\Omega_n(Q)$ in the form of an expansion in powers of $n^{-\frac{1}{2}}$. Following Ref. 7 we define

$$\phi(\alpha_\nu) = \int \exp\,[-\alpha_\nu Q^\nu]\Omega_n(Q)\, d_4\, Q. \qquad (2)$$

The function

$$\Omega_n^{(\alpha)}(Q) = \Omega_n(Q) \exp\,[-\alpha_\nu Q^\nu]/\phi(\alpha_\nu) \qquad (3)$$

is positive-definite and normalized to unity and, as shown by Lurcat and Mazur, may be treated as the frequency function of the vector variable Q, being a sum of n independent random variables k_i (vector means here 4-vector). Thus $\Omega_n(Q)$ can be approximated by an Edgeworth series. It turns out that in practical calculations it is sufficient to keep the first few terms of the series only. Let us define

$$A_\nu = \int Q_\nu \Omega_n^{(\alpha)}(Q)\, d_4\, Q. \qquad (4)$$

Lurcat and Mazur approximation is a pretty good one even for small n, if the parameter α_ν is chosen so as to make $A_\nu = Q_\nu$. In our case the problem

[1] L. Van Hove, Nuovo Cimento **28** 798 (1963).
[2] O. Czyzewski and A. Krzywicki, Nuovo Cimento, **30**, 603 (1963).
[3] L. Van Hove, Rev. Mod. Phys. **36**, 655 (1964).
[4] A. Krzywicki, Nuovo Cimento **32**, 1067 (1964).
[5] E. Fermi, Progr. Theoret. Phys. (Kyoto) 5, 570 (1950).
[6] For a discussion of the physical aspects of the problem see Ref. 4.
[7] F. Lurcat and P. Mazur, Nuovo Cimento **31**, 140 (1964).

has less symmetry, which complicates the calculation considerably. For Q_T not too large one gets, however, a reasonable approximation specifying α, by the condition

$$A_\nu = Q_\nu, \qquad \nu = 0, 1 \qquad \alpha_T \to 0. \tag{5}$$

The result of the calculation, made along the lines of Ref. 7 but much more cumbersome due to the weaker symmetry of the problem, is given in the next section.

The following notation will be used:

$$\begin{aligned}
\alpha &= (\alpha_0^2 - \alpha_L^2)^{\frac{1}{2}}, \\
W &= (Q_0^2 - Q_L^2)^{\frac{1}{2}}, \\
\varphi_i(\alpha) &= \pi \int dk_T\, k_T f_i(k_T) K_0[\alpha(k_T^2 + \mu_i^2)^{\frac{1}{2}}] \\
{}^ih_{n,m}(\alpha) &= \frac{\pi(-1)^n}{\varphi_i(\alpha)} \int dk_T\, k_T f_i(k_T)(\alpha k_T)^{2m} \\
&\quad \times [\alpha(k_T^2 + \mu_i^2)^{\frac{1}{2}}]^n K_n[\alpha(k_T^2 + \mu_i^2)^{\frac{1}{2}}] \\
Z &= 2(\alpha Q_T)^2 / \{\sum_i {}^ih_{0,1}(\alpha)\},
\end{aligned} \tag{6}$$

where $K_n(x)$ denotes as usual the modified Bessel function

$$K_n(x) = \int_0^\infty e^{-x \cosh t} \cos(nt)\, dt.$$

3. THE RESULT OF THE CALCULATION

The condition (5) can be written in the form

$$W = -\frac{1}{\alpha} \sum_i {}^ih_{1,0}(\alpha), \qquad \alpha_T = 0. \tag{7}$$

For α determined from the above equation, $\Omega_n(Q)$ is given by the following formula [$O(n^{-\frac{3}{2}})$ indicates the order of magnitude of terms independent of Q_T.]:

$$\Omega_n(Q) = \omega_n(W) e^{-\frac{1}{2}Z} \times \left\{1 + \sum_{m=0}^{2} G_n^{(m)} \left(\frac{Z}{F_{0,2} - F_{1,0}}\right)^m + O(n^{-\frac{3}{2}})\right\}, \tag{8}$$

where

$$\omega_n(W) = \frac{\alpha^3 e^{\alpha W} \prod_i \varphi_i(\alpha)}{(2\pi)^2 (F_{0,2} - F_{1,0})(WF_{2,0}/\alpha)^{\frac{1}{2}}}, \tag{9}$$

and

$$\begin{aligned}
G_n^{(0)} &= \frac{F_{4,0}}{8F_{2,0}^2} + \frac{(3F_{2,0} + F_{0,4} - 3F_{1,0} - 6F_{1,2})}{3(F_{0,2} - F_{1,0})^2} \\
&+ \frac{3(F_{2,0} - F_{1,0})}{8F_{1,0}^2} - \frac{(F_{3,0} + 2F_{1,0} - 2F_{2,0} - F_{2,2})}{2F_{2,0}(F_{0,2} - F_{1,0})} \\
&+ \frac{(F_{3,0} + 2F_{1,0} - 2F_{2,0})}{4F_{2,0}F_{1,0}} - \frac{(F_{2,0} - F_{1,0} - F_{1,2})}{2F_{1,0}(F_{0,2} - F_{1,0})} \\
&- \frac{5F_{3,0}^2}{24F_{2,0}^3} + \frac{(F_{2,0} - F_{1,0} - F_{1,2})(F_{2,0} - F_{1,0})}{2F_{2,0}F_{1,0}(F_{0,2} - F_{1,0})} \\
&- \frac{3(F_{2,0} - F_{1,0})^2}{8F_{2,0}F_{1,0}^2} + \frac{F_{3,0}(F_{2,0} - F_{1,0} - F_{1,2})}{2F_{2,0}^2(F_{0,2} - F_{1,0})} \\
&- \frac{(F_{2,0} - F_{1,0} - F_{1,2})^2}{F_{2,0}(F_{0,2} - F_{1,0})^2} - \frac{F_{3,0}(F_{2,0} - F_{1,0})}{4F_{1,0}F_{2,0}^2},
\end{aligned} \tag{10}$$

$$\begin{aligned}
G_n^{(1)} &= \frac{(F_{3,0} + 2F_{1,0} - 2F_{2,0} - F_{2,2})}{4F_{2,0}} \\
&+ \frac{(F_{2,0} - F_{1,0} - F_{1,2})}{4F_{1,0}} \\
&- \frac{(3F_{2,0} + F_{0,4} - 3F_{1,0} - 6F_{1,2})}{3(F_{0,2} - F_{1,0})} \\
&- \frac{F_{3,0}(F_{2,0} - F_{1,0} - F_{1,2})}{4F_{2,0}^2} + \frac{(F_{2,0} - F_{1,0} - F_{1,2})^2}{F_{2,0}(F_{0,2} - F_{1,0})} \\
&- \frac{(F_{2,0} - F_{1,0})(F_{2,0} - F_{1,0} - F_{1,2})}{4F_{2,0}F_{1,0}},
\end{aligned}$$

$$\begin{aligned}
G_n^{(2)} &= \frac{(3F_{2,0} + F_{0,4} - 3F_{1,0} - 6F_{1,2})}{24} \\
&\quad - \frac{(F_{2,0} - F_{1,0} - F_{1,2})^2}{8F_{2,0}}.
\end{aligned}$$

