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Degenerate Bose System. III. Dilute Gas of Hard Spheres*

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The general formalism developed in the preceding two papers of this series is applied to the dilute gas of Bose hard spheres. The well-known results of Lee, Huang, and Yang for the ground state of this model gas are duplicated. The possibility of including a weak attraction in addition to the repulsive cores is considered, and it is shown that the simple scattering length approximation is valid for positive scattering lengths.

1. INTRODUCTION

IN the preceding two papers of this series,[1,2] we have developed a general quantum statistical theory of the degenerate Bose system. This work extended the x-ensemble formulation of quantum statistics, developed by Lee and Yang[3] for the theoretical study of a Bose system in which a single quantum state is macroscopically occupied. The single quantum state for a Bose system at rest is the lowest, or zero-momentum state and the quantity x is the density of zero-momentum particles.

In the present paper, our goal is to apply the general result of our previous papers to a specific and well-known problem. This is the dilute Bose gas of hard spheres. Although Secs. 2 and 3 of this paper are valid for all temperatures T, our principal objective is to duplicate the ground-state ($T=0$) results of Lee, Huang, and Yang.[4,5] One may inquire, of course, as to the value of studying this model. One answer is that the problem that is of great interest is liquid helium II, and helium atoms have repulsive cores due to their electronic structure. Moreover, London[6] has shown that the consideration of these repulsive cores is essential to the microscopic understanding of helium II. The other answer is that this simplified model is of great value for investigating the details of the general theory, before proceeding to apply the theory to helium II. Thus, the object of this paper is not so much to reproduce well-known results, but to show how these results may be derived from our theory. A general theory is not of value until it can be shown that it is "usable." This is particularly true of a new and difficult theory, such as the one which we are using.

It is to be emphasized that the theory which we apply here is not restricted to the imperfect Bose gas, or to the dilute hard-sphere Bose gas. It is just as applicable to the helium II problem as it is to the low-density Bose hard-sphere gas. Thus, in Sec. 2, where we derive the first-order expression for the quasiparticle energies $\epsilon_+(\mathbf{k})$ and $\epsilon_-(\mathbf{k})$ for a Bose hard-sphere gas, we have in mind that the corresponding derivation for helium II will only require a simple generalization of this derivation. Similarly, in the determination of the important functions $A_i^{(<)}(t,\mathbf{k})$, $A_i^{(>)}(t,\mathbf{k})$, and $\zeta(t,\mathbf{k})$, we have in mind that these functions can be determined for helium II in analogy with the procedure of Sec. 2. In fact, in Sec. 7 we indicate these generalizations quite explicitly.

Section 3 is devoted to the rather simple calculation of the functions $N_{\mu,\nu}'$, which give the dominant contribution of the Bose statistics to the line factors $\mathcal{G}_{\mu,\nu}'$ of the theory. Then, in Sec. 4, the zero-momentum self-energy quantity $\Delta^{(0)}$ is calculated to first order for the ground-state problem, and discussed for general T. It is found that at $T=0$ the $N_{\mu,\nu}'$ do not contribute to $\Delta^{(0)}$, in keeping with the general belief that the ground state of a Bose gas is the same as the ground state of a Boltzmann gas.[7]

In Sec. 5 the Lee, Huang, Yang expression for the ground-state energy of a dilute hard-sphere Bose gas is derived. In this calculation, the assumption that the chemical potential $g=-\Delta^{(0)}$, made at the beginning of Sec. 2, is shown to be correct. For the ground state, this checks our interpretation that $-\Delta^{(0)}$ is the energy per particle of the zero-momentum superfluid. As expected, we find that the $N_{\mu,\nu}'$ do not contribute to the ground-state energy.

The Lee, Huang, Yang expressions for the momentum distribution and the pair-distribution function are derived in Sec. 6. One interesting point here is that the very low-momentum behavior of the momentum distribution for $T\neq 0$ is found to vary as p^{-2}. This result is not predicted by the Lee, Huang, Yang expression, because their expression is only valid for all $\mathbf{p}$ in the *limit* $T\to 0$.

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[1] F. Mohling, Phys. Rev. **135**, A831 (1964). Hereafter referred to as MI.

[2] F. Mohling, Phys. Rev. **135**, A855 (1964). Hereafter referred to as MII.

[3] T. D. Lee and C. N. Yang, Phys. Rev. **117**, 897 (1960).

[4] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957). See also T. D. Lee and C. N. Yang, *ibid.* **112**, 1419 (1958).

[5] Elliott H. Lieb, Phys. Rev. **130**, 2518 (1963), has given a review of the imperfect Bose gas problem, as well as an independent derivation of the Lee, Huang, Yang ground-state energy expression for the hard-sphere Bose gas.

[6] F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II, pp. 30–35.

[7] See footnote 15 of Ref. 5.

$$\mathcal{K}'_{1,1}(t_2,t_1,k)=\mathcal{K}'_{1,1}(t_2,t_1,k)_0+\mathcal{K}'_{1,1}(t_2,t_1,k)_1+\mathcal{K}'_{1,1}(t_2,t_1,k)_2+\cdots$$

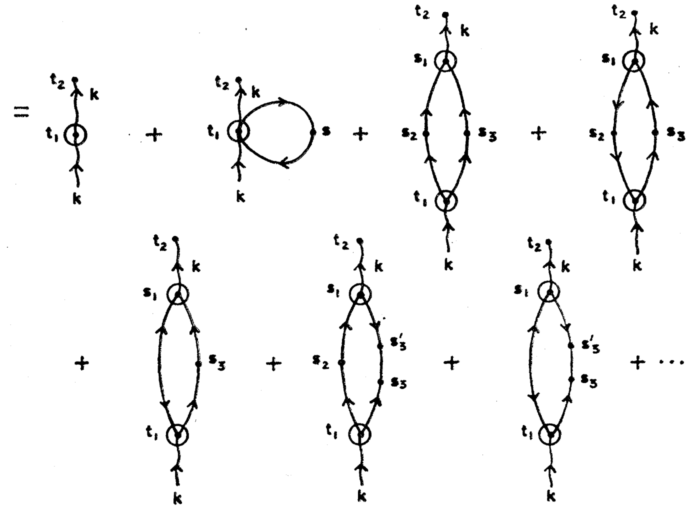

FIG. 1. The graphical expansion of $\mathcal{K}_{1,1}'(t_2,t_1,\mathbf{k})$, with the single first-order and the six second-order transformed master (1,1) L graphs shown explicitly. The graphical notation is that of MI. The symmetry number of each of the graphs shown is 1 except that of the third graph, which is 2.

The question of short-range attractive interactions outside of the repulsive cores is examined in Sec. 7. It is shown that the simple replacement $a\rightarrow a_s$, where a is the hard-sphere diameter and a_s is the two-particle interaction scattering length, is correct provided that $a_s>0$. For a negative scattering length the system collapses, thereby invalidating the low-density approximation which has been made.

The interpretation of the double quasiparticle spectrum, $\epsilon_+(\mathbf{k})$ and $\epsilon_-(\mathbf{k})$, is not considered in this paper. This interesting consequence of the theory[8] is left as a subject for further investigation. The understanding of the nonzero temperature behavior of a dilute Bose gas[4] has also been left for further study. Finally, it should be emphasized that although we believe that the generalization of the present calculation to helium II is straightforward, it nevertheless remains to be done. In particular, the physical interpretation of the results of such

$$\mathcal{K}'_{0,2}(t_2,t_1,k)=\mathcal{K}'_{0,2}(t_2,t_1,k)_0+\mathcal{K}'_{0,2}(t_2,t_1,k)_1+\mathcal{K}'_{0,2}(t_2,t_1,k)_2+\cdots$$

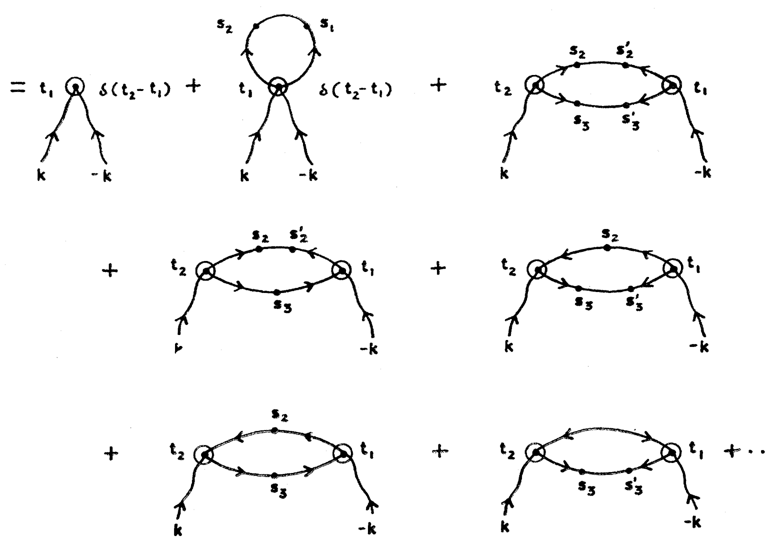

FIG. 2. The graphical expansion of $\mathcal{K}_{0,2}'(t_2,t_1,\mathbf{k})$, with the single first-order and the six second-order transformed master (0,2) L graphs shown explicitly. The graphical notation is that of MI. The symmetry numbers of the second and third graphs are each 2, and the symmetry number of each of the remaining graphs shown is 1. The first two graphs contribute to the function $K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})$, in which case the external lines are free-particle lines.

