

# Quantum Statistics of Interacting Particles; Thermodynamic Quantities and Pair Distribution Function\*

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An alternative approach to the quantum statistics of interacting particles is proposed. It consists of calculating the equilibrium thermodynamical quantities of the many-body system via the pair distribution function with the assumption that the particles interact with each other only through pair central forces. The proposed approach has some advantage over the usual treatment via the partition function in that the pair distribution function is easier to deal with than the partition function in certain circumstances particularly when the collective motion description of the system is desirable. This is because only the pair distribution function can be expressed directly in terms of the collective interaction which is closely connected with collective elementary excitation, such as a plasmon in the electron gas and a phonon in the hard-sphere Boson gas. The equation of state as well as the internal energy are obtained in the form of integrals of the pair distribution function. The close analogy between the pair distribution function and the two-body propagator, which appears in the quantum field theory, makes it possible to analyze the former by the use of Feynman diagrams identical with those usually introduced for the latter. The collective interaction, which is

defined by the sum of the direct and the indirect interactions, is introduced as a particular partial sum of the perturbation series of the pair distribution function. This is used in rewriting the pair distribution function in terms of the collective interaction.

It is shown that, while the simple chain approximation to the collective interaction in the electron gas is responsible for the transfer of a plasmon, the same approximation to the collective pseudo-interaction in the hard-sphere Boson system has a relation similar to that of transfer of a phonon, both cases occurring at low temperatures. The explicit calculation of the pair distribution functions for these systems at the absolute zero temperature is carried out up to the first order in the collective interaction (simple chain approximation.) These results are used to calculate the ground-state energies. For the electron gas the energy thus obtained confirms Gell-Mann-Bruckner's calculation of the correlation energy. For the hard-sphere Bosons the calculated energy reproduces the result of Lee, Huang, and Yang. The extension of the calculation to the finite temperature case is also indicated. In particular the classical Debye-Huckel equation of state for the electron gas is briefly discussed.

## 1. INTRODUCTION

IN the previous investigation by one of the authors (S. F.)<sup>1</sup> a close analogy is established between the  $l$ -body reduced density matrices in the grand canonical ensemble and the  $l$ -body propagators in the quantum field theory. In particular the pair distribution function was shown to be expressed in terms of a two-body propagator defined in the position-reciprocal temperature space. The analogy is a natural extension of that between the grand partition function and the vacuum fluctuation.<sup>2,3</sup> If the vacuum fluctuation and the two-body propagator are to be examined in the spirit of Feynman's diagrammatic method, it can be said that the latter is easier to handle than the former. This is particularly so when one counts the number of those diagrams which contribute to the quantity in question. Furthermore if one wishes to investigate the behavior of the collective motion of a certain many-body system, it is much simpler to deal with the two-body propagator. This is because only the two-body propagator may be expressed directly in terms of the collective interaction which is closely related to the transfer of a collective elementary excitation. This argument with the aforementioned analogy leads us to reconsider the importance of the pair distribution function as a possible tool for an investigation into the thermodynamic properties. Of course the pair distribution function  $n^{(2)}(r)$  has its own

physical meaning: it gives the relative probability of finding two particles separated by a distance  $r$ . However it is also known, at least for the classical case, that the equilibrium properties such as the internal energy and the pressure of a many-body system can be obtained from integrals of the pair distribution function provided that the system consists of particles interacting with pair forces only. This is also true for the quantum-mechanical case. As a matter of fact the internal energy was shown to be given in terms of the pair distribution function in reference 1. As another example the equation of state is presented in the form of an integral of the quantum-mechanical pair distribution function in Sec. 2. We believe that many important thermodynamic quantities such as the chemical potential, thermal compressibility, and surface energy of the system are also derivable from the pair distribution function for the quantum-statistical as well as the classical case.

The previous investigation<sup>1</sup> concerning the construction of the pair distribution function from the two-body propagator defined in the position-reciprocal temperature space is briefly summarized in Sec. 3. Since the two-body propagator mentioned above has the same operators which are to be averaged as the one usually introduced in the quantum field theory<sup>4</sup> (i.e., defined in the position time space), it is concluded that essentially the same Feynman diagrams emerge for the quantum-statistical case. A similar idea was first expressed by Matsubara<sup>2</sup> in his treatment of quantum statistics via the grand partition function. In fact Green's functions

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<sup>1</sup> S. Fujita, Phys. Rev. **115**, 1335 (1959).

<sup>2</sup> T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955).

<sup>3</sup> E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).

<sup>4</sup> E.g., S. S. Schweber, H. A. Bethe, and F. de Hoffmann, *Mesons and Fields* (Row, Peterson, Evanston, Illinois, 1955), Vol. 1, p. 394.

introduced in his theory are essentially the same as our propagators. Our formalism is different from his in that while he investigated the vacuum field fluctuation diagrams representing contributions to the grand partition function we are primarily concerned with the two-body scattering diagrams in order to treat the pair distribution function.

We give in Sec. 4 a short account of the graphical representation of the perturbation series for the propagator *a la* Feynman.<sup>5</sup> Since the actual computation of diagrams is simplified by working in momentum-energy space, we introduced the momentum-energy representation together with the position-reciprocal temperature representation of propagators. For later reference we give at the end of Sec. 4 two tables, one for the correspondence between diagram elements and propagator kernel elements in position-reciprocal temperature space, and one for the same in momentum-energy space.

In dealing with the many-body system it is sometimes of essential importance to find a certain appropriate descriptive method for its collective motion. Liquid helium and the electron gas at low temperatures are notable examples of such systems. In this connection L. Landau<sup>6</sup> pointed out that the behavior of such a system can be most conveniently described in terms of elementary excitations, e.g., phonons in liquid helium and plasmons in the electron gas. Here the elementary excitation is a physical quasi-particle which has a definite momentum-energy relation and which plays a role similar to that of a light quantum (photon) as carrier of an energy-momentum in the scattering process of particles. In other words it acts as if it produced a new interaction between particles. To study this situation Feynman's diagrammatic analysis is very useful, since it tells us clearly what type of subdiagrams out of the whole perturbation series for the propagator contributes to the new interaction—a relevant type is the one with two outer quantum lines plus closed particle loops with or without inner quantum lines. The collective (or modified) interaction is defined as a collection of these contributions. Fortunately this collective interaction is discussed in detail by J. Hubbard<sup>7</sup> for the case of the quantum-mechanical many-body problem. The extension to the quantum-statistical case is straightforward. Summing up subseries corresponding to the collective interaction, we obtain the two-body propagator expressed in terms of the collective interaction without any approximation. As expected we see from the explicit calculation that the simple chain approximation to the collective interaction for the electron gas is closely related to the transfer of a plasmon.

Because of the singular nature of the interaction we cannot develop the perturbation theory for the hard-sphere Bose gas which can be regarded as a simplified

model of liquid helium. However, it was shown by T. D. Lee, K. Huang, and C. N. Yang<sup>8,9</sup> that the low-temperature and low-density behavior of the hard-sphere system can be conveniently analyzed by introducing the so-called pseudo-interaction (pseudo-potential). Adopting this interaction we examined the momentum-energy transfer between particles and found that the simple chain approximation to the collective pseudo-interaction is closely connected with the transfer of a phonon.

The next two sections 6 and 7 are devoted to the application of the present theory to the electron gas and the hard-sphere Bose gas. In Sec. 6 we calculate the zeroth- and first-order terms in the collective interaction (simple chain approximation) of the pair distribution function of the electron gas at the absolute zero temperature. This is used to calculate the ground-state energy from the formula for the internal energy discussed in Sec. 2. The result is compared with Gell-Mann-Bruckner's<sup>10,11</sup> calculation of the correlation energy. Using the same procedure we evaluate in Sec. 7 the pair distribution function and the internal energy of the hard-sphere Bose gas at the absolute zero temperature. The result agrees with that of Lee, Huang, and Yang.<sup>8,9</sup>

Final remarks are given in Sec. 8, together with a short discussion of the Debye-Huckel equation for the electron gas at high temperatures. Throughout the text the following units are chosen: twice the mass  $M$  of a particle and the Planck's constant  $\hbar$  divided by  $(2\pi)$  are set to unity:

$$2M = \hbar = 1.$$

## 2. PAIR DISTRIBUTION FUNCTION AND EQUATION OF STATE

Let us consider a system of identical particles interacting with pair central forces only. The Hamiltonian of the system will be given by

$$H = H_0 + gH_I \quad (2.1)$$

$$= - \int d^3r \psi^\dagger(\mathbf{r}) \nabla^2 \psi(\mathbf{r}) + \frac{1}{2} g \int \int d^3r d^3r' \psi^\dagger(\mathbf{r}) \times \psi^\dagger(\mathbf{r}') v(|\mathbf{r} - \mathbf{r}'|) \psi(\mathbf{r}') \psi(\mathbf{r}), \quad (2.2)$$

where  $g$  and  $v(r)$  are the coupling strength and pair potential, respectively, and the integration extends over the volume of normalization. The field operators  $\psi(\mathbf{r})$ 's and their Hermitean conjugates  $\psi^\dagger(\mathbf{r})$ 's satisfy the following commutation relations:

$$[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')]_{\mp} \equiv \psi(\mathbf{r}) \psi^\dagger(\mathbf{r}') \mp \psi^\dagger(\mathbf{r}') \psi(\mathbf{r}) = \delta^{(3)}(\mathbf{r} - \mathbf{r}') \\ [\psi(\mathbf{r}), \psi(\mathbf{r}')]_{\mp} = [\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')]_{\mp} = 0, \quad (2.3)$$

<sup>8</sup> Kerson Huang and C. N. Yang, Phys. Rev. **105**, 767, 776 (1957); T. D. Lee, Kerson Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).

<sup>9</sup> T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1119 (1957); **113**, 1165 (1959).

<sup>10</sup> M. Gell-Mann and K. A. Bruckner, Phys. Rev. **106**, 364 (1957); P. Nozieres and D. Pines, Phys. Rev. **111**, 442 (1958).

<sup>11</sup> The identity between this and the usual definition was established in reference 1.

<sup>5</sup> R. P. Feynman, Phys. Rev. **76**, 749; 769 (1949).

<sup>6</sup> L. Landau, J. Phys. U. S. S. R. **5**, 71 (1941).

<sup>7</sup> J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957); **A243**, 336 (1958).

where upper sign is for Bosons, the lower sign for Fermions, and  $\delta^{(3)}(\mathbf{r})$  is the three-dimensional delta function. From a fundamental theorem of statistical mechanics, a grand canonical average of an arbitrary physical quantity  $G$  is given by

$$\langle G \rangle = \text{Tr}\{G e^{-\beta H + \alpha N}\} / \text{Tr}\{e^{-\beta H + \alpha N}\}, \quad (2.4)$$

where  $\beta$  is the reciprocal temperature  $(kT)^{-1}$ ,  $k$  being Boltzmann's constant, and  $e^\alpha$  is the fugacity of the system.  $N$  is the number operator defined by

$$N = \int d^3r \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}). \quad (2.5)$$

In particular, the internal energy of the system is given by the grand canonical average of the Hamiltonian:

$$E \equiv \langle H \rangle_{\text{av}} = \text{Tr}\{H e^{-\beta H + \alpha N}\} / \text{Tr}\{e^{-\beta H + \alpha N}\}. \quad (2.6)$$

Substitution of (2.1) gives

$$E = \langle H_0 \rangle_{\text{av}} + g \langle H_I \rangle_{\text{av}}. \quad (2.7)$$

The average of the potential part of the Hamiltonian is readily expressed in terms of the pair distribution function defined by<sup>11</sup>

$$n^{(2)}(\mathbf{r}, \mathbf{r}') \equiv \frac{\text{Tr}\{\psi(\mathbf{r})\psi(\mathbf{r}')e^{-\beta H + \alpha N}\psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r})\}}{\text{Tr}\{e^{-\beta H + \alpha N}\}}. \quad (2.8)$$

Substituting the explicit expression for  $H_I$  from (2.2) into (2.4) one obtains

$$\begin{aligned} \langle H_I \rangle_{\text{av}} &= -\frac{1}{2} \int \int d^3r d^3r' v(|\mathbf{r} - \mathbf{r}'|) \\ &\quad \times \frac{\text{Tr}\{\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r})e^{-\beta H + \alpha N}\}}{\text{Tr}\{e^{-\beta H + \alpha N}\}} \\ &= \frac{1}{2} V \int d^3r v(r) n^{(2)}(r). \end{aligned} \quad (2.9)$$

On the other hand a direct substitution of the kinetic energy part of the Hamiltonian into (2.4) leads to

$$\begin{aligned} \langle H_0 \rangle_{\text{av}} &= - \int d^3r \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \nabla^2 [\text{Tr}\{\psi(\mathbf{r})e^{-\beta H + \alpha N}\psi^\dagger(\mathbf{r}')\} / \\ &\quad \text{Tr}\{e^{-\beta H + \alpha N}\}] \\ &= - \int d^3r \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \nabla^2 \rho^{(1)}(\mathbf{r}; \mathbf{r}'), \end{aligned} \quad (2.10)$$

where  $\rho^{(1)}(\mathbf{r}; \mathbf{r}')$  defined above may be called the  $(\mathbf{r}, \mathbf{r}')$  element of the one-body reduced density matrix. Although the diagonal elements of the reduced density matrix  $\rho^{(1)}$  give precisely the density of the system, the off-diagonal elements are not familiar quantities.

To avoid the use of off-diagonal elements one makes use of the following relation between the internal energy

and the pair distribution function:

$$E(\beta) = E_0(\beta) + \frac{1}{2} V \int_0^g dg' \int d^3r v(r) \frac{\partial}{\partial \beta} n^{(2)}(r; \beta, g') \quad (2.11)$$

where  $E_0(\beta)$  is the kinetic energy of the free particle system with the same statistics as that of the system in question and  $n^{(2)}(r; \beta, g')$  is to be calculated with the coupling strength  $= g'$ . This relation was obtained from (2.6) by differentiating it with respect to  $g$  and rearranging the result properly and integrating back again.<sup>1</sup>

Comparing (2.7) and (2.11), one finds

$$\begin{aligned} \langle H_0 \rangle_{\text{av}} &= E - g \langle H_I \rangle_{\text{av}} \\ &= E_0 + \frac{1}{2} V \int_0^g dg' \int d^3r v(r) \frac{\partial}{\partial \beta} n^{(2)}(r; \beta, g') \\ &\quad - \frac{1}{2} V g \int d^3r v(r) n^{(2)}(r; \beta, g), \end{aligned} \quad (2.12)$$

where the last step is obtained by substituting  $\langle H_I \rangle_{\text{av}}$  from (2.9). Now the average of the kinetic energy part of the Hamiltonian is expressed in terms of the pair distribution function explicitly. The immediate application of this will be found in the following derivation of the equation of state.