F's can be expressed in terms of h's as follows:

$$\begin{aligned}
F_{1,0} &= \sum_i {}^ih_{1,0} \\
F_{2,0} &= \sum_i ({}^ih_{2,0} + {}^ih_{1,0} - {}^ih_{1,0}^2) \\
F_{0,2} &= \sum_i (\tfrac{1}{2}\,{}^ih_{0,1} + {}^ih_{1,0}) \\
F_{3,0} &= \sum_i ({}^ih_{3,0} + 3\,{}^ih_{2,0} + 2\,{}^ih_{1,0}^3 \\
&\qquad - 3\,{}^ih_{2,0}\,{}^ih_{1,0} - 3\,{}^ih_{1,0}^2) \\
F_{1,2} &= \sum_i ({}^ih_{2,0} + \tfrac{1}{2}\,{}^ih_{1,1} - {}^ih_{1,0}^2 - \tfrac{1}{2}\,{}^ih_{0,1}\,{}^ih_{1,0}) \\
F_{4,0} &= \sum_i ({}^ih_{4,0} + 6\,{}^ih_{3,0} + 12\,{}^ih_{2,0}\,{}^ih_{1,0}^2 + 3\,{}^ih_{2,0} \\
&\quad + 12\,{}^ih_{1,0}^3 - 4\,{}^ih_{3,0}\,{}^ih_{1,0} - 18\,{}^ih_{2,0}\,{}^ih_{1,0} \\
&\quad - 3\,{}^ih_{2,0}^2 - 3\,{}^ih_{1,0}^2 - 6\,{}^ih_{1,0}^4) \\
F_{2,2} &= \sum_i ({}^ih_{3,0} + {}^ih_{2,0} + \tfrac{1}{2}\,{}^ih_{2,1} + {}^ih_{1,0}^2\,{}^ih_{0,1} \\
&\quad + \tfrac{1}{2}\,{}^ih_{1,1} + 2\,{}^ih_{1,0}^3 - 3\,{}^ih_{2,0}\,{}^ih_{1,0} \\
&\quad - \tfrac{1}{2}\,{}^ih_{2,0}\,{}^ih_{0,1} - {}^ih_{1,1}\,{}^ih_{1,0} \\
&\quad - \tfrac{1}{2}\,{}^ih_{1,0}\,{}^ih_{0,1} - {}^ih_{1,0}^2) \\
F_{0,4} &= \sum_i (3\,{}^ih_{2,0} + \tfrac{3}{8}\,{}^ih_{0,2} + 3\,{}^ih_{1,1} \\
&\quad - \tfrac{3}{4}\,{}^ih_{0,1}^2 - 3\,{}^ih_{0,1}\,{}^ih_{1,0} - 3\,{}^ih_{1,0}^2).
\end{aligned} \tag{11}$$

The numerical calculation of $\Omega_n(Q)$ can easily be performed with the help of an electronic computer. One first solves Eq. (7) to get the value of the parameter α. The h's are found by integration from (6).

The calculation of F's and of the $\Omega_n(Q)$ is then almost immediate. The calculation is particularly fast in the case of equal masses of produced particles (see Ref. 4).

$$\mu_i = \mu,$$

since then only six h's need to be calculated ($h_{1,0} = -\alpha W/n$).

The accuracy of the approximation is expected to be roughly the same as in Ref. 7 for $Z \lesssim 1$.

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Composite Particles in a Relativistic Model of Two-Body Scattering

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(Received 7 July 1964)

The relativistic model of two-particle scattering recently described by Jordan, Macfarlane, and Sudarshan is extended to include bound states. The projection operator associated with the bound-state manifold is explicitly given. This relates the structure of the composite particle to the scattering amplitude. There is a discussion of the conditions the phase shifts have to satisfy in order that they can be fitted with the model. Explicit solutions are derived for a large class of phase shifts.

I. INTRODUCTION

IN a recent article Jordan, Macfarlane, and Sudarshan (JMS)[1] described a quantum mechanical model for two interacting, spinless particles which is Lorentz invariant, satisfies the asymptotic condition, and gives a nontrivial scattering amplitude. The model is based on a pair of unitary wave operators which satisfy

$$\lim_{t=\mp\infty} e^{iH_0 t}\Omega_\pm e^{-iH_0 t} = 1$$

and establish a unitary equivalence between the "free" and interacting generators of the Poincaré group. In this paper, we describe how a slight modification of the formalism gives rise to a bound state in the interacting system. The wave operators will be slightly altered so that they are no longer unitary but only isometric. The complement of the range of $\Omega_\pm$ will be a subspace irreducible under the Poincaré group and will thus describe an elementary particle[2] with definite mass and spin. The bound state particle will however have an internal structure as can be seen by going to the nonrelativistic limit.

The next section contains a short review of the JMS model whereupon we discuss the modifications necessary to include bound states. This is followed by a section on the inverse problem, i.e., the problem of fitting an experimentally given scattering amplitude with the model.

The notations used closely adhere to Ref. 1, which may be consulted for more detail.

II. THE CASE OF NO BOUND STATES

The Hilbert space of two spinless particles with masses m_1 and m_2 is the space of functions $f(\mathbf{p}_1, \mathbf{p}_2)$ of the momentum variables $\mathbf{p}_1$ and $\mathbf{p}_2$ with the inner product

$$(f, g) = \int f(\mathbf{p}_1, \mathbf{p}_2)^* g(\mathbf{p}_1, \mathbf{p}_2) \frac{1}{2W_1}\frac{1}{2W_2} d^3p_1\, d^3p_2, \quad (1)$$

where $(W_1)^2 = (\mathbf{p}_1)^2 + (m_1)^2$ and $(W_2)^2 = (\mathbf{p}_2)^2 + (m_2)^2$. The "free" generators of the Poincaré group are given by

$$\begin{aligned} H_0 &= W_1 + W_2, \\ \mathbf{P}_0 &= \mathbf{p}_1 + \mathbf{p}_2, \\ \mathbf{J}_0 &= -i\mathbf{p}_1 \times (\partial/\partial\mathbf{p}_1) - i\mathbf{p}_2 \times (\partial/\partial\mathbf{p}_2), \\ \mathbf{N}_0 &= -iW_1(\partial/\partial\mathbf{p}_1) - iW_2(\partial/\partial\mathbf{p}_2). \end{aligned} \quad (2)$$

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[1] T. F. Jordan, A. J. Macfarlane, and E. C. G. Sudarshan, Phys. Rev. 133, B487, subsequently referred to as JMS. The possibility of having a relativistically invariant description of a finite quantum mechanical system was first discussed by L. L. Foldy, Phys. Rev. 122, 275 (1961). See also the more recent article by R. Fong and J. Sucher, J. Math. Phys. 5, 456 (1964).