[8] The possibility of a double quasiparticle spectrum has previously been suggested by Elliot H. Lieb and Werner Liniger, Phys. Rev. **130**, 1605 (1963); Elliot H. Lieb, *ibid.* **130**, 1616 (1963).

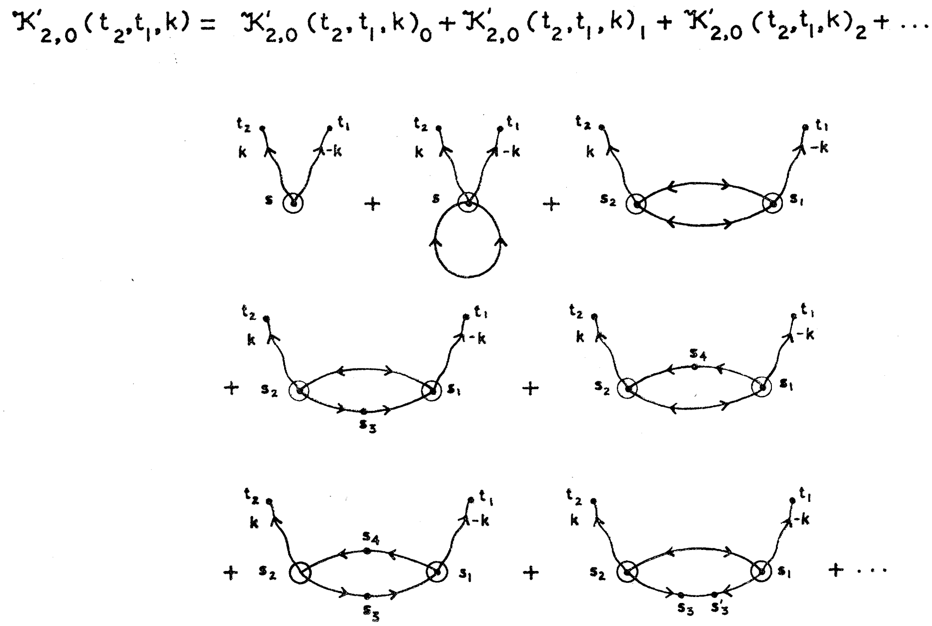

FIG. 3. The graphical expansion of $\mathcal{K}_{2,0}'(t_2,t_1,\mathbf{k})$, with the single first-order and the six second-order transformed master (2,0) L graphs shown explicitly. The graphical notation is that of MI. The symmetry numbers of the second and third graphs are each 2, and the symmetry number of each of the remaining graphs shown is 1. The first two graphs contribute to the function $K_{2,0}{}^{(1)\prime}(t_2,t_1,\mathbf{k})$, in which case the external lines are free-particle lines.

a calculation in terms of a simple quasiparticle model, and the correlation of this interpretation with the existing macroscopic theories are questions which we have not even touched upon in this paper.

2. FIRST-ORDER CALCULATION OF ε_+ AND ε_-

The first quantities which must be calculated in any application of the transformed theory of MII are the functions $\mathcal{K}_{\mu,\nu}'(t_2,t_1,\mathbf{k})$, where $\mu+\nu=2$. In Figs. 1–3, we show the graphical expansion of these three functions, using the graphical notation of MI. It is to be noted that in each case there is one first-order transformed master (μ,ν) L graph and six second-order graphs. The *order* of a graph is henceforth defined to be the number of independent momenta in the graph instead of the number of cluster vertices. The reason for this change in nomenclature is that for the dilute Bose gas of hard spheres each order of graphs then corresponds for $T\to 0$ to an extra power of $(na^3)^{1/2}$ in the power-series expansion of the function being considered. [This statement is based on a dimensional argument and it does not take into account logarithmic dependences on the parameter $(na^3)^{1/2}$.]

In this paper we shall only be interested in the first-order calculation of the functions $\mathcal{K}_{\mu,\nu}'(t_2,t_1,\mathbf{k})$. From Figs. 1–3 and Sec. V of MII we find for the first-order terms $\mathcal{K}_{\mu,\nu}'(t_2,t_1,\mathbf{k})_0$ the expressions

$$\mathcal{K}_{1,1}'(t_2,t_1,\mathbf{k})_0=[(1+B^{(0)})x\Omega\exp\beta(g+\Delta^{(0)})]\int_0^\beta ds\, G_{\text{out}}'(s)\;{}^{t_2 s}\!\begin{bmatrix}\mathbf{k} & 0\\ \mathbf{k} & 0\end{bmatrix}'_{t_1} G_{\text{in}}'(t_1)\,,$$

$$\mathcal{K}_{0,2}'(t_2,t_1,\mathbf{k})_0=\tfrac{1}{2}[x\Omega\exp2\beta(g+\Delta^{(0)})]\int_0^\beta ds_1ds_2G_{\text{out}}'(s_1)G_{\text{out}}'(s_2)\;{}^{s_2s_1}\!\begin{bmatrix}0 & 0\\ \mathbf{k} & -\mathbf{k}\end{bmatrix}'_{t_1}\delta(t_2-t_1)\,,\tag{1}$$

$$\mathcal{K}_{2,0}'(t_2,t_1,\mathbf{k})_0=\tfrac{1}{2}[(1+B^{(0)})^2x\Omega]\int_0^\beta ds\;{}^{t_1t_2}\!\begin{bmatrix}\mathbf{k} & -\mathbf{k}\\ 0 & 0\end{bmatrix}'_{s}[G_{\text{in}}'(s)]^2.$$

In these expressions we shall immediately make the approximations $B^{(0)}=0$, $G_{\text{in}}'(s)=1$, and $G_{\text{out}}'(s)=\delta(\beta-s)$. These approximations correspond to the neglect of higher order terms in the parameter $(na^3)^{1/2}$. Moreover, we shall henceforth adopt the assumption of Eq. (115) in MII that

$$g=-\Delta^{(0)}.\tag{2}$$

This assumption can always be checked by comparing the calculation of $\Delta^{(0)}$ (Sec. 4) with the final thermodynamic expressions for the system (Sec. 5). The assumption is based on our interpretation of $-\Delta^{(0)}$ as the self-energy per particle of the zero-momentum superfluid of the system. With the aid of this assumption, the above approximations, and Eqs. (41), (43), (44), (48), and (49) of MII, the functions $\mathcal{K}_{\mu,\nu}'(t_2,t_1,\mathbf{k})_0$ of Eqs. (1) can be rewritten as

$$\mathcal{K}_{1,1}'(t_2,t_1,\mathbf{k})_0 \cong (x\Omega)\zeta^{-1}(t_2,\mathbf{k})\zeta(t_1,\mathbf{k}) \sum_{i=+,-} i\Bigg[A_i^{(<)}(t_2,\mathbf{k}) \Bigg\{ {}^{\beta}_{(i,0)}\begin{bmatrix} \mathbf{k} & 0 \\ \mathbf{k} & 0 \end{bmatrix}'_{t_1} - \theta(t_2-t_1)\, {}^{t_2}_{(i,0)}\begin{bmatrix} \mathbf{k} & 0 \\ \mathbf{k} & 0 \end{bmatrix}'_{t_1} \Bigg\} + A_i^{(>)}(t_2,\mathbf{k})\, {}^{t_2}_{(i,0)}\begin{bmatrix} \mathbf{k} & 0 \\ \mathbf{k} & 0 \end{bmatrix}'_{t_1} \theta(t_2-t_1) \Bigg], \quad (3)$$

$$\mathcal{K}_{0,2}'(t_2,t_1,\mathbf{k})_0 \cong \tfrac{1}{2}(x\Omega)\zeta(t_1,\mathbf{k}) \exp[-t_1\epsilon_1(-\mathbf{k})]\delta(t_2-t_1)\, {}^{\beta}_{(0,0)}\begin{bmatrix} 0 & 0 \\ \mathbf{k} & -\mathbf{k} \end{bmatrix}'_{t_1}, \quad (4)$$

$$\mathcal{K}_{2,0}'(t_2,t_1,\mathbf{k})_0 \cong \tfrac{1}{2}(x\Omega)\zeta^{-1}(t_2,\mathbf{k}) \int_0^{t_1} ds \sum_{i=+,-} i\Bigg[A_i^{(<)}(t_2,\mathbf{k}) \Bigg\{ {}^{t_1}_{(i,1)}\begin{bmatrix} \mathbf{k} & -\mathbf{k} \\ 0 & 0 \end{bmatrix}'_{s} - {}^{t_2}_{(i,1)}\begin{bmatrix} \mathbf{k} & -\mathbf{k} \\ 0 & 0 \end{bmatrix}'_{s} \theta(t_2-s) \Bigg\} \theta(t_1-t_2) + A_i^{(>)}(t_2,\mathbf{k}) \Bigg\{ {}^{t_2}_{(i,1)}\begin{bmatrix} \mathbf{k} & -\mathbf{k} \\ 0 & 0 \end{bmatrix}'_{s} \theta(t_1-t_2) + {}^{t_1}_{(i,1)}\begin{bmatrix} \mathbf{k} & -\mathbf{k} \\ 0 & 0 \end{bmatrix}'_{s} \theta(t_2-t_1) \Bigg\} \theta(t_2-s) \Bigg]. \quad (5)$$