In deriving the equation of state it is simplest to use a virial theorem in both classical and quantum theories. This virial theorem states that for a system in equilibrium the average value of the virial of the external and internal forces exerted on the system is equal to minus twice the average value of the kinetic energy of the system. If the theorem is applied to a gas enclosed in a vessel of volume  $V$  under an external pressure  $p$ , the virial of the external forces is  $-3pV$  and the virial of the pair central forces is equal to

$$\Xi \equiv \sum_i \mathbf{r}_i \cdot \mathbf{F}_i = -\frac{1}{2} \sum_{i \neq k} \sum_{\mathbf{r}_{ik}} \frac{\partial v(r_{ik})}{\partial r_{ik}}.$$

In short the virial theorem states that

$$-2\langle H_0 \rangle_{\text{av}} = -3pV + \langle \Xi \rangle_{\text{av}}$$

or

$$pV = \frac{2}{3} \langle H_0 \rangle_{\text{av}} + \frac{1}{3} \langle \Xi \rangle_{\text{av}}. \quad (2.13)$$

The average of the virial of the internal force is

$$\langle \Xi \rangle_{\text{av}} = -\frac{1}{2} g V \int d^3r r [dv(r)/dr] n^{(2)}(r; \beta, g). \quad (2.14)$$

Substituting  $\langle H_0 \rangle_{\text{av}}$  and  $\langle \Xi \rangle_{\text{av}}$  from (2.12) and (2.14) into (2.13), one obtains the equation of state in the following form:

$$\begin{aligned} pV &= \frac{2}{3} E_0 - \frac{1}{6} V g \int d^3r [2v(r) + r(d/dr)v(r)] n^{(2)}(r; \beta, g) \\ &\quad + \frac{1}{3} V \int_0^g dg' \int d^3r v(r) \frac{\partial}{\partial \beta} n^{(2)}(r; \beta, g'). \end{aligned} \quad (2.15)$$

This form is a desirable one. The product of the pressure and the volume can now be obtained from the knowledge of the pair distribution function provided one knows the kinetic energy of the corresponding free-particle system. The latter may be given by

$$E_0(\beta) = (2\pi)^{-3} V \int d^3p \, p^2 f(p), \quad (2.16)$$

where  $f(p)$  is the Bose or Fermi distribution function depending upon the statistics obeyed by the system. So far we have succeeded in deriving the formulas for the internal energy and pressure in terms of the pair distribution function in the quantum-statistical case. However it is well known in classical statistical mechanics that various thermodynamical quantities can be expressed by integrals of the pair distribution function. Among these quantities one finds the chemical potential, thermal compressibility, surface energy, and surface tension of the system, besides the two quantities so far treated.

Although we do not attempt to derive the corresponding formulas for these quantities for the case of quantum theory, we believe that the quantum-statistical formulas can be derived with relative ease, following the similar method by which the pressure is calculated in this section. Namely, in deriving these formulas it is recommended that one start with a Hamiltonian in second quantization and use a definition (2.8) of the pair distribution function as well as appropriate techniques for the problems.

### 3. PAIR DISTRIBUTION FUNCTION AND TWO-BODY PROPAGATOR

It was shown in the previous investigation<sup>1</sup> that the pair distribution function for the grand canonical ensemble can be calculated in a similar manner as the two-body propagator is done in quantum field theory. This fact follows from the definition (2.8) of the pair distribution function in second quantization. This is briefly summarized in the following. If one introduces an operator  $S(\beta)$  such that

$$e^{-\beta H} = e^{-\beta H_0} S(\beta), \quad (3.1)$$

it is well-known from operator algebra that  $S(\beta)$  be expressed formally by an infinite series:

$$S(\beta) = \sum_{n=0}^{\infty} \frac{(-g)^n}{n!} \int_0^{\beta} \cdots \int_0^{\beta} d\beta_1 \cdots d\beta_n \times P[H_I(\beta_1) \cdots H_I(\beta_n)], \quad (3.2)$$

where  $H_I(\beta')$  is the transformed interaction Hamiltonian defined by

$$H_I(\beta') \equiv e^{\beta' H_0} H_I e^{-\beta' H_0}. \quad (3.3)$$

The symbol  $P$  is an analog of Dyson's chronological operator which has the property that, operating on a product of reciprocal temperature labeled operators, it

rearranges them in the order as the reciprocal temperature sequence ( $\beta$ -sequence) of their label, the largest one in  $\beta$  occurring first in the product:

$$P[H_I(\beta_1) \cdots H_I(\beta_n)] = H_I(\beta_i) H_I(\beta_j) \cdots H_I(\beta_k) \quad \text{if } \beta_i > \beta_j > \cdots > \beta_k. \quad (3.4)$$

It is noted that  $S(\beta)$  is an analog of the scattering matrix operators  $S$  in the quantum field theory where  $S$  is defined by

$$S \equiv \sum_{n=0}^{\infty} \frac{(-ig)^n}{n!} \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} dt_1 \cdots dt_n P[H_I(t_1) \cdots H_I(t_n)]$$

with

$$H_I(t') \equiv e^{it' H_0} H_I e^{-it' H_0}. \quad (3.5)$$

If one substitutes (3.1) into (2.8), one has

$$n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{\text{Tr}\{\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)e^{-\beta H_0 + \alpha N} S(\beta)\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\}}{\text{Tr}\{e^{-\beta H_0 + \alpha N} S(\beta)\}}, \quad (3.6)$$

where the property is used that the total Hamiltonian  $H$  as well as the free-particle Hamiltonian  $H_0$  commute with the number operator  $N$ .

Defining the interaction picture field by a similarity transformation<sup>12</sup>:

$$\begin{aligned} \psi(\mathbf{r}, \beta) &\equiv e^{\beta H_0} \psi(\mathbf{r}) e^{-\beta H_0} \\ \psi^*(\mathbf{r}, \beta) &\equiv e^{\beta H_0} \psi^\dagger(\mathbf{r}) e^{-\beta H_0} \end{aligned} \quad (3.7)$$

one can rewrite (3.6) as

$$n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{\text{Tr}\{e^{-\beta H_0 + \alpha(N+2)} \psi(\mathbf{r}_2, \beta) \psi(\mathbf{r}_1, \beta) S(\beta) \psi^*(\mathbf{r}_1, 0) \psi^*(\mathbf{r}_2, 0)\}}{\text{Tr}\{e^{-\beta H_0 + \alpha N} S(\beta)\}}. \quad (3.8)$$

If one introduces a quantity defined by

$$K^{(2)}(x_3 x_4; x_1 x_2) = \frac{\text{Tr}\{e^{-\beta H_0 + \alpha N} T[\psi(x_4) \psi(x_3) S(\beta) \psi^*(x_1) \psi^*(x_2)]\}}{\text{Tr}\{e^{-\beta H_0 + \alpha N} S(\beta)\}}, \quad (3.9)$$

where  $T$  is an analog of Wick's chronological operator  $T = \delta_P P$ ,  $\delta_P$  being the sign plus or minus according to whether the permutation of Fermion factors is even or odd, and  $x_i \equiv (\mathbf{r}_i, \beta_i)$ , then  $n^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$  will be written as

$$n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = e^{2\alpha} K^{(2)}(\mathbf{r}_1 \beta, \mathbf{r}_2 \beta; \mathbf{r}_1 0, \mathbf{r}_2 0). \quad (3.10)$$

This shows an analogy between the pair distribution function and the two-body propagator.

Fortunately the property of the propagator has been studied in great detail in the case of quantum field theory, where the two-body propagator in position-time

<sup>12</sup> As a result of this definition  $\psi^*(\mathbf{r}, \beta)$  is not the Hermitean conjugate of  $\psi(\mathbf{r}, \beta)$ . However,  $\psi^*(\mathbf{r}, -\beta) = e^{-\beta H_0} \psi^\dagger(\mathbf{r}) e^{\beta H} = (\psi(\mathbf{r}, \beta))^\dagger$ .

space is defined by

$$K^{(2)}(x_3x_4; x_1x_2) \equiv \frac{\langle \Phi_0 | T\{\psi(x_4)\psi(x_3)S\psi^*(x_1)\psi^*(x_2) | \Phi_0 \rangle}{\langle \Phi_0 | S | \Phi_0 \rangle}. \quad (3.11)$$

Here  $|\Phi_0\rangle$  stands for the vacuum state,  $S$  is the  $S$  matrix defined in (3.5), and, in this case, the fourth component of the 4-vectors  $x_i$  is time instead of reciprocal temperature. If one substitutes a series expansion of  $S$  into the above propagator, each term may be represented by a well-known Feynman diagram. Since the definition (3.9) has the same operators which are to be averaged as the definition (3.11), it is apparent that Feynman diagrams of the same type emerge for the both cases. The equality (3.10) forms a basis of later calculations.

#### 4. PERTURBATION THEORY FOR PAIR DISTRIBUTION FUNCTION

We have indicated in the preceding section that the evaluation of the pair distribution function could be reduced to that of a two-body propagator in position—reciprocal temperature space. The propagator introduced in the form (3.9) has already been discussed by T. Matsubara.<sup>2</sup> Its equivalent form in the Heisenberg picture has also been treated by P. Martin and J. Schwinger<sup>13</sup> and A. Klein and R. Prange.<sup>14</sup> The latter form seems especially suited for discussions of general properties of  $l$ -body reduced density matrices. We shall explore this problem in a separate publication.

In the paper quoted in the foregoing Matsubara developed a general perturbation theory for the quantum-statistical system and showed in great detail how to calculate the grand partition functions for various systems using Feynman diagrams in a manner similar to that used to calculate the vacuum expectation value of the  $S$  matrix in the quantum field theory. While it is certainly possible to formulate our problem of the pair distribution function in a standard field-theoretical manner as Matsubara did, we would instead directly proceed with the graphical representation of two-body propagator *à la* Feynman. This is partly because Matsubara's formulation can be extended to our case without serious modification and partly because the equivalence of the standard field theoretic method and Feynman's method is well-established in the usual quantum field theory.

We wish to calculate a propagator

$$K^{(2)}(\mathbf{r}_1\beta, \mathbf{r}_2\beta; \mathbf{r}_10, \mathbf{r}_20) \equiv \frac{\text{Tr}\{e^{-\beta H_0 + \alpha N} T[\psi(\mathbf{r}_2\beta)\psi(\mathbf{r}_1\beta)S(\beta)\psi^*(\mathbf{r}_10)\psi^*(\mathbf{r}_20)]\}}{\text{Tr}\{e^{-\beta H_0 + \alpha N} S(\beta)\}} \quad (4.1)$$

<sup>13</sup> P. Martin and Schwinger, Bull. Am. Phys. Soc. **3**, 202 (1958); Phys. Rev. **115**, 1342 (1959).

<sup>14</sup> A. Klein and R. Prange, Phys. Rev. **112**, 994 (1958).

following the Feynman formalism. For definiteness let us consider here a system of interacting identical particles without spin. Then the situation analyzed is that of two particles capable of interacting with each other through the virtual emission and absorption of quanta during a period 0 to  $\beta$ . The interaction function corresponding to a simple exchange of one quantum is of course  $gv(r)$  appearing in (2.2). It is assumed to be instantaneous (independent of  $r$ -variable) and  $g$  being the coupling constant. We shall examine the first few terms contributing to the propagator (amplitude function)  $K^{(2)}(34; 12)$ , which represents the probability amplitude for the one particle to proceed from position and reciprocal temperature  $x_1 \equiv (\mathbf{r}_1\beta_1)$  to  $x_3$ , while the other particle proceeds from  $x_2$  to  $x_4$ . This is best handled by employing the so-called Feynman diagrams. The diagrams may be ordered according to the power of the coupling constant  $g$  occurring in the expression we ascribe to the diagram, this power being half the number of particle vertices in the diagram. For the zeroth power of  $g$  one finds only one diagram shown in Fig. 1 where solid lines represent propagators of particles and  $\beta$  variable is measured along the vertical direction. The diagram represents a free passage of the two particles and corresponds to the following expression:

$$K_0(3; 1)K_0(4; 2) \pm K_0(4; 1)K_0(3; 2), \quad (4.2)$$

where  $K_0$  is a one-body free-particle propagator defined by

$$K_0(i; j) \equiv \frac{\text{Tr}\{e^{-\beta H_0 + \alpha N} T[\psi(x_i)\psi^\dagger(x_j)]\}}{\text{Tr}\{e^{-\beta H_0 + \alpha N}\}} \quad (4.3)$$

and the second term (exchange term) arises from the indistinguishability of the two particles. In general, the exchange term, except for the sign is always obtained from the corresponding normal term by exchanging the variables representative of the final state. The sign of the exchange term is chosen the same or opposite to that of the normal term according to whether the system obeys Bose or Fermi statistics, respectively. Thus it should be remembered that to each diagram two expressions are ascribed, one corresponding to the normal and one corresponding to the exchange scattering. Although this is the case we shall omit the mathematical expressions for the exchange terms in the following illustration. However we must remember that the exchange term should be taken into account when the propagator  $K^{(2)}$  is actually calculated.