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This representation is reducible and its reduciton implies a direct integration over the total mass and a direct summation over the spin.[3] This can be most easily effected by the introduction of new variables, viz., the total mass M, the center of mass momentum $\mathbf{K}$ and a unit vector $\mathbf{e}$ which describes the relative spin of the particles. In these new variables one has

$$f(\mathbf{p}_1, \mathbf{p}_2)=2M^{\frac{1}{2}}\lambda^{-\frac{1}{2}}(M) \sum_l \sum_{m=-l}^{l} f_{lm}(M, \mathbf{K})Y_{lm}(\mathbf{e}), \quad (3)$$

$$(f, g) = \int_{m_1+m_2}^{\infty} dM \int 1/2(M^2 + \mathbf{K}^2)^{-\frac{1}{2}}\, d^3K \times \sum_{lm} f_{lm}(M, \mathbf{K})^* g_{lm}(M, \mathbf{K}) \quad (4)$$

and

$$\begin{aligned}
(H_0 f)_{lm}(M, \mathbf{K}) &= (M^2 + \mathbf{K}^2)^{\frac{1}{2}} f_{lm}(M, \mathbf{K}),\\
(\mathbf{P}_0 f)_{lm}(M, \mathbf{K}) &= \mathbf{K} f_{lm}(M, \mathbf{K}),\\
(\mathbf{J}_0 f)_{lm}(M, \mathbf{K}) &= -i\mathbf{K} \times (\partial/\partial \mathbf{K}) f_{lm}(M, \mathbf{K}) + (\mathbf{I}f)_{lm}(M, \mathbf{K}),\\
(\mathbf{N}_0 f)_{lm}(M, \mathbf{K}) &= -i(M^2 + \mathbf{K}^2)^{\frac{1}{2}}(\partial/\partial \mathbf{K}) f_{lm}(M, \mathbf{K}) - [M + (M^2 + \mathbf{K}^2)^{\frac{1}{2}}]^{-1}\mathbf{K} \times (\mathbf{I}f)_{lm}(M, \mathbf{K}),
\end{aligned} \quad (5)$$

where $\lambda(M)$ is a given function and $\mathbf{I}$ are the three components of the intrinsic angular momentum.[2,4]

Next JMS define a pair of operators

$$(\Omega_\pm f)_{lm}(M, \mathbf{K}) = f_{lm}(M, \mathbf{K}) + \int dM' \left(\frac{M^2 + \mathbf{K}^2}{M'^2 + \mathbf{K}^2}\right)^{\frac{1}{2}} \times \frac{\varsigma_l(M)\varsigma_l(M')}{B_{l\pm}(M')(M' - M \pm i\epsilon)} f_{lm}(M', \mathbf{K}), \quad (6)$$

where

$$B_l(z) = 1 + \int dM \frac{\varsigma_l(M)^2}{M - z}. \quad (7)$$

The real functions $\varsigma_l(M)$ have to be square integrable but apart from that are arbitrary. The interacting generators L are defined by the unitary equivalence

$$L = \Omega_+ L_0 \Omega_+^\dagger,$$

where L_0 stands for the set of free or asymptotic generators as given by Eq. (5). That this defines a scattering system with $\Omega_\pm$ as a pair of wave operators, follows from the equations

$$\Omega_\pm \Omega_\pm^\dagger = 1, \quad (8)$$

$$\Omega_\pm^\dagger \Omega_\pm = 1, \quad (9)$$

$$\lim_{t \to \mp\infty} e^{iH_0 t}\Omega_\pm e^{-iH_0 t} = 1, \quad (10)$$

which have been shown to hold by JMS. The most general scattering operator which is unitary and commutes with the free generators of the Lorentz group has to be of the form $(Sf)_{lm}(M, \mathbf{K}) = e^{2i\delta_l(M)} f_{lm}(M, \mathbf{K})$. This is a consequence of Schur's lemma. In our case S comes out to be

$$\begin{aligned}
(Sf)_{lm}(M, \mathbf{K}) &= e^{2i\delta_l(M)} f_{lm}(M, \mathbf{K})\\
&= [B_{l-}(M)/B_{l+}(M)] f_{lm}(M, \mathbf{K}).
\end{aligned} \quad (11)$$

The model is Lorentz invariant in the sense that $\Omega_\pm$ are the same and satisfy the asymptotic condition (10) in all frames which can be reached by a proper, orthochronous Lorentz transformation. This follows from

$$\Omega_+ \mathbf{P}_0 \Omega_+^\dagger = \mathbf{P}_0. \quad (12)$$

In addition one has time-reversal invariance. This requires

$$i_t S = S^\dagger i_t, \quad (13)$$

where i_t is the antiunitary operator which corresponds to the transformation[3] $t \to -t$, $\mathbf{x} \to \mathbf{x}$. Equation (13) is satisfied in the model simply because

$$i_t \Omega_+ i_t = \Omega_-. \quad (14)$$

It is tempting to speculate to what extent the scattering operator S determines the wave operators $\Omega_\pm$. The answer to this question seems to be negative; if U is a unitary operator which satisfies

$$\lim_{t \to \mp\infty} e^{iH_0 t} U e^{-iH_0 t} = 1,$$

then $\Omega_+' = U\Omega_+$ and $\Omega_-' = U\Omega_+ S^\dagger$ satisfy condition (10) and moreover $\Omega_-'^\dagger \Omega_+' = S$. That such a U exists is very likely. If however $\Omega_\pm$ are further required to satisfy

$$\Omega_+ \mathbf{P}_0 \Omega_+^\dagger = \mathbf{P}_0 \quad (15)$$

and

$$i_t \Omega_+ i_t = \Omega_- \quad (16)$$

which is certainly sufficient to ensure Lorentz invariance; one can argue even if somewhat heuristically that S determines $\Omega_\pm$ uniquely, and with it the generators of the interacting system. To see this, suppose $\Gamma_\pm$ and $\Omega_\pm$ are two pairs of unitary operators, both of which satisfy equations (15) and (16) and in addition $S = \Omega_-^\dagger \Omega_+ = \Gamma_-^\dagger \Gamma_+$. One has to

[3] See, e.g., the lectures by A. S. Wightman at Les Houches in *Dispersion Relations and Elementary Particles*, edited by C. de Witt and R. Omnes, (John Wiley & Sons, Inc., New York, 1961).