The primed pair functions in these expressions are given by Eqs. (38)–(40) of MII. The subscript (0) refers to the zero-momentum energy $\epsilon_0 \equiv 0$, and its associated transformation functions. The subscript (1) refers to the energy

$$\epsilon_1(-\mathbf{k}) = \epsilon(-\mathbf{k}) - \Delta^{(1)}(-\mathbf{k}), \qquad \epsilon(\mathbf{k}) = \omega(\mathbf{k}) + \Delta^{(0)}, \quad \omega(\mathbf{k}) = \hbar^2k^2/2M, \quad (6)$$

and its associated $(-\mathbf{k})$ transformation functions [see above Eq. (66) in MII]. In this connection, we shall also set the function $B^{(1)}(-\mathbf{k}) = 0$ in the low-order calculations of this paper.

We shall also require the first-order calculation of the function $\mathcal{K}_{1,1}^{(1)\prime}(t_2,t_1-\mathbf{k})$ which, according to Eqs. (78), (48), and (49) in MII and Eq. (3), is given by

$$\mathcal{K}_{1,1}^{(1)\prime}(t_2,\, t_1,\, -\mathbf{k})_0 \cong (x\Omega) \times \exp[-t_1\epsilon_1(-\mathbf{k})]\, {}^{t_2}_{(1,0)}\begin{bmatrix} \mathbf{k} & 0 \\ \mathbf{k} & 0 \end{bmatrix}'_{t_1} \theta(t_2-t_1). \quad (7)$$

Similarly, we shall require the functions $K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})$ and $K_{2,0}^{(1)\prime}(t_2,t_1,\mathbf{k})$, which according to Figs. 2 and 3, and Eqs. (83) and (84) in MII, are given to first order by

$$K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})_0 \cong \tfrac{1}{2}(x\Omega) \exp(-t_1[\epsilon(\mathbf{k})+\epsilon(-\mathbf{k})]) \times \delta(t_2-t_1)\, {}^{\beta}_{(0,0)}\begin{bmatrix} 0 & 0 \\ \mathbf{k} & -\mathbf{k} \end{bmatrix}'_{t_1}, \quad (8)$$

$$K_{2,0}^{(1)\prime}(t_1,t_1,\mathbf{k})_0 \cong \tfrac{1}{2}(x\Omega) \int_0^{t_1} ds\, {}^{t_1}\begin{bmatrix} \mathbf{k} & -\mathbf{k} \\ 0 & 0 \end{bmatrix}_{s} \times \exp[2s\Delta^{(0)}]. \quad (9)$$

In Eq. (9), only the unprimed pair function of Eq. (6) in MII appears, and we have set $t_2 = t_1$, since this is the only case of interest for this function.

We now make the low-temperature, low-density approximations of this paper,

$$na^3 \ll 1, \quad a \ll \lambda_T, \quad (10)$$

where the thermal wavelength λ_T is defined by

$$\lambda_T = (2\pi\hbar^2\beta/M)^{1/2}, \quad (11)$$

n is the density of bosons in the system, and a is the diameter of a Bose hard-sphere atom. We then observe that the momenta of interest satisfy the inequality

$$ka \ll 1, \quad (10')$$

because the momenta are determined by the parameters of the problem to be $\lesssim \hbar/\lambda_T$ and $\lesssim \hbar(na)^{1/2}$. These last two quantities are found to govern the cutoffs of momentum integrals. It can also be seen why it is a good approximation to set the quantities $B(\mathbf{k})$, $B^{(1)}(\mathbf{k})$, and $B^{(0)}$ each equal to zero, for a dilute gas. These quantities enter into the theory as correction terms when one makes the mathematical idealization that there exist infinite repulsions between the Bose atoms.[9] (The atoms are then *hard* spheres.) The correction terms are called excluded volume terms, because they give the correction effect due to the finite size of the hard spheres on the size of the volume Ω in which the particles are moving. They give contributions which are at most $\sim(na^3)$ times the quantities which we shall calculate in this paper for the Bose hard-sphere gas.

With the aid of the approximation (10′), we may write down a greatly simplified expression for the pair functions which enter into Eqs. (3)–(9). For the primed pair function we use Eqs. (6), (38), and (39) in MII together with the explicit expression derived in Ref. 9 for the untransformed pair function. This yields the

[9] F. Mohling, Phys. Rev. **122**, 1043 (1961).

approximate expression, for a hard-sphere interaction,

$$\left[\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{matrix}\right]'^{\,t_2}_{(i,j)\,t_1} \cong -\Omega^{-1}(2\pi)^3(\hbar^2a/M\pi^2)\delta(\mathbf{k}_1+\mathbf{k}_2,\,\mathbf{k}_3+\mathbf{k}_4)\exp t_1[\epsilon_i(\mathbf{k}_1)+\epsilon_j(\mathbf{k}_2)]$$
$$\times\Big\{1-\Omega^{-1}(2\pi)^3(\hbar^2a/2M\pi^2)\sum_{\mathbf{k}_5\mathbf{k}_6}\delta(\mathbf{k}_1+\mathbf{k}_2,\,\mathbf{k}_5+\mathbf{k}_6)$$
$$\times P\left(\frac{1}{\epsilon_i(\mathbf{k}_1)+\epsilon_j(\mathbf{k}_2)-\epsilon(\mathbf{k}_5)-\epsilon(\mathbf{k}_6)}\right)\exp(t_2-t_1)[\epsilon_i(\mathbf{k}_1)+\epsilon_j(\mathbf{k}_2)-\epsilon(\mathbf{k}_5)-\epsilon(\mathbf{k}_6)]\Big\}\,, \quad (12)$$

where the factor $\delta(\mathbf{k}_i,\mathbf{k}_j)$ is a Kronecker δ function. The corresponding expression for the untransformed pair function, omitting the second term, is

$$\left[\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{matrix}\right]^{t_2}_{t_1} \cong -\Omega^{-1}(2\pi)^3(\hbar^2a/M\pi^2)\delta(\mathbf{k}_1+\mathbf{k}_2,\,\mathbf{k}_3+\mathbf{k}_4)\exp t_1[\omega(\mathbf{k}_1)+\omega(\mathbf{k}_2)-\omega(\mathbf{k}_3)-\omega(\mathbf{k}_4)]. \quad (12')$$

The second $O(a^2)$ term of (12) will be required in Secs. 4 and 5, but not at present.

Upon substituting the expressions (12) and (12′) into Eqs. (3)–(9), one obtains the following "first-order" functions:

$$\mathcal{K}_{1,1}'(t_2,t_1,\mathbf{k})_0 \cong -(W\xi)\zeta^{-1}(t_2,\mathbf{k})\zeta(t_1,\mathbf{k})\sum_{i=+,-} i\exp[t_1\epsilon_i(\mathbf{k})][A_i^{(<)}(t_2,\mathbf{k})\theta(t_1-t_2)+A_i^{(>)}(t_2,\mathbf{k})\theta(t_2-t_1)]\,, \quad (3a)$$

$$\mathcal{K}_{0,2}'(t_2,t_1,\mathbf{k})_0 \cong -\tfrac{1}{2}(W\xi)\zeta(t_1,\mathbf{k})\exp[-t_1\epsilon_1(-\mathbf{k})]\delta(t_2-t_1)\,, \quad (4a)$$

$$\mathcal{K}_{2,0}'(t_2,t_1,\mathbf{k})_0 \cong -\tfrac{1}{2}(W\xi)\zeta^{-1}(t_2,\mathbf{k})\sum_{i=+,-} iP\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)$$
$$\times\{A_i^{(<)}(t_2,\mathbf{k})[\exp t_1(\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k}))-\exp t_2(\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k}))]\theta(t_1-t_2)$$
$$+A_i^{(>)}(t_2,\mathbf{k})[\exp t_2(\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k}))-1]\theta(t_1-t_2)$$
$$+A_i^{(>)}(t_2,\mathbf{k})[\exp t_1(\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k}))-1]\theta(t_2-t_1)\}\,, \quad (5a)$$

$$\mathcal{K}_{1,1}^{(1)\prime}(t_2,\,t_1,\,-\mathbf{k})_0 \cong -(W\xi)\theta(t_2-t_1)\,, \quad (7a)$$

$$K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})_0 \cong -\tfrac{1}{2}(W\xi)\exp(-t_1[\epsilon(\mathbf{k})+\epsilon(-\mathbf{k})])\delta(t_2-t_1)\,, \quad (8a)$$