Now for the first power of  $g$  there exists a diagram shown in Fig. 2(a), where a wavy line denotes propaga-



FIG. 1. The zeroth-order scattering-free passage—Eq. (4.2).

tion of a quantum. The corresponding propagator  $K_1^{(2)}(3,4;1,2)$  is

$$K_1^{(2)}(3,4;1,2) = g \int \int K_0(3;5)K_0(4;6)\{-v(r_{56})\} \times K_0(5;1)K_0(6;2)d^3r_5d^3r_6d\beta' + (\text{exchange term}), \quad (4.4)$$

where it is understood that the  $\beta$  variables of space points 5 and 6 are the same, due to the instantaneous nature of the interaction, i.e.,  $\beta_5 = \beta_6 = \beta'$ . One can write this as an integral over both  $\beta_5$  and  $\beta_6$  if a delta function  $\delta(\beta_5 - \beta_6)$  is included to insure contribution only when  $\beta_5 = \beta_6$ . Hence the first-order effect of interaction is

$$K_1^{(2)}(3,4;1,2) = g \int \int dx_5 dx_6 K_0(3;5)K_0(4;6)\{-V(5,6)\} \times K_0(5;1)K_0(6;2) + (\text{exchange term}) \quad (4.5)$$

with

$$V(5,6) \equiv v(|r_5 - r_6|)\delta(\beta_5 - \beta_6), \quad (4.6)$$

where  $dx' \equiv d^3r'd\beta'$ . The delta function  $\delta(\beta' - \beta'')$  is defined in the finite interval  $(-\beta, \beta)$  such that

$$\int_0^\beta d\beta' F(\beta')\delta(\beta' - \beta'') = F(\beta'') \quad (4.7)$$

for an arbitrary function  $F(\beta')$  defined in  $(0, \beta)$ . It is noted that the expression (4.5) is obtained by merely looking at the diagram of Fig. 2(a) and vice versa. According to Feynman, Fig. 2(a) is interpreted as a first-order process in which the two particles exchange a quantum between them before they scatter each other to their final state 3, 4. More precisely, a particle goes

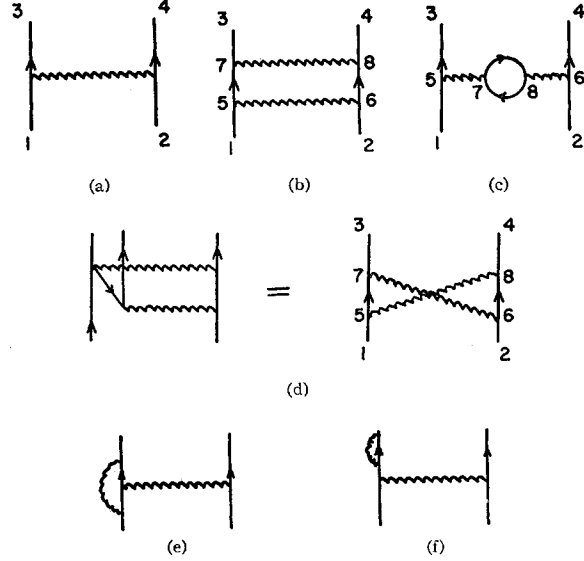


FIG. 2. (a) The first-order scattering in position-reciprocal temperature space—Eq. (4.4). (b)–(f) The two-quanta process of two-particle scattering—Eq. (4.8).

to 5 [amplitude  $K_0(5;1)$ ], emits a quantum, and then proceeds to 3 [ $K_0(3;5)$ ]; meanwhile the other particle goes to 6 [ $K_0(6;2)$ ], absorbs the quantum, and proceeds to 4 [ $K_0(4;6)$ ]. The quantum meanwhile proceeds from 5 to 6, which it does with amplitude  $-V(5,6)$ . The intermediate position and  $\beta$  variables of emission 5 and absorption 6 are to be integrated at the end. It is also noted that the negative of the four-dimensional interaction function  $-V$  is assigned to an interaction line.

Having seen this simple example we may be able to write down the corresponding quantities involving the exchange of two or more quanta between two particles. We give some examples of the two quanta process in Fig. 2(e,f) for illustration. The expressions corresponding to the three diagrams of Fig. 2(b)–(d) are given in the following:

$$K_{2b}^{(2)}(3,4;1,2) = g^2 \int \int \int \int dx_5 dx_6 dx_7 dx_8 K_0(3;7)K_0(4;8)\{-V(7;8)\}K_0(7;5) \times K_0(8;6)\{-V(5,6)\}K_0(5;1)K_0(6;2) + (\text{exchange term}) \quad (4.8a)$$

$$K_{2c}^{(2)}(3,4;1,2) = g^2 \int \int \int \int dx_5 dx_6 dx_7 dx_8 K_0(3;5)K_0(4;6)\{-V(5;7)\}K_0(7,8) \times K_0(8;7)\{-V(8;6)\}K_0(5;1)K_0(6;2) + (\text{exchange term}) \quad (4.8b)$$

$$K_{2d}^{(2)}(3,4;1,2) = g^2 \int \int \int \int dx_5 dx_6 dx_7 dx_8 K_0(3;7)K_0(4;8)K_0(7;5)K_0(8;6) \times \{-V(7,6)\}\{-V(5;8)\}K_0(5;1)K_0(6;2) + (\text{exchange term}). \quad (4.8c)$$

More examples will be found in the following sections.

The one-body free-particle propagator defined in (4.3) can be expressed in terms of either the Bose or the Fermi

distribution function by calculating the indicated trace. The result is<sup>15</sup>

$$\begin{aligned} K_0(x_2; x_1) &= V^{-1} \sum_{\mathbf{p}} (1 \pm f(\mathbf{p})) \exp[i\mathbf{p} \cdot (\mathbf{r}_2 - \mathbf{r}_1) - \mathbf{p}^2(\beta_2 - \beta_1)] \quad \text{if } \beta_2 > \beta_1 \\ &= V^{-1} \sum_{\mathbf{p}} \pm f(\mathbf{p}) \exp[i\mathbf{p} \cdot (\mathbf{r}_2 - \mathbf{r}_1) - \mathbf{p}^2(\beta_2 - \beta_1)] \quad \text{if } \beta_2 < \beta_1, \end{aligned} \quad (4.9)$$

where  $f(\mathbf{p})$  is the Bose or Fermi distribution function defined by

$$f(\mathbf{p}) = \frac{\exp(\alpha - \beta \mathbf{p}^2)}{1 \mp \exp(\alpha - \beta \mathbf{p}^2)}. \quad (4.10)$$

As was noted by Feynman, the evaluation of (4.5), as well as all the other more complicated expressions, can be very much simplified by working in the momentum and energy variables, rather than in the position and reciprocal temperature variables. For this we shall introduce the momentum-energy representation of  $K_0$  by

$$S(\mathbf{p}, s) = [is + \mathbf{p}^2 - (\alpha/\beta)]^{-1} \quad (4.11)$$

in terms of which (4.9) can be written in a simple form as<sup>16</sup>

$$K_0(x_2; x_1) = (V\beta)^{-1} \sum_{\mathbf{p}} \sum_s \exp[-(\alpha/\beta)(\beta_2 - \beta_1) + i\mathbf{p} \cdot (\mathbf{r}_2 - \mathbf{r}_1) + is(\beta_2 - \beta_1)] S(\mathbf{p}, s). \quad (4.12)$$

The summation  $s$  runs over a set of discrete values  $\{m\pi/\beta\}$  where  $m$  is the set of even or odd integers according to whether the particles obey Bose or Fermi statistics. The equivalence of (4.12) and (4.11) to (4.9) and (4.10) may be seen by simply carrying out the summation over  $s$  indicated in (4.12). This is done in Appendix A(I) using Poisson's sum formula.

It is seen from the imaginary exponential function in (4.12) that the variable  $s$  is conjugate to the reciprocal temperature  $\beta$  just as the momentum  $\mathbf{q}$  is conjugate to the position  $\mathbf{r}$ .

As an example we shall rewrite the expression (4.5) in the momentum-energy representation. For this purpose one defines the Fourier transform of the potential  $v(\mathbf{r})$  by

$$v(\mathbf{r}) = V^{-1} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} v(\mathbf{q}) \quad (4.13)$$

and expresses the delta function  $\delta(\beta' - \beta'')$  by

$$\delta(\beta' - \beta'') = \beta^{-1} \sum_t e^{it(\beta' - \beta'')}, \quad (4.14)$$

where  $t$  runs over a set of discrete values  $\{2\pi m/\beta\}$ ,  $m$  being all positive and negative integers including zero. That the expression (4.14) has the correct delta-function property (4.7) may be verified by multiplying it by a function of  $\beta'$ , and integrating with respect to  $\beta'$  over the interval  $(0, \beta)$ .

Using these results one obtains for the first term of (4.5)

$$\begin{aligned} &g(V\beta)^{-3} \sum_{\mathbf{p}_1, s_1} \sum_{\mathbf{p}_2, s_2} \sum_{\mathbf{p}_3, s_3} \sum_{\mathbf{p}_4, s_4} \sum_{\mathbf{q}, t} \exp[-\alpha(\beta_3 + \beta_4 - \beta_1 - \beta_2)/\beta] \exp(is_3\beta_3 + is_4\beta_4 - is_1\beta_1 - is_2\beta_2) \\ &\quad \times \exp(i\mathbf{p}_3 \cdot \mathbf{r}_3 + i\mathbf{p}_4 \cdot \mathbf{r}_4 - i\mathbf{p}_1 \cdot \mathbf{r}_1 - i\mathbf{p}_2 \cdot \mathbf{r}_2) \delta(s_3 - s_1 - t) \delta^{(3)}(\mathbf{p}_3 - \mathbf{p}_1 - \mathbf{q}) \delta(s_4 - s_2 + t) \delta^{(3)}(\mathbf{p}_4 - \mathbf{p}_2 + \mathbf{q}) \\ &\quad \times S(\mathbf{p}_3, s_3) S(\mathbf{p}_4, s_4) S(\mathbf{p}_1, s_1) S(\mathbf{p}_2, s_2) v(\mathbf{q}) \end{aligned} \quad (4.15)$$

$$\begin{aligned} &= g(V\beta)^{-3} \sum_{\mathbf{p}_1, s_1} \sum_{\mathbf{p}_2, s_2} \sum_{\mathbf{q}, t} \exp[-\alpha(\beta_3 + \beta_4 - \beta_1 - \beta_2)/\beta] \exp[i(s_1 + t)\beta_3 + i(s_2 - t)\beta_4 - is_1\beta_1 - is_2\beta_2] \\ &\quad \times \exp[i(\mathbf{p}_1 + \mathbf{q}) \cdot \mathbf{r}_3 + i(\mathbf{p}_2 - \mathbf{q}) \cdot \mathbf{r}_4 - i\mathbf{p}_1 \cdot \mathbf{r}_1 - i\mathbf{p}_2 \cdot \mathbf{r}_2] S(\mathbf{p}_1 + \mathbf{q}, s_1 + t) S(\mathbf{p}_2 - \mathbf{q}, s_2 - t) S(\mathbf{p}_1, s_1) S(\mathbf{p}_2, s_2) v(\mathbf{q}). \end{aligned} \quad (4.16)$$

Now Eq. (4.16) can be understood in the following way (Fig. 3). Two particles with momenta-energies  $(\mathbf{p}_1, s_1)$  and  $(\mathbf{p}_2, s_2)$  are created at  $(\mathbf{r}_1, \beta_1)$  and  $(\mathbf{r}_2, \beta_2)$ , respectively,  $[\exp(\alpha\beta_1/\beta - i\mathbf{p}_1 \cdot \mathbf{r}_1 - is_1\beta_1), \exp(\alpha\beta_2/\beta - i\mathbf{p}_2 \cdot \mathbf{r}_2$

$- is_1\beta_2)]$  and proceed with momenta energies  $(\mathbf{p}_1, s_1)$  and  $(\mathbf{p}_2, s_2)$   $[(V\beta)^{-1} S(\mathbf{p}_1, s_1) (V\beta)^{-1} S(\mathbf{p}_2, s_2)]$ . The particle 2 emits a quantum with momentum energy  $(\mathbf{q}, t)$

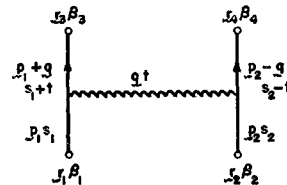


FIG. 3. The first-order scattering in momentum-energy space—Eq. (4.16).

<sup>15</sup> Expressions similar to (4.9) were introduced and discussed in their treatment by Klein and Prange<sup>14</sup> and Matsubara.<sup>2</sup> The minor discrepancy is due to the difference in the definitions.

<sup>16</sup> Note added in proof.—We are very grateful to Dr. K. Aizu for pointing out to us that the momentum-energy representation of the free-particle propagator has also been reported by E. S. Fradkin; J. Exptl. Theoret. Phys. U.S.S.R. 36, 1286 (1959) [English translation: Soviet Phys. JETP 4, 912 (1959)].

and makes its way now with momentum energy  $(\mathbf{p}_2 - \mathbf{q}, s_2 - t)[(V\beta)^{-1}S(\mathbf{p}_2 - \mathbf{q}, s_2 - t)]$  and annihilates itself at  $(\mathbf{r}_4, \beta_4)\{\exp[-\alpha\beta_4/\beta + i(\mathbf{p}_2 - \mathbf{q}) \cdot \mathbf{r}_4 + i(s_2 - t)\beta_4]\}$ . The other particle absorbs the quantum, which travels with the amplitude  $[-gv(q)]$ , and then proceeds with momentum energy  $(\mathbf{p}_1 + \mathbf{q}, s_1 + t)[(V\beta)^{-1}S(\mathbf{p}_1 + \mathbf{q}, s_1 + t)]$  and annihilates itself at  $(\mathbf{r}_3, \beta_3)\{\exp[-\alpha\beta_3/\beta + i(\mathbf{p}_1 + \mathbf{q}) \cdot \mathbf{r}_3 + i(s_1 + t)\beta_3]\}$ . One integrates over all momentum variables to get the final result.

It is apparent that one can extend this sort of interpretation to all the other complicated expressions such as (4.8a), (4.8b), and (4.8c). It is as easy to write them in the momentum-energy representation as to write them in the position-reciprocal temperature representation. Therefore instead of writing them explicitly we shall tabulate the correspondence between the various diagram elements and the kernel elements. This will be found at the end of this section.

It is noted that in the above description the momentum and energy are conserved in each event, i.e., absorption or emission of a quantum, which is exhibited explicitly by the appearance of the delta function in (4.15).

In closing this section we shall give two tables (Tables I and II), one for the correspondence between the diagram elements and the propagator kernel elements in position-reciprocal temperature space, and one for the same in momentum-energy space. It is noted that the lines rather than vertices are labeled in the momentum-energy representation. In our diagram representation *each particle line must be directed* since the reversal of the sense of direction usually gives a different contribution. On the other hand quantum lines are not necessarily directed since the sense of the direction does not affect the result. However, they may be directed sometimes for illustration.

### 5. COLLECTIVE INTERACTION

We saw in the preceding section how the two-body propagator is expanded in powers of the coupling constant and how the various terms of its expansion can be conveniently represented by Feynman diagrams. As pointed out in the Introduction, one of the reasons for introducing the diagrammatic analysis in the present

TABLE I. The correspondence between the diagram elements and the kernel elements in position-reciprocal temperature space.

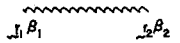
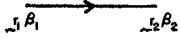
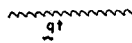
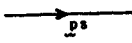
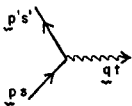



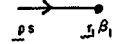
Component of diagram	Factor in the kernel element
Quantum line 	Quantum propagation function $= gv(\mathbf{r}_1 - \mathbf{r}_2) \delta(\beta_1 - \beta_2)$ $(0 \leq \beta_1, \beta_2 \leq \beta)$
Particle line (directed) 	Particle propagation function $K_0(\mathbf{r}_2, \beta_2; \mathbf{r}_1, \beta_1)$ $(0 \leq \beta_1, \beta_2 \leq \beta)$

TABLE II. The correspondence between the diagram elements and the kernel elements in momentum-energy space.