[4] A. J. Macfarlane, J. Math. Phys. 4, 490 (1963).

show that $\Gamma_+ = \Omega_+$, or $\Gamma_+^\dagger\Omega_+ = 1$. Both Ω_+ and Γ_+ commute with $\mathbf{P}_0$ and also

$$\Gamma_+^\dagger\Omega_+ = S^\dagger i_l\Gamma_+^\dagger\Omega_+ i_l S, \quad \text{or} \quad S\Gamma_+^\dagger\Omega_+ = i_l\Gamma_+^\dagger\Omega_+ i_l S.$$

Ignoring the complications due to the continuous nature of the spectrum of M, one may argue from the last equation that if $|M, \mathbf{K}, l, m\rangle$ satisfies

$$S\,|M, \mathbf{K}, l, m\rangle = e^{2i\delta_l(M)}\,|M, \mathbf{K}, l, m\rangle$$

then

$$S\Gamma_+^\dagger\Omega_+\,|M, \mathbf{K}, l, m\rangle = e^{2i\delta_l(M)} i_l\Gamma_+^\dagger\Omega_+ i_l\,|M, \mathbf{K}, l, m\rangle.$$

The most general transformation of this kind which commutes with $\mathbf{P}_0$ has to transform a special vector of the form $f_{l'm'}(M, \mathbf{K}) = \delta_{l'l}\delta_{m'm}f(M, \mathbf{K})$ into

$$(\Gamma_+^\dagger\Omega_+ f)_{l'm'}(M, \mathbf{K}) = \Big(\mu(M, \mathbf{K})\delta_{l'l}\delta_{m'm}f(M, \mathbf{K}) + \sum_i \mu_i(M, \mathbf{K})g_i(M, \mathbf{K})\Big),$$

where the μ are some functions of $\mathbf{K}$ and M and $g_i(M, K)$ have to satisfy $g_i(M', \mathbf{K}) = f(M, \mathbf{K})$, where M' is such that $\delta_{l'}(M') = \delta_l(M)$. The asymptotic condition

$$\lim_{t=-\infty} e^{iH_0t}\Gamma_+^\dagger\Omega_+ e^{-iH_0t} = 1$$

then shows that, in fact,

$$(\Gamma_+^\dagger\Omega_+ f)_{l'm'}(M, \mathbf{K}) = \delta_{l'l}\delta_{m'm}f(M, \mathbf{K}), \quad \text{i.e.,} \quad \Gamma_+^\dagger\Omega_+ = 1.$$

III. THE CASE OF BOUND STATES

In this section we discuss how the model can be extended to describe a situation where the attraction between the particles is strong enough to produce bound states in the interacting system. Each bound-state particle is characterized by its mass $\lambda_0 < m_1 + m_2$ and its spin l_0. In the previous section, the wave operator Ω_+ was defined in each spin subspace with the aid of an analytic function

$$B_l(z) = 1 + \int dM\,\frac{\mathcal{G}_l(M)^2}{M - z},$$

where $\mathcal{G}_l(M)^2 = (\pi)^{-1}\,\mathrm{Im}\,B_{l+}(M)$. The wave operator Ω_+ was then given by Eq. (6). It is clear from the proof given in the appendix of JMS that properties (9) and (10) hold equally well if one or several $B_l(z)$ are of the more general form

$$B_l(z) = \gamma_l + \int dM\,\frac{\mathcal{G}_l(M)^2}{M - z}, \tag{17}$$

where γ_l is an arbitrary real number. On the other hand the property $\Omega_\pm\Omega_\pm^\dagger = 1$ depends on whether or not the $B_l(z)$ have zeros on the first Riemann sheet. For more general $B_l(z)$ of form (17) one has only

$$\Omega_\pm\Omega_\pm^\dagger = 1 - Q = R, \tag{18}$$

where Q is a projection operator projecting onto the bound states of the system.[5] (In nonrelativistic potential scattering, the bound states correspond to the discrete eigenvalues of the Hamiltonian, whereas here we have infinite-dimensional subspaces for each discrete eigenvalue of the mass operator.) This suggests that to produce a bound state with mass λ_0 and spin l_0 one has to choose

$$\gamma_{l_0} = -\int dM\,\frac{\mathcal{G}_{l_0}(M)^2}{M - \lambda_0} \quad \text{implying} \quad B_{l_0}(\lambda_0) = 0.$$

Accordingly, we define the wave operators $\Omega_\pm$ by

$$(\Omega_\pm f)_{lm}(M, \mathbf{K}) = f_{lm}(M, \mathbf{K}) + \int dM'\Big(\frac{M^2 + \mathbf{K}^2}{M'^2 + \mathbf{K}^2}\Big)^{\frac{1}{4}} \times \frac{\mathcal{G}_l(M)\mathcal{G}_l(M')}{B_{l\pm}(M')(M' - M \pm i\epsilon)} f_{lm}(M', \mathbf{K}),$$

just as before, but now $B_{l_0}(\lambda_0) = 0$ and $B_l(z) \neq 0$ if $l \neq l_0$. [The model can be generalized to have several bound states as long as there is not more than one of them in any particular channel. One merely has to manufacture zeros in several of the functions $B_l(z)$.] As we mentioned before, the proofs of

$$\Omega_\pm^\dagger\Omega_\pm = 1,$$

$$\lim_{t\to\mp\infty} e^{iH_0t}\Omega_\pm e^{-iH_0t} = 1$$

and

$$(Sf)_{lm}(M, \mathbf{K}) = (\Omega_-^\dagger\Omega_+ f)_{lm}(M, \mathbf{K}) = [B_{l-}(M)/B_{l+}(M)]f_{lm}(M, \mathbf{K})$$

go through as in JMS. We can now evaluate $\Omega_\pm\Omega_\pm^\dagger$. We know that if none of the $B_l(z)$ have a zero it is equal to the identity. In our case $B_{l_0}(z)$ has got a zero at λ_0 and this gives rise to an extra term when opening up the contour of integration.[6] A short calculation yields

$$(Qf)_{lm}(M, \mathbf{K}) = \delta_{ll_0}\frac{\Gamma}{M - \lambda_0}\int dM'\Big(\frac{M^2 + \mathbf{K}^2}{M'^2 + \mathbf{K}^2}\Big)^{\frac{1}{4}} \times \frac{\mathcal{G}_{l_0}(M)\mathcal{G}_{l_0}(M')}{M' - \lambda_0} f_{l_0m}(M', \mathbf{K}), \tag{19}$$

where

$$(\Gamma)^{-1} = \int dM\,\frac{\mathcal{G}_{l_0}(M)^2}{(M - \lambda_0)^2}.$$

[5] See J. M. Jauch, Helv. Phys. Acta **31**, 127 (1958).
[6] See appendix of JMS.