$$K_{2,0}^{(1)\prime}(t_2,t_1,\mathbf{k})_0 \cong -\tfrac{1}{2}(W\xi)P\left(\frac{1}{\epsilon(\mathbf{k})+\epsilon(-\mathbf{k})}\right)[\exp t_1[\epsilon(\mathbf{k})+\epsilon(-\mathbf{k})]-1]\,, \quad (9a)$$

where the energy W is defined by

$$W=8\pi\hbar^2na/M\,, \quad (13)$$

and the quantity ξ is the fractional occupation of the zero-momentum state;

$$\xi=x/n\,. \quad (14)$$

We can now derive our first result from the Λ-transformation equations. Upon comparing Eq. (7a) with Eqs. (70) and (72) in MII, we find that

$$\Delta^{(1)}(-\mathbf{k})=-W\xi[1+O(a/\lambda_T)+O(na^3)^{1/2}]\,, \quad (15)$$

$$K_{1,1}^{(1)\prime}(t_2,\,t_1,\,-\mathbf{k})\cong 0\,. \quad (16)$$

Thus, there is no first-order contribution to the function $K_{1,1}^{(1)\prime}$, and from Eqs. (67) and (69) in MII we may set $G_{1,1}^{(1)\prime}(t_2,\,t_1,\,-\mathbf{k})\cong\delta(t_2-t_1)$. From Eq. (15) we see that $\Delta^{(1)}$ is independent of momentum to first approximation. The estimate of the correction terms in (15) is based on the statement about the orders of graphs in the first paragraph of this section.

Using the above result, we next write down the function $\mathcal{P}'(t_2,t_1,\mathbf{k})$ of Eq. (74) in MII. To first order, this function is

$$\mathcal{P}'(t_2,t_1,\mathbf{k})\cong\mathcal{K}_{1,1}'(t_2,t_1,\mathbf{k})_0+\int_0^\beta ds\mathcal{K}_{2,0}'(t_2,s,\mathbf{k})_0\mathcal{K}_{0,2}'(t_1,s,\mathbf{k})_0$$

$$\cong\zeta^{-1}(t_2,\mathbf{k})\zeta(t_1,\mathbf{k})\sum_{i=+,-} i\Big\{\exp t_1\epsilon_i(\mathbf{k})[A_i^{(<)}(t_2,\mathbf{k})\theta(t_1-t_2)+A_i^{(>)}(t_2,\mathbf{k})\theta(t_2-t_1)]$$

$$\times\left[-W\xi+(W\xi/2)^2P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)\right]+(W\xi/2)^2P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)\exp[(t_2-t_1)\epsilon_1(-\mathbf{k})+t_2\epsilon_i(\mathbf{k})]$$

$$\times[A_i^{(>)}(t_2,\mathbf{k})-A_i^{(<)}(t_2,\mathbf{k})]\theta(t_1-t_2)-(W\xi/2)^2P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)\exp[-t_1\epsilon_1(-\mathbf{k})]A_i^{(>)}(t_2,\mathbf{k})\Big\}\,, \quad (17)$$

where we have used Eqs. (3a)–(5a) to obtain the second line of this expression. We next wish to identify terms of the form

$$\Lambda(t_2,t_1,\mathbf{k})=\zeta^{-1}(t_2,\mathbf{k})\zeta(t_1,\mathbf{k})\sum_{i=+,-} i\Delta_i(\mathbf{k})\exp[t_1\epsilon_i(\mathbf{k})][A_i^{(<)}(t_2,\mathbf{k})\theta(t_1-t_2)+A_i^{(>)}(t_2,\mathbf{k})\theta(t_2-t_1)] \quad (18)$$

in $\mathcal{P}'(t_2,t_1,\mathbf{k})$, where the form of this function is given by Eq. (51) in MII. This can be done if we set

$$\Delta_i(\mathbf{k})=-W\xi+(W\xi/2)^2P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right). \quad (19)$$

Equation (19) determines the quantities $\Delta_i(\mathbf{k})$. Moreover, in order to insure that $\mathcal{P}'(t_2,t_1,\mathbf{k})$ will not lead to exponentially large terms when it is substituted into the basic integral equation (59) in MII of the theory (see also Sec. 2 of MII), we must set the coefficients of $\exp(t_2-t_1)\epsilon_1(-\mathbf{k})$ and $\exp[-t_1\epsilon_1(-\mathbf{k})]$ in Eq. (17) equal to zero. This results in two indentities for the determination of the $A_i^{(<)}$ and $A_i^{(>)}$, which are

$$\sum_{i=+,-} i\exp[t_2\epsilon_i(\mathbf{k})]P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)\times[A_i^{(>)}(t_2,\mathbf{k})-A_i^{(<)}(t_2,\mathbf{k})]=0, \quad (20)$$

$$\sum_{i=+,-} iP\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)A_i^{(>)}(t_2,\mathbf{k})=0.$$

The remaining two equations for the determination of the $A_i^{(<)}$ and $A_i^{(>)}$ are the *basic* identities (20) and (21) of MII. According to Eqs. (40) and (42) of MII, these two identities can be written as

$$\sum_{i=+,-} i\exp[t_2\epsilon_i(\mathbf{k})][A_i^{(>)}(t_2,\mathbf{k})-A_i^{(<)}(t_2,\mathbf{k})]=1\,,\qquad \sum_{i=+,-} i\exp[\beta\epsilon_i(\mathbf{k})]A_i^{(<)}(t_2,\mathbf{k})=0. \quad (21)$$

The four Eqs. (20) and (21) are completely equivalent to the four Eqs. (127) of MII [see also Eq. (132) of MII]. Therefore, we may immediately write down their solution, as given in Sec. 9 of MII (for the case $\tau=\beta$),

$$A_+^{(<)}(t_2)=(\Delta_--\Delta_+)^{-2}(\epsilon_++\epsilon_1)(\epsilon_-+\epsilon_1)\times\zeta(\beta)e^{\beta\epsilon_-}(e^{-t_2\epsilon_+}-e^{-t_2\epsilon_-})\,,$$

$$A_-^{(<)}(t_2)=(\Delta_--\Delta_+)^{-2}(\epsilon_++\epsilon_1)(\epsilon_-+\epsilon_1)\times\zeta(\beta)e^{\beta\epsilon_+}(e^{-t_2\epsilon_+}-e^{-t_2\epsilon_-})\,, \quad (22)$$

$$A_+^{(>)}(t_2)=(\Delta_--\Delta_+)^{-1}(\epsilon_++\epsilon_1)\zeta(t_2)\,,$$

$$A_-^{(>)}(t_2)=(\Delta_--\Delta_+)^{-1}(\epsilon_-+\epsilon_1)\zeta(t_2)\,,$$

where

$$\zeta(t)=[(\epsilon_++\epsilon_1)e^{\beta\epsilon_+}-(\epsilon_-+\epsilon_1)e^{\beta\epsilon_-}]^{-1}\times[(\epsilon_++\epsilon_1)e^{(\beta-t)\epsilon_+}-(\epsilon_-+\epsilon_1)e^{(\beta-t)\epsilon_-}]$$
$$\underset{t\to\beta}{\longrightarrow}[(\epsilon_++\epsilon_1)e^{\beta\epsilon_+}-(\epsilon_-+\epsilon_1)e^{\beta\epsilon_-}]^{-1}(\Delta_--\Delta_+). \quad (23)$$

In these equations, we have suppressed the $\mathbf{k}$ dependence of the various quantities, for simplicity of notation. In order to insert the momentum dependence into these expressions, one has only to observe that the quantity ϵ_1 is always associated with the momentum $-\mathbf{k}$.

Returning to Eq. (19) for $\Delta_i(\mathbf{k})$, we see that this equation is equivalent to Eqs. (25) and (130) in MII, provided that we set $A=-W\xi$ and $CD=(\xi W/2)^2$. Then, from Eq. (15) and Eqs. (40) and (131) in MII we have for $\epsilon_\pm(\mathbf{k})$

$$\epsilon_\pm(\mathbf{k})=\epsilon(\mathbf{k})-\Delta_\pm(\mathbf{k})=\omega(\mathbf{k})-\Delta_\pm(\mathbf{k})+\Delta^{(0)}=\pm\{[\epsilon(\mathbf{k})+\xi W]^2-(\xi W/2)^2\}^{1/2}. \quad (24)$$

Of course, this result can be derived directly from Eq. (19), but it is valuable to relate the explicit expressions of this paper with the general expressions of MII. By anticipating the result of Sec. 4, that $\Delta^{(0)}=-\frac{1}{2}(\xi W)$ to zeroth order, the expression (24) can be rewritten in the form

$$\epsilon_{\pm}(\mathbf{k})=\pm[\omega(\mathbf{k})(\omega(\mathbf{k})+\xi W)]^{1/2}$$
$$=\pm(\hbar^2/2M)k(k^2+16\pi\xi na)^{1/2}. \qquad (25)$$

This is the well-known result of Lee, Huang, and Yang,[4] except that we have obtained two functions $\epsilon_+(\mathbf{k})$ and $\epsilon_-(\mathbf{k})$ which differ only by a minus sign to first order. From Eqs. (24) and (25), we find for the quantity $(\Delta_- - \Delta_+)$, which enters into Eqs. (22) and (23),

$$[\Delta_-(\mathbf{k})-\Delta_+(\mathbf{k})]=2\epsilon_+(\mathbf{k})$$
$$=(\hbar^2/M)k(k^2+16\pi\xi na)^{1/2}. \qquad (26)$$

We finally return to Eq. (17) for $\mathcal{P}'(t_2,t_1,\mathbf{k})$. Upon comparing this expression with Eqs. (18)–(20) and with Eq. (60) in MII, we see that the function $P'(t_2,t_1,\mathbf{k})$ is zero to first order

$$P'(t_2,t_1,\mathbf{k})\cong 0. \qquad (27)$$

Therefore, according to Eqs. (55) and (59) in MII, we may also make the approximation $G'(t_2,t_1,\mathbf{k})\cong\delta(t_2-t_1)$ to first order.