Diagram element	Factor in kernel element
Quantum line 	Quantum propagation function $(V\beta)^{-1}gv(q)$
Particle line (directed) 	Particle propagation function $(V\beta)^{-1}S(\mathbf{p}, s)$
Corner 	$(V\beta)\delta^{(3)}(\mathbf{p}' - \mathbf{p} + \mathbf{q})\delta(s' - s + t)$
Creation point of a quantum 	$\exp(-i\mathbf{q} \cdot \mathbf{r}_1 - it\beta_1)$
Annihilation point of a quantum 	$\exp(i\mathbf{q} \cdot \mathbf{r}_1 + it\beta_1)$
Creation point of a particle 	$\exp[(\alpha/\beta)\beta_1 - i\mathbf{p} \cdot \mathbf{r}_1 - is\beta_1]$
Annihilation point of a particle 	$\exp[-(\alpha/\beta)\beta_1 + i\mathbf{p} \cdot \mathbf{r}_1 + is\beta_1]$

theory is to facilitate the finding of those partial sums of the perturbation series which are appropriate for the system studied. We shall consider here the so-called collective interaction as an example of such sums.

Through many theoretical and experimental investigations on the many-body systems, it has been clarified that some systems exhibit the characteristic collective motion behaviors in certain conditions. Liquid helium and the electron gas at low temperatures are notable examples of such cases. In this connection L. Landau<sup>6</sup> pointed out that the behavior of such systems can be most conveniently described in terms of elementary excitations, e.g., phonons in liquid helium and plasmons in the electron gas.

Here the elementary excitation is the name given to the physical quasi-particle which has a specific energy-momentum relation and in terms of which the behavior of the system is conveniently described; for instance, by saying that a particle having momentum  $\mathbf{p}$  and energy  $\epsilon$  changes its state to the one with momentum  $\mathbf{p} + \mathbf{q}$  and energy  $\epsilon + \kappa$  after virtual absorption of a quasi-particle with momentum  $\mathbf{q}$  and energy  $\kappa$ . It is noted that this description makes it possible to find the characteristic energy-momentum relation directly and in a much simpler way than when one calculates first the total energy and identifies the elementary excitation, for all one has to do is to examine the process of energy-momentum transfer.

As emphasized by Feynman, the virtual process is



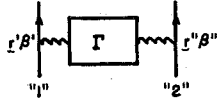


FIG. 4. Example of an indirect interaction.

most favorably handled in the Feynman formalism where energy-momentum conservation is visualized by means of Feynman diagrams (momentum representation). In this section we shall pick out special partial diagrams to construct the so-called collective (or effective or modified) interaction and examine its relation to the energy-momentum transfer by a quasi-particle. To do this we must look at the two-body scattering with a different point of view from that of the perturbation theory developed in the section. As a result we shall see that plasmons are closely connected with the simple chain approximation to the collective interaction in the electron gas.

Consider, as before, two particles in a homogeneous medium with no external field. In describing the scattering of these particles in the spirit of Feynman theory, we may say that the initial state specified by momenta and energies of the two particles has changed into the final state after an indefinite number of energy-momentum exchanges through direct interactions or through media between the two.

Let us begin with the simplest situation. Consider a case where the scattering occurs in such a way that the particle "1" emits a quantum with a definite energy momentum which is absorbed by the particle "2" after a complicated process which, however, returns all the particles involved to their original states. In a Feynman diagram, this process will be pictured in Fig. 4.

In the diagram the box stands for some set of closed particle loops and interaction lines and is to be connected to the lines of particle "1" and "2" by only the

two interaction (wavy) lines shown. This type of diagram represents the indirect interaction through the medium and adds up together with the direct interaction to form the collective interaction. In other words, let  $\Gamma$  be the structure of the box; then the collective interaction  $U(\mathbf{r}'\beta', \mathbf{r}''\beta'')$  will be defined by the infinite sum over  $\Gamma$ :

$$U(\mathbf{r}'\beta'; \mathbf{r}''\beta'') \equiv \sum_{\Gamma} W(\mathbf{r}'\beta', \mathbf{r}''\beta''; \Gamma), \quad (5.1)$$

where  $W(\mathbf{r}_1\beta', \mathbf{r}_2\beta''; \Gamma)$  is the integral of the diagram specified by  $\Gamma$  over all  $\mathbf{r}$  and  $\beta$  coordinates except the end points  $(\mathbf{r}'\beta')$  and  $(\mathbf{r}''\beta'')$ . We shall refer to such summation process as reduction of the direct and the indirect interaction to the collective interaction. Unfortunately the task of summing over  $\Gamma$  is truly hopeless, since the number of terms increases rapidly as the order of  $\Gamma$ , i.e., the number of interaction lines involved in  $\Gamma$ , increases.

At this point Hubbard<sup>7</sup> proposed another summation formula. Following Dyson's<sup>17</sup> techniques in the treatment of the elimination of photon self-energy, he could derive an integral equation for  $U$  and solved it with the assumption that there be no external fields. The result is the following. The collective interaction  $U$  is obtained by the Fourier inverse of the expression:

$$U(q, t) = \frac{v(q)}{1 + \bar{U}(q, t)v(q)} \quad (5.2)$$

$$\begin{aligned} &= v(q) - \frac{v^2(q)\bar{U}(q, t)}{1 + \bar{U}(q, t)v(q)} \\ &= v(q) - U_1(q, t), \end{aligned} \quad (5.3)$$

where  $\bar{U}(q, t)$  is the Fourier component of the following quantity:

$$\bar{U}(q, t) \equiv \int d^3(\mathbf{r}' - \mathbf{r}) d(\beta' - \beta) \bar{U}(\mathbf{x}' - \mathbf{x}) \exp[i(\mathbf{r}' - \mathbf{r}) \cdot \mathbf{q} + i(\beta' - \beta)t] \quad (5.4)$$

and

$$\bar{U}(\mathbf{x}', \mathbf{x}) = \bar{U}(\mathbf{x}' - \mathbf{x}) \equiv \sum_{\Gamma'}^{\text{proper}} \bar{W}(\mathbf{x}', \mathbf{x}; \Gamma'). \quad (5.5)$$

Here  $\bar{W}(\mathbf{x}', \mathbf{x}; \Gamma')$  is related to  $W(\mathbf{x}', \mathbf{x}; \Gamma)$  by

$$W(\mathbf{x}', \mathbf{x}; \Gamma) = \int \int dx_1 dx_2 V(\mathbf{x}' - x_1) \bar{W}(x_1, x_2; \Gamma) V(x_2 - \mathbf{x}). \quad (5.6)$$

The sum appearing in (5.5) means that the summation over proper polarization structure  $\Gamma'$  and the possibility of putting  $\bar{U}(\mathbf{x}, \mathbf{x}') = \bar{U}(\mathbf{x} - \mathbf{x}')$  is due to the homogeneity of the field (no external force). Here the adjective "proper" means the following. Let  $\Gamma$  be any polarization structure. Then it may or may not be that  $\Gamma$  consists of two or more parts which are connected only by single interaction lines. In the first case we shall say that  $\Gamma$  is an improper polarization structure; in the latter case

that it is a proper polarization structure. For example, the polarization structure shown in Fig. 5(a) is a proper structure, while that shown in Fig. 5(b) is improper.



FIG. 5(a). Example of a proper polarization structure. (b) Example of an improper polarization structure.

<sup>17</sup> F. J. Dyson, Phys. Rev. **75**, 1736 (1949).

The first few terms of the series (5.5) is graphically represented as

$$\bar{U}(x', x) = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} \quad (5.7)$$

+ (Diagrams with more interaction lines)

where the mark  $\times$  denotes the place from which an interaction line should run.

For example, if only the first term of (5.7) is retained and then substituted into (5.2), this is equivalent to taking all orders of chain diagrams shown in Fig. 6 in the original summation (5.1), which is known as the simple chain approximation. So far we have discussed the case where the over-all interactions between the particles "1" and "2" are reducible to a single collective interaction  $U$ . This is not the only possible case, however. Let us suppose a case diagrammed in Fig. 7(a), where the particle "1" emits two quanta which are absorbed by a third particle which returns to its original state after transferring a quantum to the particle "2." This type of interaction cannot be reduced to a single interaction.

However, it is apparent that the scattering diagrams appearing in Fig. 7(b) are indeed reducible to Fig. 7(a) in the same sense that the interaction shown in Fig. 5

FIG. 6. Examples of simple chain diagrams.



was reducible to the interaction  $U$ . Thus it will be a sensible approach to the scattering problem if we enumerate irreducible diagrams and replace every interaction line  $V$  by a collective interaction  $U$ . Employing this approach the calculation of the pair distribution function will be made in the later sections (6 and 7).

Returning to the discussion of the collective interaction, we notice from (5.3) that (i) it is possible from its definition to separate it into two parts, i.e., direct (original) and indirect interactions, and (ii) the direct interaction is energy-independent while the indirect interactions are not always so. In fact, the property (ii) can be restated by saying that the direct interaction is instantaneous (i.e., acting only at the same  $\beta$ ) while the indirect interactions are not.

Now it will be interesting to ask the particle interpretation of the indirect interaction. First, we notice that at each corner upon integration over  $\mathbf{r}$  and  $\beta$  coordinates there appears a 4-dimensional delta function which is interpreted as energy-momentum conservation. Since the free particle has a definite energy momentum  $(\mathbf{p}, s)$  attached to itself, we tentatively define the energy momentum of a quasi-particle as that  $(\mathbf{q}, t)$  appearing in the argument of the delta function. Next, we ask the energy-momentum relation thus defined. One notices that, in the case of the free-particle propagator, it was found by

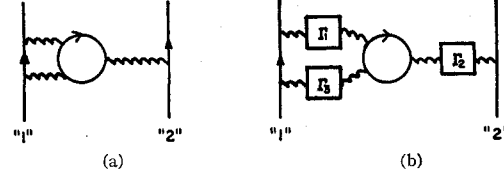


FIG. 7(a). Example of a proper many-body interaction. (b) Example of an improper many-body interaction.

identifying the pole with respect to the energy variable  $s$  of  $K_0(\mathbf{p}, s)$  except for the imaginary unit  $i$ . It may be inferred from the analogy that the energy of the quasi-particle corresponding to the collective interaction may be obtained from the pole of the momentum representation  $U(q, t)$  of the interactions. We shall examine this in the following two examples.

### (A) Electron Gas

From the work by E. Montroll and J. Ward,<sup>3</sup> it is known that the simple ring diagrams [Fig. 8(c)] give the important contributions to the grand partition function of the electron gas at both high and low temperatures. Specifically, they yield the Debye-Hueckel theory in the classical limit while at low temperatures they lead to the Gell-Mann-Bruckner equation for the correlation energy. As is readily seen, the simple ring is closely related to the simple chain. For instance, the former can be constructed using the latter in the following way. Take a simple self-energy diagram [Fig. 8(a)]. Replace its interaction line by a simple chain [Fig. 8(b)]. Then closing both ends of the particle line, one gets a simple ring [Fig. 8(c)]. Thus it would be reasonable to examine simple chain diagrams at least as an initial step.

As was noted in the passage following the expression (5.7), the momentum representation of the simple chain approximation to the collective interaction is given by

$$\frac{v(q)}{1 + \lambda(q, t)v(q)} = v(q) - \frac{v^2(q)\lambda(q, t)}{1 + \lambda(q, t)v(q)}, \quad (5.9)$$

where  $v(q)$  is the Fourier transform of the Coulomb potential

$$v(q) \equiv \int d^3r e^{i\mathbf{q} \cdot \mathbf{r}} \epsilon^2 / r = \epsilon^2 4\pi / q^2 \quad (5.10)$$

( $\epsilon$  being the electronic charge) and  $\lambda(q, t)$  is

$$\lambda(q, t) = (V\beta)^{-1} \sum_{\mathbf{p}} \sum_s [is + \mathbf{p}^2 - \alpha/\beta]^{-1} \times [-i(s+t) + (\mathbf{p} + \mathbf{q})^2 - \alpha/\beta]^{-1}. \quad (5.11)$$

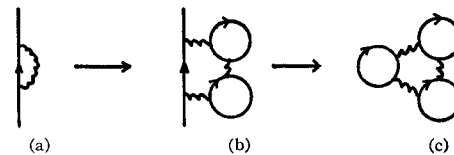


FIG. 8. Construction of a simple ring.

The last quantity  $\lambda(q, t)$  is the momentum representation of the first term of (5.7) and is written down directly with the help of Table II of the last section. The summation over  $s$  is taken on a set of discrete values  $\{(2m+1)\pi/\beta\}$ ,  $m$  being an integer. This may be evaluated by first resolving the summand into a sum of partial fractions and then applying Poisson's sum formula. Thus one gets

$$\lambda(q, t) = V^{-1} \sum_{\mathbf{p}} [(\mathbf{p} + \mathbf{q})^2 - \mathbf{p}^2 + i\epsilon]^{-1} \times [f_{\mathbf{F}}(\mathbf{p}) - f_{\mathbf{F}}(\mathbf{p} + \mathbf{q})], \quad (5.12)$$

where  $f_{\mathbf{F}}(\mathbf{p})$  is the Fermi distribution function.

If one takes a limit as  $V \rightarrow \infty$  of  $\lambda(q, t)$  in (5.11), it agrees with the  $\lambda$  introduced by Montroll and Ward within a factor  $(2\pi)^2$ . Following their calculation one obtains for  $\lambda(q, t)$

$$\lambda(q, t) = (p_0/4\pi^2) [1 - u \tan^{-1}(1/u)] \equiv (p_0/4\pi^2) R(u) \quad (5.13)$$

with

$$u \equiv t/(2qp_0) \quad (5.14)$$

as  $q \rightarrow 0$  and  $\beta \rightarrow \infty$ , where  $p_0 \equiv \epsilon_f$  is the Fermi energy at the absolute zero temperature of the ideal gas with the same mass and density as the parallel spin electron gas.