The operator Q satisfies $Q^\dagger = Q$, $Q^2 = Q$ as can be checked by straightforward computation. Therefore it is a projection operator, as it should be, and it projects onto the manifold which describes the composite particle. The equation $Qf = f$ is an integral equation in the variable M and its solutions will be denoted by f^{λ_0}. They are of the form

$$f^{\lambda_0}_{lm}(M, \mathbf{K}) = \delta_{ll_0}(\Gamma)^{\frac{1}{2}}\left(\frac{M^2 + \mathbf{K}^2}{\lambda_0^2 + \mathbf{K}^2}\right)^{\frac{1}{2}} \frac{\varsigma_{l_0}(M)}{M - \lambda_0} f^{\lambda_0}_{l_0m}(\mathbf{K}),$$

where $f^{\lambda_0}_{l_0}(\mathbf{K})$ is an arbitrary function of $\mathbf{K}$. The f^{λ_0} are normalized in such a way that

$$(f^{\lambda_0}, g^{\lambda_0}) = \int d^3K(\lambda_0^2 + \mathbf{K}^2)^{-\frac{1}{2}}\tfrac{1}{2}\sum_m (f^{\lambda_0}_{l_0m}(\mathbf{K}))^* g^{\lambda_0}_{l_0m}(\mathbf{K}).$$

The manifold f^{λ_0} describes a composite particle with mass λ_0, intrinsic spin l_0 and momentum distribution $f^{\lambda_0}_{l_0m}(\mathbf{K})$. The dependence on M reveals its internal structure as can best be seen by going to the δ-function limit in the center-of-mass system. In this limit $\mathbf{p}_1 = -\mathbf{p}_2$ and so

$$M^2 = (p_1 + p_2)^2 = m_1^2 + m_2^2 + 2[(m_1^2 + |\mathbf{p}_1|^2)^{\frac{1}{2}}(m_2^2 + |\mathbf{p}_1|^2)^{\frac{1}{2}} + |\mathbf{p}_1|^2]$$

is a function of $|\mathbf{p}_1|$ and in the nonrelativistic approximation $\varsigma_{l_0}(M)$ will give the radial distribution for particle 1.

The generators for the interacting system are given by

$$\begin{aligned} HR &= \Omega_+ H_0 \Omega_+^\dagger, \\ \mathbf{P}R &= \Omega_+ \mathbf{P}_0 \Omega_+^\dagger = \mathbf{P}_0 R = R\mathbf{P}_0, \\ \mathbf{J}R &= \Omega_+ \mathbf{J}_0 \Omega_+^\dagger = \mathbf{J}_0 R = R\mathbf{J}_0, \\ \mathbf{N}R &= \Omega_+ \mathbf{N}_0 \Omega_+^\dagger, \end{aligned}$$

where R is the projection operator $R = 1 - Q$. Notice that at this stage the interacting generators are defined only on R. It is natural to extend the definition to the whole Hilbert space by putting

$$\mathbf{P} = \mathbf{P}_0, \qquad \mathbf{J} = \mathbf{J}_0, \qquad HQ = (\lambda_0^2 + \mathbf{P}^2)^{\frac{1}{2}}Q,$$

and

$$(NQf)_{lm}(M, \mathbf{K}) = -i(\lambda_0^2 + \mathbf{K}^2)^{\frac{1}{2}}(\partial/\partial\mathbf{K})(Qf)_{lm}(M, \mathbf{K}) - [\lambda_0 + (\lambda_0^2 + \mathbf{K}^2)^{\frac{1}{2}}]^{-1}\mathbf{K} \times (\mathbf{I}Qf)_{lm}(M, \mathbf{K}),$$

where $\mathbf{I}$ is the spin. With this definition one has an irreducible representation of the Poincaré group on Q, characterized by the mass λ_0 and spin l_0.

From the equation

$$\lim_{t=\mp\infty} e^{iH_0t}\Omega_\pm e^{-iH_0t} = 1$$

follows

$$\lim_{t=\mp\infty} e^{iH_0t}e^{-iHt}R = \Omega_\pm^\dagger$$

or

$$R = \lim_{t=\mp\infty} e^{iHt}e^{-iH_0t}\Omega_\pm^\dagger.$$

The above equations imply

$$\lim_{t=\mp\infty} e^{iHt}e^{-iH_0t} = \lim_{t=\mp\infty} e^{iHt}e^{-iH_0t}\Omega_+^\dagger\Omega_+ = R\Omega_+ = \Omega_+,$$

which shows that the usual requirements of a scattering system are satisfied.

IV. THE INVERSE PROBLEM

Equation (11) suggests that a large class of scattering amplitudes can be fitted with the model. To see this one has to look for the solutions of the equation

$$e^{2i\delta_l(M)} = B_{l-}(M)/B_{l+}(M), \tag{20}$$

where we assume the phase shifts $\delta_l(M)$ to be given, with the convention $-\frac{1}{2}\pi \leq \delta_l(M) < \frac{1}{2}\pi$. The $B_l(z)$ have to satisfy three conditions:

A) $B_l(z)$ are real, analytic, regular apart from a cut on the positive real axis, with the branch point at $m_1 + m_2$.

B) $\operatorname{Im} B_{l+}(M) \geq 0$ on the cut,

C) $B_l(z) \to \gamma_l$ as $|z| \to \infty$, where γ_l are real constants.

A particular solution of Eq. (20) is the real analytic Omnes function[7]

$$D_l(z) = \gamma_l \exp\left[-(\pi)^{-1}\int_{m_1+m_2}^\infty dM\, \frac{\delta_l(M)}{M - z}\right]. \tag{21}$$

Here we assume that $\delta_l(M) \to 0$, as $M \to \infty$, sufficiently fast to make $\delta_l(M)$ integrable. The function $D_l(z)$ satisfies (A) and (C), has no zeros, and its imaginary part, as z approaches the real axis from above, is given by

$$\operatorname{Im} D_{l+}(M) = -\gamma_l \sin\delta_l(M) \times \exp\left[-(\pi)^{-1}P\int dM'\, \frac{\delta_l(M')}{M' - M}\right], \tag{22}$$

which shows that if, for all l, one has either $-\frac{1}{2}\pi \leq \delta_l(M) \leq 0$ or $0 \leq \delta_l(M) < \frac{1}{2}\pi$ then with the choice $\gamma_l = +1$ or $\gamma_l = -1$ respectively,

[7] R. Omnes, Nuovo Cimento 8, 316 (1958). The mathematical content of this section is not new. Similar equations occur in nonrelativistic potential scattering as discussed by M. Gourdin and A. Martin, Nuovo Cimento 8, 699 (1958). The author is indebted to the referee for calling his attention to this paper.

$$B_l(z) = D_l(z) = \pm 1 + \pi^{-1} \int dM \Big\{ \mp \sin \delta_l(M) \times \exp\left[-(\pi)^{-1} P \int dM' \frac{\delta_l(M')}{M' - M} \right] (M - z)^{-1} \Big\} \quad (23)$$

is a satisfactory solution with no bound states. Incidentally

$$\mathcal{G}_l(M) = \pi^{-\frac{1}{2}} \Big(\mp \sin \delta_l(M) \times \exp\left[-(\pi)^{-1} P \int dM' \frac{\delta_l(M')}{M' - M} \right] \Big)^{\frac{1}{2}}.$$