3. DETERMINATION OF $N_{\mu,\nu}'(\mathrm{p})$

The results of Sec. 2, and in particular of Eqs. (16) and (27), have demonstrated that the transformed integral equations of MII may be solvable by a simple iteration procedure. The iteration procedure is, in fact, the graphical expansion described at the beginning of Sec. 2, and it will be clarified further in the following two sections. The first-order results of Sec. 2 can, therefore, be expected to lead to meaningful expressions for the other quantities of the transformed quantum statistical theory. In this section, we shall use these results to determine the important functions $N_{\mu,\nu}'(\mathbf{p})$.

As was discussed in connection with Eqs. (16) and (27) we may write the functions G' and $G^{(1)\prime}$ as

$$G'(t_2,t_1,\mathbf{k})\cong G^{(1)\prime}(t_2,t_1,\mathbf{k})\cong\delta(t_2-t_1) \qquad (28)$$

to first order. Therefore, the first-order expressions for the functions $L_{0,2}'$ and $L_{2,0}'$, of Eqs. (81) and (82) in MII, are

$$L_{0,2}'(t_2,t_1,\mathbf{k})\cong\mathcal{K}_{0,2}'(t_2,t_1,\mathbf{k})_0-K_{0,2}^{(1)\prime}(t_2,t_1\mathbf{k})_0,$$
$$L_{2,0}'(t_2,t_1,\mathbf{k})\cong\mathcal{K}_{2,0}'(t_2,t_1,\mathbf{k})_0 -\delta(t_2,t_1)K_{2,0}^{(1)\prime}(t_1,t_1,\mathbf{k})_0. \qquad (29)$$

The functions $K_{\mu,\nu}'(\mathbf{p})$ of Eqs. (85) in MII, where $\mathbf{k}\to\mathbf{p}$ when $\mathbf{k}$ cannot be zero, are then obtained by substituting Eqs. (29), along with Eqs. (4a), (5a), and (27).

$$K_{1,1}'(\mathbf{p})\cong 0, \qquad (30)$$

$$K_{0,2}'(\mathbf{p})\cong-\tfrac{1}{2}(W\xi)\int_0^\beta dt\zeta(t,\mathbf{p})\exp[-t\epsilon_1(-\mathbf{p})]$$
$$=-\tfrac{1}{2}(W\xi)[(\epsilon_++\epsilon_1)e^{\beta\epsilon_+}-(\epsilon_-+\epsilon_1)e^{\beta\epsilon_-}]^{-1} \times(e^{\beta\epsilon_+}-e^{\beta\epsilon_-}), \qquad (31)$$

$$K_{2,0}'(\mathbf{p})\cong\mathcal{K}_{2,0}'(\beta,\beta,\mathbf{p})_0$$
$$=-\tfrac{1}{2}(W\xi)(\Delta_--\Delta_+)^{-1}(e^{\beta\epsilon_+}-e^{\beta\epsilon_-})e^{\beta\epsilon_1}. \qquad (32)$$

The second lines of Eqs. (31) and (32) are derived with the aid of Eqs. (22) and (23). As pointed out below Eqs. (85) in MII, the functions $K_{0,2}^{(1)\prime}$ and $K_{2,0}^{(1)\prime}$ do not contribute to $K_{0,2}'(\mathbf{p})$ and $K_{2,0}'(\mathbf{p})$, respectively. The limit $(t_1,t_2)\to\beta$ in Eq. (5a) can be performed by keeping either $t_1<t_2$ or $t_1>t_2$, and either choice leads to the second line of Eq. (32). In order to insert the momentum dependence into the expressions (31) and (32), one has only to observe that the quantity ϵ_1 is always associated with the momentum $-\mathbf{p}$. Of course, the distinction between $\mathbf{p}$ and $-\mathbf{p}$ is unimportant for an isotropic system, which is the case we are concerned with in this paper, and we henceforth drop the distinction. We finally observe that with the aid of Eq. (2), it is a simple matter to verify that Eqs. (31) and (32) satisfy the first of Eqs. (97) in MII.

We now turn our attention to the functions $N_{\mu,\nu}'(\mathbf{p})$. From Eqs. (91), (92) and (97)–(100) in MII, we obtain the following first-order expressions for these functions.

$$N_{1,1}'(\mathbf{p})=\nu'(\mathbf{p})\{1-[1+\nu'(\mathbf{p})]^2[K_{0,2}'(\mathbf{p})]^2\}^{-1}, \qquad (33)$$

$$N_{0,2}'(\mathbf{p})=\nu'(\mathbf{p})[1+\nu'(\mathbf{p})]K_{0,2}'(\mathbf{p})e^{-\beta\epsilon_1(\mathbf{p})} \times\{1-[1+\nu'(\mathbf{p})]^2[K_{0,2}'(\mathbf{p})]^2\}^{-1}, \qquad (34)$$

$$N_{2,0}'(\mathbf{p})=[1+\nu'(\mathbf{p})]^2K_{0,2}'(\mathbf{p}) \times\{1-[1+\nu'(\mathbf{p})]^2[K_{0,2}'(\mathbf{p})]^2\}^{-1}, \qquad (35)$$

where

$$\nu'(\mathbf{p})=\zeta(\beta,\mathbf{p})[1-\zeta(\beta,\mathbf{p})]^{-1}, \qquad (36)$$

These equations will be of value in the subsequent calculations of this paper.

The zero-momentum behavior of the $N_{\mu,\nu}'(\mathbf{p})$ is subject to the theorems of Eqs. (101) in MII. The simplest way to show that our first-order results are in agreement with these theorems is to check the first of Eqs. (102) in MII, which is equivalent to these theorems. Thus, one finds from Eqs. (30)–(32), (36), (25), and (26) that

$$\lim_{\mathbf{p}\to0}[\nu'(\mathbf{p})]^{-1}=-\lim_{\mathbf{p}\to0}[\zeta^{-1}(\beta,\mathbf{p})K_{0,2}'(\mathbf{p})]$$
$$=\tfrac{1}{2}\beta W\xi \quad \text{Q.E.D.} \qquad (37)$$

4. FIRST-ORDER CALCULATION OF $\Delta^{(0)}$

In this section we shall describe the first-order calculation of $\Delta^{(0)}$, which results in the ground-state expression

$$\Delta^{(0)}=-\tfrac{1}{2}(W\xi)[1+(40/3)(n\xi a^3/\pi)^{1/2} +O(na^3)+O(na\lambda_T^2)^{-1}]. \qquad (38)$$

This calculation will illustrate the graphical iteration procedure described at the beginning of Sec. 2.

The determination of $\Delta^{(0)}$ has been discussed in detail in Sec. 7 of MII, and it begins with the calculation of either $\mathcal{K}_{\mathrm{out}}'(t)$ or $\mathcal{K}_{\mathrm{in}}'(t)$. We shall investigate both of these quantities by writing down the 3 one-vertex terms of Fig. 5 in MII for $\mathcal{K}_{\text{out}}'(t)$ and the 3 one-vertex terms of Fig. 6 in MII for $\mathcal{K}_{\text{in}}'(t)$. These terms give all of the zeroth- and first-order contributions to these quantities. Using the rules for transformed master graphs, we obtain the expressions:

$$\mathcal{K}_{\text{out}}'(t)=\mathcal{K}_{\text{out}}'(t)_0+\mathcal{K}_{\text{out}}'(t)_1+\mathcal{K}_{\text{out}}'(t)_2+\cdots, \tag{39}$$

$$\mathcal{K}_{\text{out}}'(t)_0=\tfrac{1}{2}[(1+B^{(0)})x\Omega\exp\beta(g+\Delta^{(0)})]\int_0^\beta ds_1ds_2G_{\text{out}}'(s_1)G_{\text{out}}'(s_2)\,{}^{s_1s_2}\!\begin{bmatrix}0 & 0\\ 0 & 0\end{bmatrix}'_t G_{\text{in}}'(t),$$