So far we have not considered the effect of the electronic spin. However, since we do not include spin-dependent terms in our Hamiltonian (2.1), the spin correction for the electron gas is very simple. One allows two electrons at most to occupy each of the single-particle states specified by the momentum eigenvalues. This leads to the multiplication of each factor  $\lambda(q, t)$  appearing in the theory by 2. Thus, we have for the simple chain approximation to the collective interaction.

$$U(q, t) = v(q) - \frac{2v^2(q)\lambda(q, t)}{1 + 2\lambda(q, t)v(q)} \quad (5.15)$$

$$= v(q) + U_1(q, t). \quad (5.16)$$

Substitution from (5.10) and (5.13) gives for the indirect interaction

$$U_1(q, t) = \frac{8\epsilon^2 p_0 R(u)}{q^4 + 2\pi^{-1}\epsilon^2 q^2 p_0 R(u)}. \quad (5.17)$$

As  $q$  approaches zero,

$$u \rightarrow 0 \quad \text{and} \quad R(u) \rightarrow \frac{1}{3}(2qp_0)^2/t^2. \quad (5.18)$$

Substituting this into (5.17) one finds as the pole with respect to  $t$

$$t = \pm i(8\epsilon^2 p_0^3/3\pi)^{1/2}, \quad (5.19)$$

hence getting the energy-momentum relation for a quasi-particle

$$\epsilon = (8\epsilon^2 p_0^3/3\pi)^{1/2}. \quad (5.20)$$

This is the well-known energy of a plasmon<sup>18</sup> in the electron gas. Thus we could show that the simple chain approximation to the collective interaction is responsible for the transfer of plasmons which are principal elementary excitations of the electron gas at the very low temperatures.

## (B) Hard Sphere Bosons

Since the Fourier component of the hard sphere potential does not exist, we cannot proceed in the previously described way. However, it was shown by Lee and Yang<sup>9</sup> that the discussion of scattering of two particles can be made by grouping the special kind of diagrams without using a singular potential explicitly. This is the so-called binary collision expansion method.

Suppose we consider the scattering of two particles in the absence of other particles. The scattering will be described through an indefinite number of exchanges of quanta between the two. Diagrammatically this process will be described by the sum of the ladder diagrams:

$$\text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \dots \quad (5.21)$$

where the particle lines represent Boltzmann propagators (see Sec. 8) unlike those that appeared in Tables I and II. The matrix element  $\langle \mathbf{r}_1' \mathbf{r}_2' | \exp(-\beta H_2) - \exp[-\beta H_2^{(0)}] | \mathbf{r}_1 \mathbf{r}_2 \rangle \equiv \langle \mathbf{r}_1' \mathbf{r}_2' | U(\beta; 1, 2) | \mathbf{r}_1 \mathbf{r}_2 \rangle$  of this process can be calculated by means of a partial wave method. In the foregoing,  $H_2$  and  $H_2^{(0)}$  are the two-particle Hamiltonians defined by

$$H_2 \equiv -\nabla_1^2 - \nabla_2^2 + v(r_{12}) \quad (5.22)$$

and

$$H_2^{(0)} \equiv -\nabla_1^2 - \nabla_2^2. \quad (5.23)$$

Furthermore it was found convenient by them to introduce the so-called binary kernel  $B(\beta; 1, 2)$  defined by

$$B(\beta; 1, 2) \equiv -v(r_{12}) \exp(-\beta H_2). \quad (5.24)$$

This is related to  $U$  by

$$B(\beta; 1, 2) = \frac{\partial U(\beta; 1, 2)}{\partial \beta} - (\nabla_1^2 + \nabla_2^2) U(\beta; 1, 2) \quad (5.25)$$

and graphically written as

$$\text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \dots \quad (5.26)$$

It is important to notice that these two quantities  $U$  and  $B$  do not contain  $v$  alone and the explicit form of

<sup>18</sup> See, e.g., D. Pines, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1955), Vol. 1, p. 367.

$B(\beta; 1, 2)$  can be evaluated even if  $v = \infty$  for some spatial configuration of  $\mathbf{r}_1$  and  $\mathbf{r}_2$  as in the case of hard sphere interaction. The matrix elements of  $U$  and  $B$  in both the coordinate and momentum representation were calculated by Lee and Yang in the  $S$ -wave approximation. At the lowest temperatures the  $S$ -wave contribution will be most important. Furthermore, in the limit of low density the expansion in the hard-sphere parameter " $a$ " of the binary collision kernel will be permissible. For these cases, the first-order term in  $a$  of  $B$  is

$$B_1(\beta; 1, 2) = -8\pi a \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2) \exp(\beta \nabla_1^2 + \beta \nabla_2^2). \quad (5.27)$$

In this form, it is closely related to the pseudo-potential discussed by Huang, Yang, and Lee.<sup>8</sup> The momentum representation of  $B_1$  has a very simple form:

$$\langle \mathbf{p}_1' \mathbf{p}_2' | B_1 | \mathbf{p}_1 \mathbf{p}_2 \rangle = -a \pi^{-2} \delta^{(3)}(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2') \times \exp(-\beta p_1^2 - \beta p_2^2). \quad (5.28)$$

It is both important and interesting to notice that these matrix elements (5.27) and (5.28) would be obtained if the state of the two particles undergoes a change through a channel associated with a single pseudo-potential  $8\pi a \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2)$  except the last exponential factor, which may be taken as the propagator of the two particles.

Returning to the discussion of the many-body system the transfer of quanta between two particles will be caused not only by the direct interaction (ladder diagram), but also by other channels associated with the other particles. One of the simplest and calculable type of those channels will be a (modified) simple chain shown in Fig. 5 with the replacement of interaction lines by the ones associated with a pseudo-potential defined in the foregoing. This modified simple chain configuration was found to give the most important contribution to the ground-state energy of the hard-sphere Bose gas. With this in mind we proceed to calculate the momentum representation of the collective pseudo-interaction given by (5.9) with the replacement of hard sphere potentials by the pseudo-potentials.

Recalling the definition of the Fourier transform (5.10) of the potential, the momentum representation of the pseudo-potential is simply

$$v'(q) \equiv 8\pi a; \quad v'(r) = 8\pi a \delta^{(3)}(\mathbf{r}). \quad (5.29)$$

The quantity  $\lambda(q, t)$  is still given by (5.11). However, the summation over  $s$  should be calculated in accordance with the rule stated immediately following (4.12), i.e., with the rule for a Boson system. The result can be written in a form identical with (5.12), which was derived for a Fermion system, except that the Bose distribution function takes the place of the Fermi distribution function:

$$\lambda(q, t) = V^{-1} \sum_{\mathbf{p}} [(\mathbf{p} + \mathbf{q})^2 - \mathbf{p}^2 + it]^{-1} \times [f_B(\mathbf{p}) - f_B(\mathbf{p} + \mathbf{q})], \quad (5.30)$$

where  $f_B(\mathbf{p})$  is the Bose distribution function.

In the limit of low temperature the Bose distribution function  $f_B(\mathbf{p})$  will become a Kronecker's delta function centered around zero-momentum with the multiplicative factor  $N$ .<sup>19</sup> Using this property  $\lambda(q, t)$  is given by

$$\lambda(q, t) = n 2q^2 / (q^4 + t^2), \quad (5.31)$$

where  $n$  is the number density defined by  $n \equiv N/V$ .

Substituting  $v(q)$  and  $\lambda(q, t)$  from (5.29) and (5.31) into (5.9), one obtains

$$U'(q, t) \equiv \frac{v'(q)}{1 + \lambda(q, t)v'(q)} = \frac{8\pi a}{1 + (16\pi a n q^2) / (q^4 + t^2)}. \quad (5.32)$$

This has a pole at

$$t = \pm i q (q^2 + 16\pi a n)^{1/2} \quad (5.33)$$

giving the energy-momentum relation for a quasi-particle:

$$\epsilon = q(q^2 + 16\pi a n)^{1/2}. \quad (5.34)$$

This agrees with the phonon spectrum obtained by the previous investigators.<sup>20</sup>

## 6. THE EXPANSION OF THE PAIR DISTRIBUTION FUNCTION IN TERMS OF THE COLLECTIVE INTERACTION. THE ELECTRON GAS AT LOW TEMPERATURES

It was shown in the last section that in calculating the perturbation series for the pair distribution function it is sometimes more advantageous to rearrange it in such a way as to eliminate the polarization parts of the representative diagrams by introducing collective interactions. This seems to be the case when one wishes to investigate the many-body system from a collective motion point of view. Taking this viewpoint, we shall examine in this section the pair distribution function and the internal energy at low temperatures by choosing the electron gas as a particular example. The corresponding treatment for the hard-sphere Bosons will be found in the next section.

We found also in the last section that the simple chain approximation to the collective interaction for the electron gas is responsible for the transfer of a plasmon which is known to be an important collective excitation at the very low temperatures. Hence, it would be of great interest if we consider an expansion of the pair distribution function in terms of the collective interaction  $U$  rather than in terms of the original (Coulomb) interaction  $V$ . Here we shall calculate the zeroth- and

<sup>19</sup> This property of the distribution function is also characteristic of the Boltzmann system but not of the Fermi system. The following argument holds also for the Boltzmann system.

<sup>20</sup> Cf references 8 and 9. Also see N. Bogolyubov, J. Phys. U.S.S.R. 11, 23 (1947); N. Bogolyubov and N. Zubarev, J. Exptl. Theoret. Phys. 28, 129 (1955); K. A. Brueckner and K. Sawada, Phys. Rev. 106, 1117, 1128 (1957); R. Abe, Progr. Theoret. Phys. (Kyoto) 19, 699 (1958).

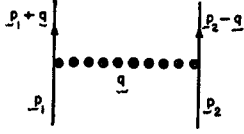


FIG. 9. The first-order diagram in  $U$  of the pair distribution function. The thick dotted line represents a collective interaction  $U$ .

the first-order term in  $U$  of the pair distribution function. Although a further refinement of the theory as well as the calculation may be made by employing usual procedures for simplifying the problem such as treatment of self-energy part and vertex part and renormalization, we shall postpone this to the later publications.

The zeroth-order term  $n_0^{(2)}(\mathbf{r}_1\mathbf{r}_2)$  of the pair distribution function is, of course, the one for the ideal gas (Fig. 1). It is given from (3.10) and (4.2)

$$\begin{aligned} n_0^{(2)}(\mathbf{r}_1\mathbf{r}_2) &= e^{2\alpha} K_0^{(2)}(\mathbf{r}_1\beta, \mathbf{r}_2\beta; \mathbf{r}_10, \mathbf{r}_20) \\ &= e^{2\alpha} K_0(\mathbf{r}_1\beta; \mathbf{r}_10) K_0(\mathbf{r}_2\beta; \mathbf{r}_20) \\ &\quad \pm e^{2\alpha} K_0(\mathbf{r}_2\beta; \mathbf{r}_10) K_0(\mathbf{r}_1\beta; \mathbf{r}_20). \end{aligned} \quad (6.1)$$

Computing the trace in (4.3), one has for the one-body free-particle propagator

$$e^\alpha K_0(\mathbf{r}\beta; \mathbf{r}'0) = V^{-1} \sum_{\mathbf{p}} f(\mathbf{p}) e^{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} \quad (6.2)$$

$$\begin{aligned} n_I^{(2)}(\mathbf{r}_1\mathbf{r}_2) &= e^{2\alpha} K_I^{(2)}(\mathbf{r}_1\beta, \mathbf{r}_2\beta; \mathbf{r}_10, \mathbf{r}_20) \\ &= (V\beta)^{-1} \sum_{\mathbf{p}_1 s} \sum_{\mathbf{p}_2 s_2} \sum_{\mathbf{q} t} \exp[i(s_1 + t)\beta + i(s_2 - t)\beta] \exp[i(\mathbf{p}_1 + \mathbf{q}) \cdot \mathbf{r}_1 + i(\mathbf{p}_2 - \mathbf{q}) \cdot \mathbf{r}_2 - i\mathbf{p}_1 \cdot \mathbf{r}_1 - i\mathbf{p}_2 \cdot \mathbf{r}_2] \\ &\quad \times S(\mathbf{p}_1 + \mathbf{q}, s_1 + t) S(\mathbf{p}_2 - \mathbf{q}, s_2 - t) S(\mathbf{p}_1, s_1) S(\mathbf{p}_2, s_2) \{-U(\mathbf{p}, t)\} + (\text{exchange term}), \end{aligned} \quad (6.6)$$

where the second term (exchange term) is, except for the sign, equal to the quantity obtained from the first term by exchanging the pair of position vectors  $(\mathbf{r}_1, \mathbf{r}_2)$  of the final state. Since

$$\exp(is_1\beta + is_2\beta) = \exp[i(2m+1)\pi + i(2n+1)\pi] = 1 \text{ for integers } m \text{ and } n, \quad (6.7)$$

the summations over  $s_1$  and  $s_2$  can be carried out in the same way as the summation over  $s$  in (5.11). Introducing a new quantity  $\lambda(q, t; \mathbf{r})$  defined by

$$\begin{aligned} \lambda(q, t; \mathbf{r}) &= (V\beta)^{-1} \sum_{\mathbf{p} s} e^{i\mathbf{p} \cdot \mathbf{r}} S(\mathbf{p} + \mathbf{q}, s + t) S(\mathbf{p}, s) \\ &= V^{-1} \sum_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{r}} [(\mathbf{p} + \mathbf{q})^2 - \mathbf{p}^2 + it]^{-1} [f(\mathbf{p}) - f(\mathbf{p} + \mathbf{q})], \end{aligned} \quad (6.8)$$

one can rewrite the right-hand side of (6.6) as

$$n_I^{(2)}(\mathbf{r}_1\mathbf{r}_2) = -(V\beta)^{-1} \sum_{\mathbf{q} t} e^{i\mathbf{q} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} U(q, t) [\lambda^2(q, t; 0) \pm \lambda^2(q, t; \mathbf{r}_1 - \mathbf{r}_2)] \quad (6.9)$$

$$\equiv n_{Ia}^{(2)}(\mathbf{r}_1\mathbf{r}_2) \pm n_{Ib}^{(2)}(\mathbf{r}_1\mathbf{r}_2). \quad (6.10)$$

It is noted that  $\lambda(q, t; 0)$  coincides with  $\lambda(q, t)$  defined in (5.11):

$$\lambda(q, t; 0) = \lambda(q, t). \quad (6.11)$$

Adding contributions from (6.5) and (6.10), one obtains for the pair distribution function up to the first order in  $U$

where  $f(\mathbf{p})$  is the Bose or the Fermi distribution function. Substitution into (6.1) yields

$$\begin{aligned} n_0^{(2)}(\mathbf{r}_1\mathbf{r}_2) &= [V^{-1} \sum_{\mathbf{p}} f(\mathbf{p})]^2 \\ &\quad \pm [V^{-1} \sum_{\mathbf{p}} f(\mathbf{p}) e^{i\mathbf{p} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}]^2, \end{aligned} \quad (6.3)$$

which is London-Placzek's<sup>21</sup> formula for the ideal gas. In the present approximation of the calculation the first term may be taken as the square of the density  $n$ . Hence one has, alternatively,

$$n_0^{(2)}(\mathbf{r}_1\mathbf{r}_2) = n^2 \pm [V^{-1} \sum_{\mathbf{p}} f(\mathbf{p}) e^{i\mathbf{p} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}]^2 \quad (6.4)$$

$$\equiv n^2 \pm n_{0b}^{(2)}(\mathbf{r}_1\mathbf{r}_2). \quad (6.5)$$

Next, we shall consider the first-order term  $e^{2\alpha} K_I^{(2)}(\mathbf{r}_1\beta, \mathbf{r}_2\beta; \mathbf{r}_10, \mathbf{r}_20)$  in the collective interaction. It may be represented by a graph shown in Fig. 9, where a thick dotted line denotes the collective interaction  $U$ . Its mathematical expression may be written down immediately from Table II. However, noting that the only difference from Fig. 2(a) is the replacement of the original (Coulomb) interaction  $V$  by the collective interaction  $U$ , one may guess it easily from (4.16);

$$\begin{aligned} n^{(2)}(\mathbf{r}_1\mathbf{r}_2) &= n^2 \pm n_{0b}^{(2)}(\mathbf{r}_1\mathbf{r}_2) \\ &\quad + n_{Ia}^{(2)}(\mathbf{r}_1\mathbf{r}_2) \pm n_{Ib}^{(2)}(\mathbf{r}_1\mathbf{r}_2). \end{aligned} \quad (6.12)$$

The discussions so far are only applicable to spinless Bose or Fermi gases. We shall specialize ourselves in the electron gas problem for the remainder of this section.