To produce a bound state one has to notice that

$$D_l(z) = \frac{M(z)}{N(z)} \gamma_l \exp\left[-(\pi)^{-1} \int dM \frac{\delta_l(M)}{M - z} \right],$$

where $M(z)$ and $N(z)$ are arbitrary polynomials, is also a solution of Eq. (20). Because of condition (C) one must have $\lim_{|z|\to\infty} M(z)/N(z) = 1$. Let us now suppose that for some l, say l_0, $\delta_{l_0}(M)$ satisfies $-\frac{1}{2}\pi \leq \delta_{l_0}(M) < 0$ if $m_1 + m_2 < M \leq M_0$ and $0 < \delta_{l_0}(M) < \frac{1}{2}\pi$ if $M > M_0$, where M_0 is a real number $M_0 > m_1 + m_2$. The phase shift $\delta_{l_0}(M)$ has a jump of magnitude π at $M = M_0$. This introduces a singularity in $\int dM\, \delta_{l_0}(M)/(M - z)$ and an easy calculation shows that in the neighborhood of M_0

$$-\frac{1}{\pi} \int dM \frac{\delta_{l_0}(M)}{M - z} \sim +\log (z - M_0).$$

Consequently, the function

$$D_{l_0}(z) = \frac{z - \lambda_0}{z - M_0} \gamma_{l_0} \exp\left[-(\pi)^{-1} \int dM \frac{\delta_{l_0}(M)}{M - z} \right]$$

remains finite as $z \to M_0$ and has a zero at $z = \lambda_0$, $\lambda_0 < m_1 + m_2$. Its imaginary part on the real axis $M \geq m_1 + m_2$ is given by

$$\operatorname{Im} D_{l_0+}(M) = -\gamma_{l_0}(M - \lambda_0)/(M - M_0) \sin \delta_{l_0}(M) \times \exp\left[-(\pi)^{-1} P \int dM' \frac{\delta_{l_0}(M')}{M' - M} \right] \geq 0 \quad (24)$$

provided $\gamma_{l_0} < 0$. Choosing $\gamma_{l_0} = -1$ we obtain that

$$B_{l_0}(z) = D_{l_0}(z) = -1 + \frac{1}{\pi} \int dM \frac{M - \lambda_0}{(M - z)(M - M_0)} \times \sin \delta_{l_0}(M) \exp\left[-(\pi)^{-1} P \int dM' \frac{\delta_{l_0}(M')}{M' - M} \right] \quad (25)$$

is a satisfactory solution with a zero at $z = \lambda_0$, i.e., with one bound state.

This kind of argument can be generalized. If $\delta(M)$ passes through $+\frac{1}{2}\pi$ from the opposite direction, the discontinuity in $\delta(M)$ produces a pole in the Omnes function. In general, one can fit with the model any set of phase shifts which satisfies in each channel $n_1 = 0$, $n_2 \leq n_3$ where n_1, n_2, and n_3 are the number of times $\delta_l(M)$ passes through 0, $\frac{1}{2}\pi$, and $-\frac{1}{2}\pi$ respectively. As $n_1 + n_2 \geq n_3 - 1$ we see that a sufficient condition for having a bound state is that $n_2 - n_3 = -1$.

V. CONCLUSIONS

Our conclusions may be summarized as follows:

(1) In the relativistic scattering of two spinless particles, in so far as they constitute a closed system, the scattering amplitude determines the wave operators $\Omega_\pm$ and the interacting generators uniquely, provided $\Omega_\pm$ are further required to satisfy $\Omega_+ \mathbf{P}_0 \Omega_+^\dagger = \mathbf{P}_0$ and $i_t \Omega_+ i_t = \Omega_-$ which is sufficient to ensure invariance under arbitrary Lorentz transformations. This we proved only for the case of no bound states but analogous results can probably be derived even for the more general case.

(2) The model constructed by JMS can be extended to include bound states. The projection operator associated with the bound-state manifold can be calculated, giving a direct relation between the scattering amplitude and the structure of the composite particle.

(3) A large class of phase shifts can be fitted with the model. The phase shifts have to go to zero sufficiently fast and one has to have $n_1 = 0$, $n_2 \leq n_3$, where n_1, n_2, and n_3 denote the number of times the phase shift goes through 0, $\frac{1}{2}\pi$, and $-\frac{1}{2}\pi$ in any particular channel.

An extension of the model to spin-$\frac{1}{2}$ particles would make it possible in principle to calculate the relativistic deuteron wavefunction from proton–neutron scattering data. However, the spin-$\frac{1}{2}$ case will be more involved, because of the spin degeneracy in the reduction of the two-particle space.[3,4] Work on the extension of this model to remove the restriction $\delta_l(M) \to 0$ and to include spin $\frac{1}{2}$ is now in progress.

Note added after the completion of the manuscript: Work on the inclusion of resonance states and the removal of the condition $\delta_l(M) \to 0$ as $M \to \infty$ has now been completed. The results are being published in the Arkiv för Fysik by the author.

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Fourier Series Expansion for the General Power of the Distance between Two Points

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The general power $r^n = (r_1^2 - 2r_1 r_2 \cos\omega + r_2^2)^{n/2}$ of the distance between two points is expressed as a Fourier series $\sum R_{n,l}(r_1, r_2) \cos l\omega$. Following Sack's method, the radial functions $R_{n,l}$ are obtained as power series in $r_</r_>$. Symmetrical expressions in r_1 and r_2 and recurrence relations are found for $R_{n,l}$.

1. INTRODUCTION

EXPANSIONS for powers of the distance $r = (r_1^2 - 2r_1r_2\cos\omega + r_2^2)^{\frac{1}{2}}$, [$\cos\omega = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1 - \phi_2)$] between two points with spherical polar coordinates r_1, θ_1, ϕ_1 and r_2, θ_2, ϕ_2 have been considered by several authors. The expansion of the first inverse power as a series in the Legendre coefficients $P_l(\cos\omega)$ is well known. Chapman[1] generalized this expansion to any real power n of the distance for applications in the kinetic theory of gases. His method was first to express r^n as a binomial series in powers of $\{2r_1r_2/(r_1^2 + r_2^2)\}\cos\omega$, and then to substitute for the powers of $\cos\omega$ the appropriate series of Legendre coefficients $P_l(\cos\omega)$, and for those of $(r_1^2 + r_2^2)$ the corresponding binomial series. After rearranging and interchanging orders of summation, he could prove the validity of his final expansion. Later Sack,[2] obviously unaware of Chapman's work, used a different method to obtain the same results for applications in the theory of molecular structure. However, Sack obtained further results, e.g., the expressions for $\log r$ and of certain functions of r. He also obtained expansions for r^n symmetrical in r_1 and r_2.