$$\mathcal{K}_{\text{out}}'(t)_1=\sum_{\mathbf{k}}\int_0^\beta ds_1ds_2\mathcal{G}_{1,1}'(t,s_1,\mathbf{k})G_{\text{out}}'(s_2)\,{}^{s_2s_1}\!\begin{bmatrix}0 & \mathbf{k}\\ 0 & \mathbf{k}\end{bmatrix}'_t,$$

$$\mathcal{K}_{\text{out}}'(t)_2=\tfrac{1}{2}(1+B^{(0)})\exp[-\beta(g+\Delta^{(0)})]\sum_{\mathbf{k}}\int_0^\beta ds_1ds_2\mathcal{G}_{0,2}'(s_2,s_1,\mathbf{k})\,{}^{s_2s_1}\!\begin{bmatrix}\mathbf{k} & -\mathbf{k}\\ 0 & 0\end{bmatrix}_t G_{\text{in}}'(t), \tag{40}$$

$$\mathcal{K}_{\text{in}}'(t)=\mathcal{K}_{\text{in}}'(t)_0+\mathcal{K}_{\text{in}}'(t)_1+\mathcal{K}_{\text{in}}'(t)_2+\cdots, \tag{41}$$

$$\mathcal{K}_{\text{in}}'(t)_0=\tfrac{1}{2}[(1+B^{(0)})x\Omega\exp\beta(g+\Delta^{(0)})]\int_0^\beta ds_1ds_2G_{\text{out}}'(s_2)\,{}^{ts_2}\!\begin{bmatrix}0 & 0\\ 0 & 0\end{bmatrix}'_{s_1}[G_{\text{in}}'(s_1)]^2,$$

$$\mathcal{K}_{\text{in}}'(t)_1=\sum_{\mathbf{k}}\int_0^\beta ds_1ds_2\mathcal{G}_{1,1}'(s_1,s_2,\mathbf{k})\,{}^{ts_2}\!\begin{bmatrix}0 & \mathbf{k}\\ 0 & \mathbf{k}\end{bmatrix}'_{s_1}G_{\text{in}}'(s_1),$$

$$\mathcal{K}_{\text{in}}'(t)_2=\tfrac{1}{2}(1+B^{(0)})^{-1}\exp\beta(g+\Delta^{(0)})\sum_{\mathbf{k}}\int_0^\beta ds_1ds_2G_{\text{out}}'(s_2)\,{}^{ts_2}\!\begin{bmatrix}0 & 0\\ \mathbf{k} & -\mathbf{k}\end{bmatrix}'_{s_1}\mathcal{G}_{2,0}'(s_1,s_1,\mathbf{k}). \tag{42}$$

The first factors in $\mathcal{K}_{\text{out}}'(t)_2$ and $\mathcal{K}_{\text{in}}'(t)_2$ are due to the definitions of $\mathcal{K}_{\text{out}}'(t)$ and $\mathcal{K}_{\text{in}}'(t)$ by Eqs. (106) in MII.

We see from Eqs. (40) and (42) that the first-order calculation of $\mathcal{K}_{\text{out}}'(t)$ and $\mathcal{K}_{\text{in}}'(t)$ requires expressions for the line factors $\mathcal{G}_{\mu,\nu}'(t_2,t_1,\mathbf{k})$. From Eqs. (93)–(96) in MII, and with the aid of Eqs. (28) and (29), we obtain the first-order expressions for these line factors.

$$\begin{aligned}\mathcal{G}_{1,1}'(t_2,t_1,\mathbf{k})\cong{}&\delta(t_2-t_1)+N_{2,0}'(\mathbf{p})\int_0^\beta ds\mathcal{K}_{0,2}'(t_1,s,\mathbf{p})+N_{0,2}'(\mathbf{p})\mathcal{K}_{2,0}'(t_2,\beta,\mathbf{p})\delta(\beta-t_1)+N_{1,1}'(\mathbf{p})\delta(\beta-t_1)\\&+N_{1,1}'(-\mathbf{p})\mathcal{K}_{2,0}'(t_2,\beta,\mathbf{p})\int_0^\beta ds\mathcal{K}_{0,2}'(t_1,s,\mathbf{p})R(\beta,-\mathbf{p}),\end{aligned} \tag{43}$$

$$\begin{aligned}\mathcal{G}_{0,2}'(t_2,t_1,\mathbf{k})\cong{}&[\mathcal{K}_{0,2}'(t_2,t_1,\mathbf{k})-K_{0,2}{}^{(1)\prime}(t_2,t_1,\mathbf{k})]+2N_{1,1}'(\mathbf{p})\delta(\beta-t_2)\int_0^\beta ds\mathcal{K}_{0,2}'(s,t_1,\mathbf{p})\\&+N_{0,2}'(\mathbf{p})\delta(\beta-t_2)\int_0^\beta dsG_0(\beta,s,-\mathbf{p})G_0{}^{(1)-1}(s,t_1,-\mathbf{p})\\&+N_{2,0}'(\mathbf{p})\int_0^\beta ds_2ds_1\mathcal{K}_{0,2}'(t_2,s_2,\mathbf{p})\mathcal{K}_{0,2}'(s_1,t_1,\mathbf{p}),\end{aligned} \tag{44}$$

$$\begin{aligned}\mathcal{G}_{2,0}'(t_2,t_1,\mathbf{p})\cong{}&[\mathcal{K}_{2,0}'(t_2,t_1,\mathbf{k})-\delta(t_2,t_1)K_{2,0}{}^{(1)\prime}(t_1,t_1,\mathbf{k})]+2N_{1,1}'(\mathbf{p})\mathcal{K}_{2,0}'(\beta,t_1,\mathbf{p})\\&+N_{2,0}'(\mathbf{p})R^{-1}(t_1,-\mathbf{p})+N_{0,2}'(\mathbf{p})\mathcal{K}_{2,0}'(t_2,\beta,\mathbf{p})\mathcal{K}_{2,0}'(\beta,t_1,\mathbf{p}).\end{aligned} \tag{45}$$

In these expressions, the function $R(t,\mathbf{p})$ is given by Eq. (91) in MII as

$$R(t,\mathbf{p})=\zeta^{-1}(t,\mathbf{p})\exp[-t\epsilon_1(\mathbf{p})]. \tag{46}$$

The functions $K_{0,2}{}^{(1)\prime}$ and $K_{2,0}{}^{(1)\prime}$ of Eq. (29) occur only in the first terms of Eqs. (44) and (45), because they are wiggly-line double-bond subtraction terms [see discussion below Eq. (84) in MII].

Rather than write down a number of lengthy equations required in the derivation of the general first-order expression for $\Delta^{(0)}$, we shall describe the steps of this derivation in detail. These steps, which use only expressions and manipulations already given, are as follows:

(1) One first sets $B^{(0)}=0$ and $g=-\Delta^{(0)}$ in Eqs. (40) and (42). The justification for this step has been given in Sec. 2.

(2) One next uses Eqs. (41), (44), (48), and (49) of MII, and the approximate expression (12) for the pair function to obtain simplified forms for $\mathcal{K}_{\text{out}}'(t)_0$ and $\mathcal{K}_{\text{in}}'(t)_0$. We shall write these particular expressions down, using $\epsilon_0=0$, in order to clarify the discussion of the subsequent steps.

$$\begin{aligned}\mathcal{K}_{\text{out}}'(t)_0&\cong-\tfrac{1}{2}(W\xi)\int_t^\beta ds_1ds_2G_{\text{out}}'(s_2)G_{\text{out}}'(s_1)G_{\text{in}}'(t)-\tfrac{1}{8}(n\Omega)^{-1}(W^2\xi)\sum_{\mathbf{k}}P\left(\frac{1}{\epsilon(\mathbf{k})}\right)\exp(\beta-t)[-2\epsilon(\mathbf{k})],\\ \mathcal{K}_{\text{in}}'(t)_0&\cong-\tfrac{1}{2}(W\xi)\int_0^t ds_1\int_{s_1}^\beta ds_2G_{\text{out}}'(s_2)[G_{\text{in}}'(s_1)]^2-\tfrac{1}{8}(n\Omega)^{-1}(W^2\xi)\sum_{\mathbf{k}}P\left(\frac{1}{\epsilon(\mathbf{k})}\right)\int_0^t ds\exp(t-s)[-2\epsilon(\mathbf{k})].\end{aligned}\tag{47}$$

The second terms in each of these expressions are first-order terms, and for these terms, only, is it justified to set

$$G_{\text{out}}'(s)\cong\delta(\beta-s),\quad G_{\text{in}}'(s)\cong 1.\tag{48}$$

(3) The zeroth-order calculation of $\Delta^{(0)}$, resulting in the term $-\frac{1}{2}(W\xi)$, is now straightforward. According to Eqs. (109) and (112) of MII, and the associated discussion in Sec. 7 of MII, one has only to set *one* $G_{\text{out}}'(s)\cong\delta(\beta-s)$ and *one* $G_{\text{in}}'(s)\cong1$ in each of the expressions (47) to obtain the zeroth-order term in $\Delta^{(0)}$. Both expressions (47) yield the same result, as they must. We see that $K_{\text{in}}'(t)$ and $K_{\text{out}}'(t)$ are both zero to zeroth order, and this justifies the use of the approximations (48) in Sec. 2. As we shall see in step (8), however, it does not justify the use of these approximations in the first terms of the expressions (47).