Since the electron has spin of magnitude  $\frac{1}{2}$ , certain modifications are necessitated in our formalism. However, they are very simple, because we still assume the spin-independent Hamiltonian (2.1). The only effects of

<sup>21</sup> F. London, J. Chem. Phys. **11**, 203 (1943); G. Placzek, *Second Berkeley Symposium on the Mathematical Statistics and Probability*, p. 581 (1950).

the electronic spin on our formalism are: (i) to allow two electrons in each state specified by the electronic momentum; and (ii) to throw out the exchange terms for the antiparallel spin electron encounter. The consideration of these two leads to the doubling of every value  $\lambda$  which appears in the theory, and the reduction by a factor  $\frac{1}{2}$  of all the exchange terms in formula (6.12). Hence, we have for the electron gas

$$n^{(2)}(\mathbf{r}_1\mathbf{r}_2) = n^2 - \frac{1}{2}n_{0b}^{(2)}(\mathbf{r}_1\mathbf{r}_2) + n_{Ia}^{(2)}(\mathbf{r}_1\mathbf{r}_2) - \frac{1}{2}n_{Ib}^{(2)}(\mathbf{r}_1\mathbf{r}_2) \quad (6.13)$$

with the change of  $\lambda$  into  $2\lambda$  implicitly contained in  $n_{Ia}^{(2)}(\mathbf{r}_1\mathbf{r}_2)$  and  $n_{Ib}^{(2)}(\mathbf{r}_1\mathbf{r}_2)$ . We shall evaluate this at the absolute zero temperature.

The second term is the correlation due to the exchange effect of the noninteracting Fermi particles. It was evaluated by London.<sup>20</sup>

$$n_{0b}^{(2)}(\mathbf{r}_1\mathbf{r}_2) = n^2 \frac{9\pi [J_{\frac{1}{2}}(x)]^2}{2x^3} \quad (6.14)$$

with

$$x \equiv 2\pi p_0 r. \quad (6.15)$$

This is also known as the Wigner-Seitz formula.<sup>22</sup>

The third term was given in (6.9). In the calculation, we shall adopt the simple chain approximation for the collective interaction discussed in the last section. Thus substituting  $U$  from (5.15) one gets

$$n_{Ia}^{(2)}(r) = -(V\beta)^{-1} \sum_{q,t} e^{i\mathbf{q}\cdot\mathbf{r}} 4\lambda^2(q,t) v(q) \times [1 + 2v(q)\lambda(q,t)]^{-1} \quad (6.16)$$

with  $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$  and  $r \equiv |\mathbf{r}|$ . As  $V \rightarrow \infty$  and  $\beta \rightarrow \infty$ , one may approximate the above sums by the corresponding integrals:

$$\begin{aligned} V^{-1} \sum_{\mathbf{q}} &\rightarrow (2\pi)^{-3} \int d^3q \\ \beta^{-1} \sum_t &\rightarrow (2\pi)^{-1} \int_{-\infty}^{+\infty} dt. \end{aligned} \quad (6.17)$$

Hence one has

$$n_{Ia}^{(2)}(r) = (2\pi)^{-4} \int d^3q dt e^{i\mathbf{q}\cdot\mathbf{r}} 4\lambda^2(q,t) v(q) \times [1 + 2v(q)\lambda(q,t)]^{-1}. \quad (6.18)$$

If the distance  $r$  is sufficiently large, the important contribution to the integral over  $\mathbf{q}$  will come only from the small  $\mathbf{q}$  domain of integration due to the oscillating function  $e^{i\mathbf{q}\cdot\mathbf{r}}$ . Substituting  $\lambda(q,t)$  and  $v(q)$  from (5.15) and (5.10), one has

$$\begin{aligned} n_{Ia}^{(2)}(r) &= -\frac{1}{(2\pi)^4} \int d^3q e^{i\mathbf{q}\cdot\mathbf{r}} \\ &\times \int dt \frac{(\epsilon^2 p_0^2 R^2(u))/(\pi^2 q^2)}{1 + [2\epsilon^2 p_0 R(u)]/(\pi q^2)}. \end{aligned} \quad (6.19)$$

To simplify the complicated expression, we shall use the conventional units for the electron gas. First, the inverse density is set equal to

$$n^{-1} \equiv (4/3)\pi r_0^3. \quad (6.20)$$

The dimensionless parameter  $r_s$  is defined by

$$r_s \equiv r_0/r_B, \quad (6.21)$$

where  $r_B$  is the Bohr radius

$$r_B \equiv 2/\epsilon^2. \quad (6.22)$$

Now in these units the expression (6.19) after angular integrations is given by

$$\begin{aligned} n_{Ia}^{(2)}(r) &= -\frac{9}{4\pi} n^2 \int_0^\infty dQ Q^3 \frac{\sin Q p_0 r}{Q p_0 r} \\ &\times \int_{-\infty}^{+\infty} du \frac{4\alpha r_s R^2(u)}{\pi Q^2 + 4\alpha r_s R(u)}, \end{aligned} \quad (6.23)$$

where  $\alpha$  is a numerical factor defined by

$$\alpha \equiv (4/9\pi)^{\frac{1}{2}}. \quad (6.24)$$

A rough estimate of the integral will be made in the following way. The method is originally due to A. Glick.<sup>23</sup> Consider an integral

$$I(Q) \equiv \int_{-\infty}^{+\infty} du \frac{4\alpha r_s R^2(u)}{\pi Q^2 + 4\alpha r_s R(u)}. \quad (6.25)$$

For  $4\alpha r_s/(\pi Q^2) \ll 1$  this will be approximately given by

$$\begin{aligned} I(Q) &\cong \frac{4\alpha r_s}{\pi Q^2} \int_{-\infty}^{+\infty} du R^2(u) \\ &= (8/3)\alpha r_s Q^{-2} (1 - \ln 2). \end{aligned} \quad (6.26)$$

On the other hand for  $4\alpha r_s/(\pi Q^2) \gg 1$ ,  $I(Q)$  will become

$$I(Q) \cong \int_{-\infty}^{+\infty} du R(u) = \frac{\pi}{2} \quad (6.27)$$

As an approximation, we shall take in place of  $I(Q)$  a function  $I'(Q)$  which have the same limiting values as  $I(Q)$ . The simplest one is

$$I'(Q) = (\pi/2) \{1 + 3\pi Q^2 [16\alpha r_s (1 - \ln 2)]^{-1}\}^{-1}. \quad (6.28)$$

Substituting this into (6.23), one can read the integral

<sup>22</sup> E. Wigner and F. Seitz, Phys. Rev. 43, 804 (1933).

<sup>23</sup> A. Glick (private communication).

from a standard mathematical table:

$$\begin{aligned} \frac{n_{Ia}^{(2)}(r)}{n^2} &= -\frac{32\alpha^2 r_s^2 (1-\ln 2)}{\pi^2} \int_0^\infty dy \sin y (1 - \{y^2 + [16\alpha r_s^3 \rho_0^2 (1-\ln 2)] / (3\pi)\}^{-1})^{-1} 3\pi [16\alpha r_s^3 \rho_0^2 (1-\ln 2)]^{-1} \\ &= -\frac{32\alpha^2 r_s^2 (1-\ln 2)}{\pi^2} \left\{ \frac{1}{x^2} - \frac{1}{2x} [e^{-x} \bar{\text{Ei}}(x) - e^x \text{Ei}(-x)] \right\} \text{ for large } r \end{aligned} \quad (6.29)$$

with

$$x \equiv \left( \frac{16r_s(1-\ln 2)}{3\pi\alpha} \right)^{\frac{1}{2}} \frac{r}{r_0}. \quad (6.30)$$

The formula (6.29) is valid only for a large value of  $r$  as stated before.

The fourth term in the right-hand side of (6.13) is given by

$$\frac{1}{2} n_{Ib}^{(2)}(r) = -\frac{1}{2} (V\beta)^{-1} \sum_{\mathbf{q}'} e^{i\mathbf{q} \cdot \mathbf{r}} 4\lambda^2(q, t; \mathbf{r}) v(q) [1 + 2v(q)\lambda(q, t)]^{-1}. \quad (6.31)$$

The quantity  $\lambda(q, t; \mathbf{r})$  was given in (6.8). Due to the oscillating function  $e^{i\mathbf{p} \cdot \mathbf{r}}$  in its expression, it approaches zero rapidly as  $r \rightarrow \infty$ . Hence the function  $n_{Ib}^{(2)}(r)$  approaches zero more rapidly than the function  $n_{Ia}^{(2)}(r)$ . We do not attempt here to calculate  $n_{Ib}^{(2)}(r)$  in any detail. More accurate calculation of  $n_{Ia}^{(2)}(r)$  as well as  $n_{Ib}^{(2)}(r)$  is in contemplation and will be published elsewhere.

We shall hereafter evaluate the ground-state energy of the electron gas using the general theory developed in Sec. 2.

It is well known that as the temperature approaches zero every thermodynamical average becomes a pure quantum-mechanical average, i.e., an average using the ground-state wave function. As a particular example, the relation (2.11) between the internal energy and the pair distribution function becomes the well-known relation between the ground-state energy  $E$  and the ground-

state pair distribution function  $n^{(2)}(\mathbf{r}; g)$ :

$$E(g) = E(0) + \frac{1}{2} V \int_0^g dg' \int d^3r v(r) n^{(2)}(\mathbf{r}; g'), \quad (6.32)$$

$E(0)$  being the ground-state energy of the corresponding ideal gas. The derivation of the latter from the former is very simple when one works in the canonical ensemble.

In the electron gas the square of the electronic charge may be chosen as the natural coupling strength. For convenience, we shall introduce a parameter such that

$$g \equiv \epsilon^2 \kappa. \quad (6.33)$$

Then as the coupling is switched on at zero and increased up to the full strength  $\epsilon^2$ ,  $\kappa$  takes a value from zero to one.

Using this convention and substituting (6.13) into (6.32), one has

$$\begin{aligned} E(g) &= E(0) + \frac{1}{2} V \epsilon^2 \int_0^1 d\kappa \int d^3r n^{(2)}(\mathbf{r}; \kappa) r^{-1} \\ &= E(0) + \frac{1}{2} V \epsilon^2 \int d^3r n^2 r^{-1} - \frac{1}{4} V \epsilon^2 \int d^3r n_{Ib}^{(2)}(\mathbf{r}) r^{-1} \\ &\quad + \frac{1}{2} V \epsilon^2 \int_0^1 d\kappa \int d^3r n_{Ia}^{(2)}(\mathbf{r}, \kappa) r^{-1} - \frac{1}{4} V \epsilon^2 \int_0^1 d\kappa \int d^3r n_{Ib}^{(2)}(\mathbf{r}; \kappa) r^{-1}. \end{aligned} \quad (6.34)$$

Before going into the calculation, we must comment on the Coulomb energy of the electron gas. Since the pair distribution function  $n^{(2)}(r)$  approaches  $n^2$  at large distances  $r$  the first integral on the right side of (6.34) diverges quadratically. To avoid this, we subtract from (6.34) a quantity defined by

$$\frac{1}{2} V \epsilon^2 \int d^3r n^2 r^{-1} \quad (6.35)$$

and consider only the rest of the ground-state energy. The quantity appeared in (6.25) is usually called the Coulomb energy. The subtraction corresponds physi-

cally to the following situation. Suppose, we have an electron gas with a uniformly distributed background of positive charge just sufficient to keep the whole system electrically neutral. This system has an extra energy due to the interaction between the electrons and the background in addition to those given by (6.34). This extra energy is exactly the same as (6.35) in magnitude and opposite in sign. Thus the total energy of the whole system becomes finite. The introduction of a positively charged background is also required from the practical standpoint, for the system investigated by means of the electron gas is usually electrically neutral, e.g., electrons in a metal. Hence, hereafter we consider a system

comprising an electron gas with a uniformly charged background.