It is equally important in the applications to obtain a Fourier series expansion for r^n, i.e., an expansion in which the dependence of the different terms on ω appears as $\cos l\omega$ and which is appropriate in two dimensions. Hobson,[3] obtained this expansion for the particular case $n = -1$ by writing $r^{-1} = (r_1 - r_2e^{-i\omega})^{-\frac{1}{2}}(r_1 - r_2e^{i\omega})^{-\frac{1}{2}}$, and multiplying the two series resulting from the binomial expansions. In a previous paper,[4] in the course of obtaining an integral equation for the associated Legendre function of the first kind, Fourier series for r^{-1} and r^{-3} were obtained in which the dependence on r_1 and r_2 appears as series of $P_n^m(1 - r_1^2)^{\frac{1}{2}}P_n^m(1 - r_2^2)^{\frac{1}{2}}$ ($|r_1|$ and $|r_2|$ are assumed to be both less than unity[5]).

The object of this paper is to obtain this Fourier expansion for r^n. For this purpose, we have at our disposal the three methods of Chapman, Sack, and Hobson, all of which may be adapted to the present problem. Sack's method is chosen and is followed closely, because it does not involve any multiplication or rearrangement of series. His notation is used and reference should be made to his paper (referred to hereafter as I) for definitions not given here.

2. MATHEMATICAL DERIVATION

Following the method used in I, we express $V_n = r^n$ as

$$V_n = \sum_l R_{n,l}(r_1, r_2)\cos l\omega, \tag{1}$$

where the R's are homogeneous functions of degree n in the variables r_1 and r_2 and may be expressed as

$$R_{n,l} = r_<^l r_>^{n-l} G_{nl}(r_</r_>), \tag{2}$$

since V_n is continuous when $r_< = 0$. The function $G_{nl}(x)$ is analytic for $0 \le x < 1$ and hence may be expressed as

$$G_{nl}(r_</r_>) = \sum_s C_{n,l,s}(r_</r_>)^s. \tag{3}$$

If we now define the operator ∇_λ^2 as

$$\nabla_\lambda^2 \equiv \frac{\partial^2}{\partial^2 r_\lambda} + \frac{1}{r_\lambda}\frac{\partial}{\partial r_\lambda} + \frac{1}{r_\lambda^2}\frac{\partial^2}{\partial\omega^2}, \tag{4}$$

(i.e., ∇_λ^2 is the Laplacian operator in the two-dimensional polar coordinates r_λ, ω), it can be

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[1] S. Chapman, Quart. J. Pure Appl. Math. 185, 16 (1916).

[2] R. A. Sack, J. Math. Phys. 5, 245 (1964).

[3] E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics*, (Cambridge University Press, London, 1951), p. 443.

[4] A. A. Ashour, J. Math. Phys. 5, 1421 (1964).

[5] This is no serious limitation since r_1 and r_2 can be expressed as ax_1 and ax_2 where a is chosen such that $|x_1|$ and $|x_2|$ are both less than one.

shown by direct differentiation that

$$\nabla_1^2 V_n = \nabla_2^2 V_n = n^2 V_{n-2}. \tag{5}$$

From (1) and (5), we then obtain

$$\frac{\partial^2 R_{n,l}}{\partial r_1^2} + \frac{1}{r_1}\frac{\partial R_{n,l}}{\partial r_1} - \frac{l^2}{r_1^2} R_{n,l} = \frac{\partial^2 R_{n,l}}{\partial r_2^2} + \frac{1}{r_2}\frac{\partial R_{n,l}}{\partial r_2} - \frac{l^2}{r_2^2} R_{n,l} \tag{6}$$

Substituting from (2) and (3) into (6) and equating coefficients of equal powers of $r_</r_>$, we obtain

$$(s+2)(2l+s+2)C_{n,l,s+2} = (n-s)(n-s-2l)C_{n,l,s}. \tag{7}$$

For exactly the same reasons given in I, we conclude from (7) that all coefficients $C_{n,l,s}$ vanish when s is odd, and that the sequence of even coefficients start with $s = 0$. Hence

$$C_{n,l,2\nu} = [(-\tfrac{1}{2}n)_\nu (l - \tfrac{1}{2}n)_\nu / \nu!\,(l+1)_\nu] C_{n,l,0}. \tag{8}$$

From (2), (3), and (8) we obtain

$$R_{n,l}(r_1, r_2) = K(n, l) r_<^l r_>^{n-l} F(-\tfrac{1}{2}n, l - \tfrac{1}{2}n; l+1; (r_</r_>)^2), \tag{9}$$

where $K(n, l)$ is a suitable function of n and l to be determined, and F is the Gauss hypergeometric function defined in I. It can be proved in exactly the same manner as in I that

$$K(n, l) = f(l)(-\tfrac{1}{2}n)_l. \tag{10}$$

The determination of the unknown factor $f(l)$ is not direct as in I. This is because in the present analysis the expansion of V_n is not preknown for any special value of n (except the trivial case $n = 0$), while in I, the expansion for V_{-1} is known. However, by examining the expansions for positive even n, we find, in view of

$$(-2\cos\omega)^{n/2} = (2 - \delta^0_{n/2})(-)^{n/2}\cos\tfrac{1}{2}n\omega + \cdots,$$

that

$$f(l) = (2 - \delta_l^0)/l!, \tag{11}$$

where δ_l^m is the Kronecker symbol. This result will further be verified when considering the expansion of $\log r$ in the next section. Thus we finally obtain

$$R_{n,l}(r_1, r_2) = [(2 - \delta_l^0)/l!](-\tfrac{1}{2}n)_l r_>^n (r_</r_>)^l \times F(-\tfrac{1}{2}n, l - \tfrac{1}{2}n; l+1; (r_</r_>)^2). \tag{12}$$

The above expression agrees, for the special case $n = -1$, with that obtained by Hobson.[3]

3. THE EXPANSION FOR $\log r$

The function $\log r$ is a solution of Laplace's equation in either (r_1, ω) or (r_2, ω). Also

$$(\log r)_{\omega=0} = \log(r_> - r_<) = \log r_> - \sum_{l=1}^{\infty} \frac{1}{l}\left(\frac{r_<}{r_>}\right)^l. \tag{13}$$

Hence it follows that

$$\log r = \log r_> - \sum_1^\infty \frac{1}{l}\left(\frac{r_<}{r_>}\right)^l \cos l\omega. \tag{14}$$

As a check to previous results and also to verify the value of $f(l)$, we find $\log r$ using the formula

$$\log r = \lim_{n\to 0}\frac{\partial r^n}{\partial n} = \sum_l R_{\log,l}(r_1, r_2)\cos l\omega. \tag{15}$$

Equations (12) and (15) give

$$R_{\log,0} = \log r_>, \qquad R_{\log,l} = -(1/l)(r_</r_>)^l, \quad l > 0, \tag{16}$$

in agreement with (14).

4. PROPERTIES OF THE RADIAL FUNCTIONS

n Even Integer

If n is a positive even integer, then due to the factor $(-\frac{1}{2}n)_l$, the radial functions $R_{n,l}$ vanish identically for $l > \frac{1}{2}n$, and hence the series for V_n will have $\frac{1}{2}n + 1$ terms only. The hypergeometric function appearing in each of these terms will be a polynomial since both $l - \frac{1}{2}n$ and $-\frac{1}{2}n$ are either negative integers or zero.