(4) The use of the approximations (48) in the second and third of Eqs. (40) and (42) is now justified.

(5) One nexts substitutes the line factor expressions (43)–(45) into the second and third of Eqs. (40) and (42). It is well to observe in this connection that for $T\neq0$, all of the terms in Eqs. (43)–(45) can be expected to, and do, give first-order terms. We also note that the use of the $K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})$ term of (44) in $\mathcal{K}_{\text{out}}'(t)_2$ causes the corresponding pair function to be an untransformed pair function [see Eq. (83) in MII and subsequent discussion]. The temperature integration of this term then yields two further terms, one of which cancels the second term in $\mathcal{K}_{\text{out}}'(t)_0$, Eq. (47). A similar situation exists with the $K_{2,0}^{(1)\prime}(s_1,s_1,\mathbf{k})$ term in $\mathcal{K}_{\text{in}}'(t)_2$, Eq. (42). We finally observe that the next to last term of Eq. (44) is associated with an integral which only has the effect of changing a Λ-transformation function from $G_0^{(1)}$ to G_0 in the transformed pair function of $\mathcal{K}_{\text{out}}'(t)_2$. This situation has been discussed in connection with Eq. (94) in MII.

(6) One inserts Eqs. (45) and (46) from MII, together with an approximation of the type (12) for the functions $g_{i,j}(\mathbf{k}_1\mathbf{k}_2|\mathbf{k}_3\mathbf{k}_4)$ into the expressions derived in step (5) for $\mathcal{K}_{\text{out}}'(t)_1$, $\mathcal{K}_{\text{out}}'(t)_2$, $\mathcal{K}_{\text{in}}'(t)_1$, and $\mathcal{K}_{\text{in}}'(t)_2$.

(7) One writes the functions $\Delta^{(0)}$, $K_{\text{out}}'(t)$, and $K_{\text{in}}'(t)$ as a series of terms corresponding to the series for $\mathcal{K}_{\text{out}}'(t)$, Eq. (39), and $\mathcal{K}_{\text{in}}'(t)$, Eq. (41).

$$\Delta^{(0)}=\Delta_0^{(0)}+\Delta_1^{(0)}+\Delta_2^{(0)}+\cdots,\tag{49}$$

$$K_{\text{out}}'(t)=K_{\text{out}}'(t)_0+K_{\text{out}}'(t)_1+K_{\text{out}}'(t)_2+\cdots,\tag{50}$$

$$K_{\text{in}}'(t)=K_{\text{in}}'(t)_0+K_{\text{in}}'(t)_1+K_{\text{in}}'(t)_2+\cdots.\tag{51}$$

The second and third terms in these series can be written down, after comparing the final expressions obtained in step (6) with the general forms for $\mathcal{K}_{\text{out}}'(t)$, Eq. (109) in MII, and $\mathcal{K}_{\text{in}}'(t)$, Eq. (112) in MII. It is important to keep in mind the discussion at the end of Sec. 7 in MII when deriving these terms. The final expressions which one obtains are still much too lengthy to be written down. However, in the low-temperature limit $na\lambda_T^2\gg1$, one can easily extract from these terms the ground-state contributions to $\Delta^{(0)}$. This limit corresponds to the neglect of the $\epsilon_-(\mathbf{k})$ exponential terms, because when $na\lambda_T^2\gg1$, then

$$\exp[\beta\epsilon_-(\mathbf{k})]\ll1,\quad(\mathbf{k}\neq0).\tag{52}$$

The reason for this is that the largest cutoff momentum when $T\to0$, in all the integrals which occur, is the momentum $\hbar(na)^{1/2}$. This fact combined with Eq. (25) then yields the inequality (52). One finds for $\Delta_1^{(0)}$ and $\Delta_2^{(0)}$ when $T\to0$ the expressions

$$\Delta_1^{(0)}\underset{T\to0}{\longrightarrow}-W(n\Omega)^{-1}\sum_{\mathbf{k}}(\Delta_--\Delta_+)^{-1}(\epsilon_-+\epsilon_1)\underset{\Omega\to\infty}{\longrightarrow}-(8/3)W(n\xi^3a^3/\pi)^{1/2},\tag{53}$$

$$\Delta_2^{(0)}\underset{T\to0}{\longrightarrow}\tfrac{1}{4}\xi W^2(n\Omega)^{-1}\sum_{\mathbf{k}}[(\Delta_--\Delta_+)^{-1}-(2\epsilon)^{-1}]\underset{\Omega\to\infty}{\longrightarrow}-4W(n\xi^3a^3/\pi)^{1/2},\tag{54}$$

where W is defined by Eq. (13). These terms are just those which one obtains by keeping in the line factors (43)–(45) only the first terms, which do not depend on the $N_{\mu,\nu}'(\mathbf{p})$. This is a very reasonable result, because it is generally believed that the ground state of a Bose gas can be understood by considering only the case of Boltzmann statistics,[7] and this case corresponds to neglecting the "statistics" terms $N_{\mu,\nu}'$.

(8) The expressions for $K_{\text{out}}'(t)_1$, $K_{\text{out}}'(t)_2$, $K_{\text{in}}'(t)_1$,

and $K_{in}'(t)_2$ will not be written down here, but it is important to observe that they must be substituted into the first terms of Eqs. (47) in order to calculate $\Delta_0^{(0)}$, $K_{out}'(t)_0$, and $K_{in}'(t)_0$ to first order. This is a somewhat lengthy calculation, which yields nonzero first-order expressions for each of these three quantities. However, in the limit (52) one finds that the first-order contribution to $\Delta_0^{(0)}$ vanishes, and one obtains only the zeroth-order term

$$\Delta_0^{(0)} \underset{T\to 0}{\longrightarrow} -\tfrac{1}{2}(W\xi)\,. \qquad (55)$$

Equations (53)–(55) can now be substituted into Eq. (49) to give the result (38), written down at the beginning of this section.

The purpose of the lengthy discussion given in this section, of the derivation of Eq. (38), has been twofold. On the one hand, we have shown the simple approximations which will yield this result, thereby justifying our iteration procedure. On the other hand, we have given an indication of the complexity of the problem when one considers finite temperatures $T\neq 0$. It is a tedious, but straightforward, calculation to obtain the general first-order expression for $\Delta^{(0)}$. It will be of considerable interest to study this expression in various temperature regions in order to extract knowledge of the microscopic physics of the hard-sphere Bose gas at finite temperatures.

5. FIRST-ORDER CALCULATION OF GROUND-STATE ENERGY

In this section we shall only consider the derivation of the first-order expression for the energy of a hard-sphere Bose gas near $T=0$, i.e., when $na\lambda_T^2\gg 1$. Our considerations will depend partly on the insight gained into the mathematical structure of the theory from the calculation of Sec. 4. In quantum statistics, the calculation of any thermodynamic quantity such as the energy begins with a determination of the grand potential f. From Eq. (125) in MII, we have for Ωf the expression

$$\begin{aligned}\Omega f(x,\beta,g,\Omega)\cong&\tfrac{1}{2}\sum_{\mathbf{p}}\ln[(1+\langle n(\mathbf{p})\rangle)(1+\nu'(\mathbf{p}))]+x\Omega[(1+B^{(0)})\exp\beta(g+\Delta^{(0)})-1]\\&-x\Omega(1+B^{(0)})\exp\beta(g+\Delta^{(0)})\left[\int_0^\beta dtK_{out}'(t)K_{in}'(t)+\int_0^\beta dt_1dt_2G_{out}'(t_2)\Lambda^{(0)}(t_2,t_1)G_{in}'(t_1)\right]\\&+\Omega F(x,\beta,g,\Omega)+\sum_{\mathbf{k}}\int_0^\beta dt_1\int_0^{t_1}dt_2G_{1,1}^{(t_1)\prime}(t_1,t_2,\mathbf{k})[P^{(t_1)\prime}(t_2,t_1,\mathbf{k})+\Lambda^{(t_1)}(t_2,t_1,\mathbf{k})]\\&-\tfrac{1}{2}\sum_{\mathbf{k}}\int_0^\beta dt_1dt_2\{\sum_{\substack{(\mu,\nu)\\ \mu+\nu=2}}(1+\delta_{\mu,\nu})\mathcal{G}_{\nu,\mu}'(t_1,t_2,\mathbf{k})\mathcal{K}_{\mu,\nu}'(t_2,t_1,\mathbf{k})+K_{2,0}^{(1)\prime}(t_1,t_2,\mathbf{k})K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})\}\,,\end{aligned}\qquad (56)$$

where the sum $\sum_{(\mu,\nu)}$ in the last term is over the three possibilities for which $\mu+\nu=2$, and where we have used Eq. (30).