Returning to (6.34), we shall consider term by term separately. The first term is the kinetic energy of the free Fermions with the correction due to the electronic spin.

$$E(0) = \frac{3}{5} N \epsilon_f. \quad (6.36)$$

In the conventional units used for the electron gas, this is expressed as

$$E(0) = \frac{3}{5} \alpha^{-2} r_s^{-2}. \quad (6.37)$$

The second term (Coulomb energy) is discarded by the reason stated above. The third is usually called the exchange energy. Substitution from (6.4) yields:

$$\begin{aligned} E_{0b} &\equiv -\frac{1}{4} \epsilon^2 V (2\pi)^{-6} \int d^3 r r^{-1} \int \int d^3 p d^3 p' f_F(\mathbf{p}) f_F(\mathbf{p}') \exp[i(\mathbf{p}-\mathbf{p}') \cdot \mathbf{r}] \\ &= -\pi \epsilon^2 V (2\pi)^{-6} \int \int d^3 p d^3 p' f_F(\mathbf{p}) f_F(\mathbf{p}') (\mathbf{p}-\mathbf{p}')^{-2}. \end{aligned} \quad (6.38)$$

At the zero temperature the Fermi distribution function  $f_F(\mathbf{p})$  takes the value one inside the Fermi sphere and zero outside so that one has only to carry out the above integration over the interception of the two Fermi spheres. The integration is tedious but elementary and gives

$$E_{0b}/N = -\epsilon^2 p_0^4 V (4\pi^3)^{-1} \quad (6.39)$$

$$= -\frac{3}{2} (\pi \alpha r_s)^{-1}. \quad (6.40)$$

Now consider the fourth term of (6.34). Substitution from (6.9) and integration over the coupling strength give rise to

$$\begin{aligned} E_{Ia} &\equiv -\frac{1}{2} V \epsilon^2 (2\pi)^{-4} \int d^3 r r^{-1} \int d^3 q dt e^{i\mathbf{q} \cdot \mathbf{r}} \{ 2\lambda(q, t) - v^{-1}(q) \ln[1 + 2v(q)\lambda(q, t)] \} \\ &= -\frac{1}{2} V (2\pi)^{-4} \int d^3 q dt \{ 2v(q)\lambda(q, t) - \ln[1 + 2v(q)\lambda(q, t)] \}. \end{aligned} \quad (6.41)$$

Substituting  $\lambda(q, t)$  from (5.13) into this and employing the conventional units, one obtains,

$$E_{Ia}/N = -\frac{3}{4\pi} \frac{1}{\alpha^2 r_0^2} \int_0^1 dQ Q^3 \int_{-\infty}^{+\infty} du \left\{ \frac{4\alpha r_s}{\pi Q^2} R(u) - \ln \left[ 1 + \frac{4\alpha r_s}{\pi Q^2} R(u) \right] \right\}. \quad (6.42)$$

This is exactly the formula (M-W, 6-12) obtained by Montroll and Ward<sup>3</sup> for the change in the ground state energy due to the electron interactions up to the ring integral approximation. It also appears in the Gell Mann-Bruckner theory of the correlation energy and was evaluated there to be given by

$$\begin{aligned} E_{Ia}/N &= \frac{2}{\pi^2} (1 - \ln 2) \left( \ln \frac{4\alpha r_s}{\pi} - 0.551 - \frac{1}{2} \right) \\ &+ (\text{vanishing terms as } r_s \rightarrow 0). \end{aligned} \quad (6.43)$$

What is noteworthy in the foregoing is the logarithmic dependency of the energy with the respect to  $r_s$ . It is known from the dimensional analysis<sup>3</sup> that in the low-temperature limit the perturbation expansion becomes equivalent to the high-density expansion, the appropriate parameter being the dimensionless quantity  $r_s$ , inversely proportional to the cube root of the density. However, a straightforward perturbation expansion was found to yield a divergence due to the long-range Coulomb force. To relieve this situation Gell-Mann and Bruckner have proposed the following high-density

expansion formula:

$$\begin{aligned} E/N &= A r_s^{-2} + B r_s^{-1} + D \ln r_s \\ &+ C + F r_s \ln r_s + G r_s + \dots \end{aligned} \quad (6.44)$$

and calculated the coefficients  $C$  and  $D$  exactly. The value of the coefficient  $D$  is exactly the same as the one appearing in (6.43). On the other hand, our formula (6.34) is essentially the expansion in terms of the collective interaction, which is closely related to the collective excitation (plasmon) as remarked in the last section. It has no divergence whatsoever but is not by itself the high-density expansion of Gell-Mann-Bruckner. However, it is very interesting to notice that the terms appearing in (6.34) give successively the first three of the expansion (6.45). In other words, we can read the coefficients  $A$ ,  $B$ , and  $D$  from (6.37), (6.40), and (6.43):

$$\begin{aligned} A &= \frac{3}{5} \alpha^{-2} = 2.21 \quad B = -3/(2\pi\alpha) = -0.916 \\ D &= 2(1 - \ln 2)/\pi^2 = 0.0622. \end{aligned} \quad (6.45)$$

This is one of the main advantages of the present theory and gives a support to the expansion method in powers of the collective interaction.



In order to calculate the constant  $C$ , it is necessary to evaluate more accurately that part of the integral (6.41), which contributes to the energy of the zeroth order in  $r_s$  and add another contribution from the last term of (6.34). These will be easily identified as

$$\epsilon_a^{(2)} = -\frac{1}{2}VN^{-1}(2\pi)^{-4} \int d^3q dt \frac{1}{2} [2v(q)\lambda(q,t)]^2 \quad (6.46)$$

$$\epsilon_b^{(2)} = \frac{1}{4}VN^{-1}(2\pi)^{-4} \int d^3q dt \times \int d^3r (\epsilon^2/r) e^{i\mathbf{q}\cdot\mathbf{r}} 2v(q)\lambda^2(q,t; \mathbf{r}). \quad (6.47)$$

According to Gell-Mann and Bruckner the correction due to the exact evaluation of  $\epsilon_a^{(2)}$  and the numerical integration of  $\epsilon_b^{(2)}$  are the following:

$$\delta \equiv \epsilon_a^{(2)} - \left[ \frac{3}{4\pi} \frac{1}{\alpha^2 r_0^2} \left( \frac{4\alpha r_s}{\pi} \right)^2 \times \int_0^1 \frac{dQ}{Q} \int_{-\infty}^{+\infty} du R^2(u) \right] \quad (6.48)$$

$$= -0.0508$$

$$\epsilon_b = 0.046. \quad (6.49)$$

Adding these to the constant term in (6.43), one obtains the value  $C$  as follows:

$$C = -0.096. \quad (6.50)$$

## 7. A HARD SPHERE BOSE SYSTEM AT THE ABSOLUTE ZERO TEMPERATURE

In this section we shall investigate the ground-state behavior of a hard-sphere Bose system following the same procedure employed for the electron gas.

We have seen in Sec. 5 that the simple chain approximation to the collective pseudo-interaction for a hard-sphere Bose system is closely related to the transfer of a phonon just as the same approximation to the collective interaction for the electron gas is related to the transfer of a plasmon. As we did for the electron gas in the last section, we start by calculating the first two terms of the collective pseudo-interaction expansion of the pair distribution function for a hard-sphere Bose system. The graphs representative of these two terms are the same as for the electron gas, i.e., Fig. 1 and Fig. 9 except that the thick dotted line in the second figure should represent the collective pseudo-interaction given by (5.32) instead of the collective interaction. Let us compute these one by one.

The zeroth-order term of  $n^{(2)}(\mathbf{r})$  represented in Fig. 1 is nothing but the free-Boson pair distribution function.

From (6.5) this is given by

$$n_0^{(2)}(\mathbf{r}) = n^2 + [V^{-1} \sum_{\mathbf{p}} f_B(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{r}}]^2, \quad (7.1)$$

where  $f_B(\mathbf{p})$  is the Bose distribution function.

At the absolute zero temperature  $f_B(\mathbf{p})$  becomes a Kronecker's delta function with the multiple factor  $N$  centered at  $\mathbf{p}=0$ . Therefore, we would get  $2n^2$  for  $n_0^{(2)}(\mathbf{r})$  from (7.1) irrespective of the spatical configuration of the two particles. This is in contradiction with the familiar notion that every pair distribution function, as required from its probability interpretation, must approach the square  $n^2$  of the density if the system remains uniformly distributed. We are not able to resolve this contradiction at the moment. However, we shall note here as a special feature characteristic of the ground-state Bose system that the exchange term of any order in  $U'$  contributes the same amount to  $n^{(2)}(\mathbf{r})$  as the corresponding normal (scattering) term by virtue of the delta-function nature of the Bose distribution function. Hence, we have only to compute the normal scattering terms. As for the contradiction we shall tentatively renormalize the pair distribution function  $n^{(2)}(\mathbf{r})$  such that

$$n^{(2)}(\mathbf{r}) \rightarrow n^2 \quad \text{as } \mathbf{r} \rightarrow \infty, \quad (7.2)$$

since we can in no sense doubt the correctness of probabilistic physical argument. Although this is equivalent to discarding the exchange term (or the normal term) in the calculation of  $n^{(2)}(\mathbf{r})$  at the absolute zero temperature, a different situation will arise at finite temperatures. In actuality below the  $\lambda$  point of the Bose condensation the exchange term in (7.1) does not vanish but approaches  $n^2(N_0/N)$  ( $N_0/N$  being the fraction of the zero-momentum particles) at infinite separation because of the degeneracy of the ground single-particle state. Therefore, the renormalization of  $n^{(2)}(\mathbf{r})$  becomes necessary at finite temperatures for a free-Boson system and therefore, must be required for an interacting Boson system.

Since we shall deal with the zero-temperature case in the following we shall calculate only the normal scattering terms and treat them as if they were the only contributions to the specified diagram.

Thus, the zeroth-order contribution to the pair distribution function is, after renormalization, given by

$$n_0^{(2)}(\mathbf{r}) = n^2. \quad (7.3)$$

For the first-order term in  $U'$  (Fig. 9) of the pair distribution function one has from (6.8)

$$n_1^{(2)}(\mathbf{r}) = - (V\beta)^{-1} \sum_{\mathbf{q}, t} e^{i\mathbf{q}\cdot\mathbf{r}} U'(q, t) \lambda^2(q, t). \quad (7.4)$$

The quantity  $\lambda(q, t)$  was calculated in (5.31) and the simple chain approximation to the collective pseudo-interaction  $U'(q, t)$  is also given in (5.32). Substituting these expressions in the foregoing, one gets

$$n_1^{(2)}(\mathbf{r}) = - (V\beta)^{-1} \sum_{\mathbf{q}, t} e^{i\mathbf{q}\cdot\mathbf{r}} 32\pi a n^2 q^4 (q^4 + t^2 + 16\pi a n q^2)^{-1} (q^4 + t^2)^{-1}. \quad (7.5)$$

Approximating the sums by the corresponding integrals [cf (6.17)] and then integrating over angular coordinates, one obtains

$$\begin{aligned} n_{I(r)}^{(2)} &= -\frac{8}{\pi^2} \frac{an^2}{\alpha} \int_0^\infty dq \frac{\sin qr}{q^4} \int_{-\infty}^{+\infty} dt \left( \frac{1}{q^4 + t^2} - \frac{1}{q^4 + t^2 + \alpha q^2} \right) \\ &= -\frac{8}{\pi^2} \frac{an^2}{\alpha} \int_0^\infty dq \frac{\sin qr}{q^2} \left( 1 - \frac{1}{(1 + \alpha/q^2)^{1/2}} \right) \end{aligned} \quad (7.6)$$

with

$$\alpha \equiv 16\pi an. \quad (7.7)$$

If one introduces a dimensionless variable by

$$y = qr, \quad (7.8)$$

one can rewrite (7.6) as

$$n_I^{(2)}(r) = -\frac{8}{\pi} \frac{an^2}{\alpha r^3} \int_0^\infty dy \frac{\sin y}{y^2} \{1 - [1 + (\alpha r^2/y^2)]^{-1}\}. \quad (7.9)$$

For small distances such that

$$r \ll \alpha^{-1/2} = (16\pi an)^{-1/2} \equiv r_c, \quad (7.10)$$

the expression (7.9) reduces to

$$\begin{aligned} n_I^{(2)}(r) &= -\frac{8}{\pi} \frac{an^2}{\alpha r^3} \int_0^\infty dy \frac{\sin y}{y} \frac{1}{2} \alpha r^2 \\ &= -2n^2(a/r) \quad \text{for } r \ll r_c. \end{aligned} \quad (7.11)$$

In the other limiting case, i.e., for large separations the expression (7.9) becomes

$$\begin{aligned} n_I^{(2)}(r) &\rightarrow -\frac{8}{\pi} \frac{an^2}{\alpha r^3} \int_0^\infty dy \frac{\sin y}{y} \sin y \left( 1 - \frac{r_c}{r} y \right) \\ &= -n^2 (4\pi^{1/2} a^{1/2} n^{1/2})^{-1} r^{-4} \quad \text{for } r \gg r_c, \end{aligned} \quad (7.12)$$

where the integral was evaluated by inserting an integrating factor  $e^{-\gamma y}$  into the integrand and subsequently taking the limit  $\gamma \rightarrow 0$ .

Adding contributions from (7.3), (7.11), and (7.12) one obtains for the pair distribution function up to the first order in  $U'$

$$n^{(2)}(r) = n^2 [1 - 2(a/r)] \quad \text{for } a \ll r \ll r_c \quad (7.13a)$$

$$= n^2 [1 - (4\pi^{1/2} a^{1/2} n^{1/2})^{-1} r^{-4}] \quad \text{for } r \gg r_c. \quad (7.13b)$$

This result is consistent with the calculation of Lee, Huang, and Yang<sup>8</sup> employing the pseudo-potential method. They obtained

$$n^{(2)}(r) = n^2 [1 - (a/r)]^2 + O(a/r_c) \quad \text{for } a < r \ll r_c \quad (7.14a)$$

$$= n^2 + O(r^{-4}) \quad \text{for } r \gg r_c. \quad (7.14b)$$

Our formula (7.13a) agrees with (7.14a) up to the order  $a/r$  while (7.13b) coincides with (7.14b) completely. The formula (7.14a) can be understood in the following way.

For small separation the direct interaction, which is singular near  $r=0$ , acts comparatively stronger than the indirect interaction through a medium. The  $S$ -wave solution of the Schrödinger equation for two hard spheres in a large box has the form

$$\psi(r) = cr^{-1} \sin k(r-a) \quad \text{for } r > a, \quad (7.15)$$

where  $r$  is the distance between the two particles and  $k$  a relative momentum eigenvalue subject to a certain boundary condition and  $c$  a constant. If the direct interaction is predominant as mentioned above, the pair

distribution function at small separations will have the form

$$n^{(2)}(r) \propto |\psi(r)|^2 \propto [1 - (a/r)]^2 \quad \text{for } r \cong a. \quad (7.16)$$

This agrees with (7.14a). Thus it seems to be necessary to take into account more precise behavior of the two-body pseudo-interaction at least for the direct interaction contribution to  $n^{(2)}(r)$ .

The quantity  $r_c$  defined in (7.10) has the dimension of length and could be called the correlation length. It measures the extension of the correlation between particles introduced by the hard-sphere interaction.