If we apply the transformation (20a) in I to the hypergeometric function in the expression (12) for $R_{n,l}$, we obtain

$$R_{n,l}(r_1, r_2) = \frac{(2 - \delta_l^0)}{l!}\left(-\frac{n}{2}\right)_l r_>^n \left(\frac{r_<}{r_>}\right)^l \left[1 - \left(\frac{r_<}{r_>}\right)^2\right]^{n+1} \times F(l + 1 + \tfrac{1}{2}n, 1 + \tfrac{1}{2}n; l+1; (r_</r_>)^2). \tag{17}$$

It is clear from (17) that if n is an even *negative* integer, the hypergeometric function involved will again break and reduce to a polynomial, but the series for V_n will be infinite. In particular

$$V_{-2} = \frac{1}{(r_>^2 - r_<^2)}\left\{1 + 2\sum_1^\infty \left(\frac{r_<}{r_>}\right)^l \cos l\omega\right\}. \tag{18}$$

It is clear from (18) that $(r_2^2 - r_1^2)/(r_1^2 - 2r_1 r_2\cos\omega + r_2^2)$ is a two-dimensional solution of Laplace's equation in the polar coordinates r_1 (or r_2) and ω, as can easily be verified by direct differentiation.

Symmetrical Expressions in r_1 and r_2

Application of the transformations (26a) and (26b) in I to the hypergeometric function in (12) yields

$$R_{n,l}(r_1, r_2) = \frac{(2-\delta_l^0)(-n/2)_l}{l!}(r_1r_2)^l(r_1^2+r_2^2)^{n/2-l} \times F\left(\frac{l}{2}-\frac{n}{4}, \frac{l}{2}-\frac{n}{4}+\frac{1}{2}; l+1; \frac{4r_1^2r_2^2}{(r_1^2+r_2^2)^2}\right), \quad (19a)$$

$$R_{n,l}(r_1, r_2) = \frac{(2-\delta_l^0)(-n/2)_l}{l!}(r_1r_2)^l(r_1+r_2)^{n-2l} \times F\left(l-\frac{n}{2}, l+\frac{1}{2}; 2l+1; \frac{4r_1r_2}{(r_1+r_2)^2}\right). \quad (19b)$$

These expressions are symmetrical in r_1 and r_2. To find the same for $\log r$ we use (15) and (19). Thus we obtain

$$R_{\log,l} = -\frac{1}{l}\left\{\frac{r_1r_2}{(r_1^2+r_2^2)}\right\}^l F\left(\frac{l}{2}, \frac{l+1}{2}; l+1; \frac{4r_1^2r_2^2}{(r_1^2+r_2^2)^2}\right) \quad (20a)$$

$$= -\frac{1}{l}\left\{\frac{r_1r_2}{(r_1+r_2)^2}\right\}^l F\left(l, l+\tfrac{1}{2}; 2l+1; \frac{4r_1r_2}{(r_1+r_2)^2}\right) \quad l>0 \quad (20b)$$

and

$$R_{\log,0} = \tfrac{1}{2}\log(r_1^2+r_2^2) - \frac{1}{4}\sum_{s=1}^{\infty}\frac{(1/2)_s}{s\cdot s!}\left(\frac{2r_1r_2}{(r_1^2+r_2^2)}\right)^{2s} \quad (21a)$$

$$= \log(r_1+r_2) - \frac{1}{2}\sum_{s=1}^{\infty}\frac{(1/2)_s}{s\cdot s!}\left\{\frac{4r_1r_2}{(r_1+r_2)^2}\right\}^s. \quad (21b)$$

The expressions (20) can be summed to yield (16b) by means of (B.2.8.6).[6] Also the series in (21a) and (21b) can be summed to give $R_{\log,0} = \log r_>$ in agreement with (16).

Recurrence Relations

Application of (B.2.8.31) to (19b) gives the recurrence relation

$$R_{n+2,l} = \{(n+2)/[(n+2)^2-4l^2]\} \times \{2(n+1)(r_1^2+r_2^2)R_{n,l} - n(r_1^2-r_2^2)^2R_{n-2,l}\}, \quad (22)$$

and of (B.2.8.35) to (19a) yields

$$(r_1^2+r_2^2)R_{n,l} = 2(1+\delta_l^1)r_1r_2R_{n,l-1} + [(n+2+2l)/(n+2)]R_{n+2,l}, \quad (l>0). \quad (23)$$

Also, application of (B.2.9.3) and (B.2.8.45) to (12) obtains

$$(r_1^2+r_2^2)R_{n,l} = (r_1r_2/2l)\{(n+2l+2)R_{n,l+1} + (1+\delta_l^1)(2l-n-2)R_{n,l-1}\}, \quad (l>0). \quad (24)$$

From (23) and (24) we finally obtain

$$R_{n+2,l} = [(n+2)/2l]r_1r_2 \times \{R_{n,l+1} - (1+\delta_l^1)R_{n,l-1}\}, \quad (l>0). \quad (25)$$

In Ref. 4, the writer obtained the following expressions for $R_{-1,l}$ and $R_{-3,l}$:

$$R_{-1,l}(r_1, r_2) = \frac{\pi}{2}(2-\delta_l^0)\sum_{s=0}^{\infty}(4s+2l+1) \times \left\{\frac{1\cdot3\cdot5\cdots2s-1}{2\cdot4\cdot6\cdots2s+2l}\right\}^2 P_{2s+l}^l(\xi_1)P_{2s+l}^l(\xi_2), \quad (26a)$$

$$R_{-3,l}(r_1, r_2) = -\frac{\pi(2-\delta_l^0)}{2\xi_1\xi_2}\sum_{s=0}^{\infty}(4s+2l+3) \times \left\{\frac{1\cdot3\cdot5\cdots2s+1}{2\cdot4\cdot6\cdots2s+2l}\right\}^2 P_{2s+l+1}^l(\xi_1)P_{2s+l+1}^l(\xi_2), \quad (26b)$$

where $r_\lambda = (1-\xi_\lambda^2)^{\frac{1}{2}}$ ($\lambda = 1$ or 2 and $|r_\lambda|$ is assumed less than one). The expressions (26) may be used with the recurrence relations (22)–(25) to obtain similar expansions[7] for $R_{n,l}$ when n is an odd integer, positive or negative. As an example, we take $n = -1$ in (22) and obtain

$$R_{1,l} = -[(\xi_1^2-\xi_2^2)^2/(4l^2-1)]R_{-3,l}, \quad (27)$$

in agreement with (17) for $n = 1$ and $n = -3$ (B.2.9.1).

[6] Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill Book Company, Inc., New York, 1953). Sections and formulas in this reference will be referred to (as in I) by the letter B.

[7] Such expressions are useful in finding solutions for Fredholm integral equations with kernel $R_{n,l}$ and interval of integration 0 to 1 (or −1 to 1).