Now again using the formula (6.32), we shall calculate the ground-state energy from the pair distribution func-

tion. As we shall treat the pseudo-interaction  $8\pi a\delta^{(3)}(\mathbf{r})$  as if it were a real interaction, the hard-sphere diameter  $a$  could be taken as the coupling strength  $g$  in the formula (6.32). Introducing a parameter  $\kappa$  such that  $g=a\kappa$  and substituting  $n^{(2)}$  from (7.3) and (7.4) into (6.32), one has

$$E = E(0) + \frac{1}{2}V \int_0^1 d\kappa \int d^3r v'(\mathbf{r}) \times \{n^2 - (V\beta)^{-1} \sum_{q,t} e^{iq \cdot \mathbf{r}} \lambda^2(q,t) U'(q,t)\}. \quad (7.17)$$

The ground-state energy for the free Bose system can be taken as zero.

$$E(0) = 0. \quad (7.18)$$

Replacing the summation over  $t$  by the corresponding integral and substituting  $v'(\mathbf{r})$ ,  $\lambda(q,t)$ , and  $U'(q,t)$  from (5.29), (5.31), and (5.32), respectively, one obtains

$$E = 4\pi a n N - \frac{1}{2}(2\pi)^{-1} \sum_q \int dt \times \left\{ \frac{\alpha q^2}{q^4 + t^2} - \ln \left( 1 + \frac{\alpha q^2}{q^4 + t^2} \right) \right\} \quad (7.19)$$

with  $\alpha$  defined in (7.7). Integration over  $t$  gives rise to

$$E = 4\pi a n N - \frac{1}{2} \sum_q \{q_0^2 + q^2 - q(q^2 + 2q_0^2)^{\frac{1}{2}}\} \quad (7.20)$$

with

$$q_0^2 \equiv 8\pi a n. \quad (7.21)$$

The foregoing summation is divergent. However, a remedy for the situation is well known. In fact, the formula (7.20) is identical with Eq. (19) of reference 8, where Lee, Huang, and Yang derived it using the same pseudo-interaction (pseudo-potential) as ours. Reasoning that they should have used the correct pseudo-potential  $[8\pi a\delta^{(3)}(\mathbf{r})(\partial/\partial\mathbf{r})\mathbf{r} = v'(\mathbf{r})]$ , they then subtracted the spurious term  $q_0^4/(2q^2)$  in the summand, thus removing the above divergence, and finally obtained the following result:

$$E = 4\pi a n N - \frac{1}{2} \sum_q [q_0^2 + q^2 - q(q^2 + 2q_0^2)^{\frac{1}{2}} - q_0^4/(2q^2)] \\ = 4\pi a n N [1 + (128/15\sqrt{\pi})(a^3 n)^{\frac{1}{2}}]. \quad (7.22)$$

According to their analysis this subtraction corresponds to dropping the term proportional to  $a^2$  in the formula (7.20) after its expansion in powers of  $a$ . This can be understood in the following way. The contribution of the order  $a^2$  in our theory can be identified by its graphical representation shown in Fig. 10(a), where each wavy line in this case denotes a pseudo-interaction. The thin dotted line means that the ends of particle lines should be connected, indicating the extra integration performed over the position variables of the ends. If we recall that the pseudo-interaction originates from a set of ladder diagrams, we should have included the con-

tribution Fig. 10(a) in the contribution Fig. 10(b) which is of the order  $a$ . This explains the above subtraction.

It is interesting to note that the expression (7.22) is the low-density expansion in contrast to the high-density expansion (6.34) for the electron gas case although both cases were treated in a similar fashion. This apparent paradox, however, can be resolved from a dimensional argument. For the electron gas at low temperatures the appropriate dimensionless expansion parameter was shown to be  $(\epsilon^2 n^{-1})$  while for the hard sphere gas it is clearly  $(na^3)$ . Hence an expansion in powers of the coupling strength (the hard sphere diameter  $a$  is regarded as a coupling strength of the pseudo-interaction) necessarily means a high-density expansion for the electron gas and a low-density expansion for the Bose gas.

### 8. FINAL REMARKS. DEBYE-HUCKEL EQUATION OF STATE

Although the general formulation presented in Secs. 2-4 is valid for all temperatures, the subsequent applications of the theory to the electron gas and the hard-sphere Bose gas were made only at the absolute zero temperature. The extension of these calculations to the finite but very low temperature case is especially simple. To do this, we must recalculate the quantity  $\lambda(q,t)$  in (6.8). However, this is easily done because the low-temperature behavior of the Bose or Fermi distribution function  $f(\mathbf{p})$  is well known, e.g., in the works by F. London<sup>24</sup> and A. Sommerfeld.<sup>25</sup>

In order to calculate the internal energy from the pair distribution we must, of course, use the temperature-dependent formula (2.11) in the place of (6.32). The calculation of the specific heats of the electron gas and the hard-sphere Bose gas will be reported in a subsequent publication.

As a last application of the present theory, we shall briefly discuss the classical Debye-Huckel equation of state for the electron gas embedded in a uniform background of positive charge. First, we note that our quantum statistical one-body free-particle propagator approaches in the classical limit to the Boltzmann propagator introduced by Montroll and Ward;<sup>3</sup> that is,

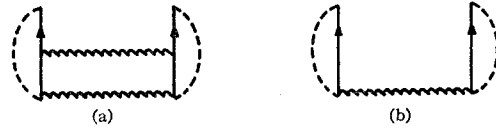


FIG. 10. The diagrams of orders  $a$  and  $a^2$  for the energy. The thin dotted lines mean that the ends of the particle lines should be connected, indicating those integrations completed over the position variables of the ends.

<sup>24</sup> F. London, Proc. Roy. Soc. (London) **153**, 576 (1936); Phys. Rev. **54**, 947 (1938).

<sup>25</sup> A. Sommerfeld and H. Bethe, "Elektronentheorie der Metalle," *Handbuch der Physik* (Springer-Verlag Berlin), Vol. 24, No. 2, p. 346 (1933). Also see, C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York), second edition, p. 256 (1956).

as  $\beta \rightarrow 0$ ,

$$\begin{aligned} K_0(x_2; x_1) &\rightarrow V^{-1} \sum_{\mathbf{p}} \exp[i\mathbf{p} \cdot (\mathbf{r}_2 - \mathbf{r}_1) - \mathbf{p}^2(\beta_2 - \beta_1)] \quad \beta_2 > \beta_1 \\ &\rightarrow 0 \quad \beta_2 < \beta_1. \end{aligned} \quad (8.3)$$

Using this propagator one can calculate the collective interaction and the pair distribution function for the high-temperature dilute electron gas in the same manner as we did for the low-temperature case in Secs. 5 and 6. The same calculation was previously carried out by S. Fujita, A. Isihara, and E. Montroll<sup>26</sup> using the "toron" method. By adopting the simple chain approximation to the collective interaction  $U$ , they obtained the Debye screened Coulomb potential

$$U(r) = e^2 r^{-1} e^{-\kappa r} \quad (8.2)$$

with

$$\kappa \equiv (4\pi\beta n e^2)^{1/2}. \quad (8.3)$$

Up to the first order in the screened Coulomb interaction, the pair distribution function was shown to be

$$n^{(2)}(r) = n^2 (1 - \beta e^2 r^{-1} e^{-\kappa r}) \quad \text{for large } r. \quad (8.4)$$

As an application of the formula (2.15), we shall derive the equation of state from this pair distribution function. The kinetic energy  $E_0$  of the free-particle system is  $\frac{3}{2} N k T$ . The square of the electronic charge  $e$  may be regarded as the coupling parameter. Then we have

$$\begin{aligned} \frac{pV}{N} &= \frac{3}{2} k T - \frac{1}{6N} e^2 \int d^3r \frac{1}{r} n^2 \left( 1 - \beta \frac{e^2}{r} e^{-\kappa r} \right) + \frac{1}{3N} \int_0^{\epsilon^2} d(\epsilon'^2) \int d^3r \frac{1}{r} \frac{\partial}{\partial \beta} \left[ n^2 \left( 1 - \beta \frac{e^2}{r} e^{-\kappa r} \right) \right] \\ &= k T \left( 1 - \frac{1}{3} \pi^{1/2} n^{1/2} \beta^{1/2} e^3 \right) + (\text{the term which cancels with the contribution from the background}). \end{aligned} \quad (8.5)$$

This is the classical Debye-Huckel equation of state.

#### APPENDIX A. MOMENTUM REPRESENTATION OF THE ONE-BODY FREE-PARTICLE PROPAGATOR

The equivalence between the two expressions (4.9) and (4.12) for the one-body free-particle propagator will be shown by carrying out the summation over  $s$  indicated in the latter. Comparison of these two expressions requires showing that

$$\begin{aligned} \beta^{-1} \sum_{n=-\infty}^{+\infty} \exp[-\alpha(\beta_2 - \beta_1)\beta^{-1} + i(2n + \epsilon)(\beta_2 - \beta_1)\pi/\beta] [i(2n + \epsilon)\pi\beta^{-1} + \mathbf{p}^2 - \alpha/\beta]^{-1} \\ = [1 \mp \exp(\alpha - \beta \mathbf{p}^2)]^{-1} \exp[-\mathbf{p}^2(\beta_2 - \beta_1)] \quad \beta_2 > \beta_1 \\ = \pm \exp(\alpha - \beta \mathbf{p}^2) [1 \mp \exp(\alpha - \beta \mathbf{p}^2)] \exp[-\mathbf{p}^2(\beta_2 - \beta_1)] \quad \beta_2 < \beta_1, \end{aligned} \quad (A.1)$$

where  $\epsilon$  is to be taken as 0 for a Boson and 1 for a Fermion. The summation on the left-hand side can be calculated in a straightforward manner by employing Poisson's sum formula.<sup>27</sup> The formula states that

$$\beta^{-1} \sum_{n=-\infty}^{+\infty} f\left(\frac{2n\pi}{\beta}\right) = (2\pi)^{-1/2} \sum_{m=-\infty}^{+\infty} F(\beta m), \quad (A.2)$$

where the function  $F$  is the Fourier inverse of  $f$ :

$$F(x) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} dy e^{-iuy} f(y). \quad (A.3)$$

In order to apply this formula to the summation in question one has to calculate the Fourier inverse of a function:

$$f(y) = \exp[-\alpha(\beta_2 - \beta_1)\beta^{-1} + i\epsilon\pi(\beta_2 - \beta_1)/\beta] \exp[iy(\beta_2 - \beta_1)] [iy + \mathbf{p}^2 - (\alpha/\beta) + i\epsilon\pi/\beta]^{-1}. \quad (A.4)$$

This is readily evaluated by using Cauchy's integral theorem. Noting that the only pole of the integrand is located at  $y = i(\mathbf{p}^2 - \alpha/\beta) - \epsilon\pi/\beta$  and choosing the appropriate contour of integration, one finds aside from the constant factor

$$\begin{aligned} \int_{-\infty}^{+\infty} dy \frac{\exp[iy(\beta_2 - \beta_1 - x)]}{iy + \mathbf{p}^2 - (\alpha/\beta) + i\epsilon\pi/\beta} &= 2\pi \exp\{- (\beta_2 - \beta_1 - x)[\mathbf{p}^2 - (\alpha/\beta) + i\epsilon\pi/\beta]\} \quad \beta_2 - \beta_1 - x > 0 \\ &= 0 \quad \beta_2 - \beta_1 - x < 0 \end{aligned} \quad (A.5)$$

<sup>26</sup> S. Fujita, A. Isihara, and E. Montroll, *Bull. classe sci. Acad. roy. belg.* 44, 1080 (1958).

<sup>27</sup> P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 467.

when

$$\mathbf{p}^2 - \alpha/\beta > 0. \quad (\text{A.6})$$

If  $\mathbf{p}^2 - \alpha/\beta < 0$ , then the integration (A.5) is replaced by

$$\begin{aligned} \int_{-\infty}^{+\infty} dy \frac{\exp[iy(\beta_2 - \beta_1 - x)]}{iy + \mathbf{p}^2 - (\alpha/\beta) + i\epsilon\pi/\beta} &= 0 & \beta_2 - \beta_1 - x > 0 \\ &= -2\pi \exp\{-(\beta_2 - \beta_1 - x)[\mathbf{p}^2 - (\alpha/\beta) + i\epsilon\pi/\beta]\} & \beta_2 - \beta_1 - x < 0. \end{aligned} \quad (\text{A.7})$$

However, it turns out that both cases lead to the identical result (A.1) eventually. Hence we shall give here only the proof of (A.1) when  $\mathbf{p}^2 - \alpha/\beta > 0$ . The proof of the other case can be done in a similar manner.

From (A.4) and (A.5) one sees that

$$\begin{aligned} F(\beta m) &= (2\pi)^{\frac{1}{2}} \exp[-\alpha(\beta_2 - \beta_1)\beta^{-1} + i\epsilon(\beta_2 - \beta_1)\pi/\beta] \exp\{-(\beta_2 - \beta_1 - \beta m)[\mathbf{p}^2 - (\alpha/\beta) + i\epsilon\pi/\beta]\} \\ &= 0 \quad \beta_2 - \beta_1 - \beta m < 0 \end{aligned} \quad (\text{A.8})$$

since  $\beta_1$  and  $\beta_2$  are restricted to the interval  $(0, \beta)$ ,  $|\beta_2 - \beta_1| \leq \beta$ . Summing  $F$  over  $m$ , one gets for the right-hand side of (A.2)

$$(2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{+\infty} F(\beta m) = \begin{cases} \exp[-(\beta_2 - \beta_1)\mathbf{p}^2] \sum_{m=-\infty}^0 \exp(i\epsilon\pi m) \exp[(\alpha - \beta\mathbf{p}^2)m] & \beta_2 > \beta_1 \\ \exp[-(\beta_2 - \beta_1)\mathbf{p}^2] \sum_{m=-\infty}^{-1} \exp(i\epsilon\pi m) \exp[(\alpha - \beta\mathbf{p}^2)m] & \beta_2 < \beta_1. \end{cases} \quad (\text{A.9})$$

Noting that

$$\begin{aligned} e^{i\epsilon\pi m} &= (+1)^m \quad \epsilon = 0 \\ &= (-1)^m \quad \epsilon = 1, \end{aligned} \quad (\text{A.10})$$

one finally obtains

$$\begin{aligned} (2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{+\infty} F(\beta m) &= \exp[-(\beta_2 - \beta_1)\mathbf{p}^2] [1 \mp \exp(\alpha - \beta\mathbf{p}^2)]^{-1} \quad \beta_2 > \beta_1 \\ &= \pm \exp[-(\beta_2 - \beta_1)\mathbf{p}^2] \exp(\alpha - \beta\mathbf{p}^2) [1 \mp \exp(\alpha - \beta\mathbf{p}^2)]^{-1} \quad \beta_2 < \beta_1. \end{aligned} \quad (\text{A.11})$$

This establishes a proof of (A.1) when  $\mathbf{p}^2 - \alpha/\beta > 0$ .

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