In Fig. 4, we show the graphical expansion of $\Omega F(x,\beta,g,\Omega)$ to second order, in terms of transformed master (0,0) graphs. The expression for the zeroth-order term in this expansion is

$$\Omega F_0(x,\beta,g,\Omega)=\tfrac{1}{4}(x\Omega)^2(1+B^{(0)})^2\exp2\beta(g+\Delta^{(0)})\int_0^\beta ds_1ds_2dtG_{out}'(s_1)G_{out}'(s_2)\,{}^{s_1s_2}\!\begin{bmatrix}0&0\\0&0\end{bmatrix}_t'[G_{in}'(t)]^2\,. \qquad (57)$$

It is unnecessary to write down the expressions for the first-order terms in ΩF, because they are cancelled by the three $\mathcal{G}_{\nu,\mu}'\mathcal{K}_{\mu,\nu}'$ terms in the grand potential. We may than set $B^{(0)}=0$ and $g=-\Delta^{(0)}$, as in Sec. 2, and write for the grand potential to first order

$$\begin{aligned}f(x,\beta,\Omega)\cong&\tfrac{1}{2}\Omega^{-1}\sum_{\mathbf{p}}\ln[(1+\langle n(\mathbf{p})\rangle)(1+\nu'(\mathbf{p}))]+F_0(x,\beta,\Omega)\\&-x\left[\int_0^\beta dtK_{out}'(t)K_{in}'(t)+\Delta^{(0)}\int_0^\beta dt_2\int_0^{t_2}dt_1G_{out}'(t_2)G_{in}'(t_1)\right]\\&+\Omega^{-1}\sum_{\mathbf{k}}\int_0^\beta dt_1dt_2\{G_{1,1}^{(t_1)\prime}(t_1,t_2,\mathbf{k})[P^{(t_1)\prime}(t_2,t_1,\mathbf{k})+\Lambda^{(t_1)}(t_2,t_1,\mathbf{k})]\theta(t_1-t_2)\\&\qquad-\tfrac{1}{2}K_{2,0}^{(1)\prime}(t_1,t_2,\mathbf{k})K_{0,2}^{(1)\prime}(t_2,t_1,\mathbf{k})\}\,,\end{aligned}\qquad (58)$$

where we have used Eq. (110) of MII. Notice that the chemical potential g no longer explicitly appears in this expression, because we have used the assumption (2). This is the situation referred to at the end of Sec. 2 in MI.

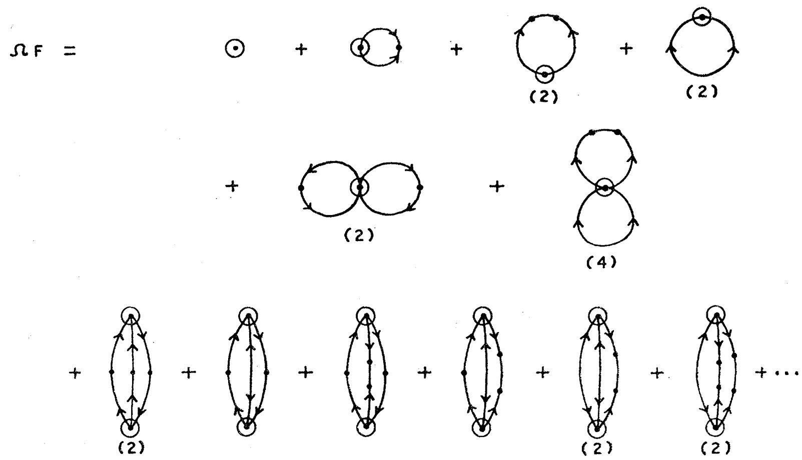

FIG. 4. The graphical expansion of $\Omega F(x,\beta,g,\Omega)$, showing the one zeroth-order, three first-order, and eight second-order transformed master (0,0) graphs. The symmetry numbers of these graphs have been indicated whenever they differ from unity. For convenience, the temperature and momentum labels of the graphs have been omitted.

It is now necessary to determine the function $\Lambda^{(\tau)}(t_2,t_1,\mathbf{k})$, where from Eq. (121) in MII

$$\Lambda^{(\tau)}(t_2,t_1,\mathbf{k})=\zeta_\tau^{-1}(t_2,\mathbf{k})\zeta_\tau(t_1,\mathbf{k})\sum_{i=+,-} i\Delta_i(\mathbf{k})\exp t_1\epsilon_i(\mathbf{k})[A_{i,\tau}^{(<)}(t_2,\mathbf{k})\theta(t_1-t_2)+A_{i,\tau}^{(>)}(t_2,\mathbf{k})\theta(t_2-t_1)]. \quad (59)$$

The determination of this function for the general parameter $\tau>(t_2,t_1)$ has been discussed in Sec. 9 of MII. One follows in complete analogy through the analysis of Sec. 2, arriving at a set of relations (22) and (23), with β replaced by τ. One also finds that

$$P^{(\tau)\prime}(t_2,t_1,\mathbf{k})\cong 0\,,$$
$$G^{(\tau)\prime}(t_2,t_1,\mathbf{k})\cong\delta(t_2-t_1)\,, \quad (60)$$

to first order. The expression (58) can therefore be further simplified to

$$f(x,\beta,\Omega)\cong\tfrac{1}{2}\Omega^{-1}\sum_{\mathbf{p}}\ln[(1+\langle n(\mathbf{p})\rangle)(1+\nu'(\mathbf{p}))]+\tfrac{1}{2}\Omega^{-1}\sum_{\mathbf{k}}\int_0^\beta dt_1\Lambda^{(t_1)}(t_1^{(-)},t_1,\mathbf{k})$$
$$-x\left[\int_0^\beta dtK_{\mathrm{out}}'(t)K_{\mathrm{in}}'(t)+\Delta^{(0)}\int_0^\beta dt_2\int_0^{t_2}dt_1G_{\mathrm{out}}'(t_2)G_{\mathrm{in}}'(t_1)\right]$$
$$-\tfrac{1}{4}W\xi^2n\int_0^\beta dt\int_t^\beta ds_1ds_2G_{\mathrm{out}}'(s_1)G_{\mathrm{out}}'(s_2)[G_{\mathrm{in}}'(t)]^2-\tfrac{1}{16}\beta(W\xi)^2\Omega^{-1}\sum_{\mathbf{k}}P\left(\frac{1}{\epsilon(\mathbf{k})}\right), \quad (61)$$

where we have substituted Eq. (57) for ΩF_0, and used Eqs. (41) and (44) of MII along with Eqs. (12), (8a), (9a), and (14) of the present paper. We observe that we may use the approximations (48) in the second term of (57), after the approximate pair-function expression (12) has been substituted. An analogous situation occurred in connection with Eqs. (47). The last term of Eq. (61), which is not well defined, combines with the $\Lambda^{(t_1)}$ term to give a well-defined final expression [see Eq. (63)]. We note that we must insert a minus sign superscript in the $\Lambda^{(t_1)}$ term, in order to indicate that the first term, and not the second term of (59) is to be used when we take the limit $t_2\to t_1$ [see also Eq. (58)]. Finally, we have used the fact that the integral of a δ function times a step function of the same argument equals $\frac{1}{2}$.

We now write down the terms $A_{i,t_1}^{(<)}(t_1)$ and $\zeta_{t_1}(t_1)$ which occur in the function $\Lambda^{(t_1)}(t_1^{(-)},t_1)$ of Eq. (59). Setting $\beta=t_2=t_1$ in Eqs. (22) and (23), we obtain (using $\epsilon_+=-\epsilon_-$)

$$A_{i,t_1}^{(<)}(t_1)=(\Delta_--\Delta_+)^{-2}(\epsilon_++\epsilon_1)(\epsilon_-+\epsilon_1)\times\zeta_{t_1}(t_1)(e^{-t_1\epsilon_+}-e^{-t_1\epsilon_-})e^{-t_1\epsilon_i}\,,$$
$$\zeta_{t_1}(t_1)=[(\epsilon_++\epsilon_1)e^{t_1\epsilon_+}-(\epsilon_-+\epsilon_1)e^{t_1\epsilon_-}]^{-1}(\Delta_--\Delta_+). \quad (62)$$

Before substituting Eqs. (59) and (62) into the grand potential (61), we consider the low-temperature limit $na\lambda_T^2\gg1$. In this case, we may set $K_{\mathrm{out}}'(t)\cong K_{\mathrm{in}}'(t)\cong 0$ everywhere in (61), because in this limit these terms give no first-order contribution to $\beta^{-1}f$. This statement is a consequence of the investigations discussed in Sec. 4. We may also omit the first term in $\beta^{-1}f$, because it gives no contribution when $na\lambda_T^2\gg1$. Then, using the inequality (52) we obtain for the very low-temperature grand potential of a dilute gas of Bose hard spheres, the final expression

$$(n\beta)^{-1}f(x,\beta,\Omega)\cong-\xi\Delta^{(0)}-\tfrac{1}{4}W\xi^2+\tfrac{1}{8}(W\xi)^2(n\Omega)^{-1}\sum_{\mathbf{k}}\left[(\epsilon_++\epsilon_1)^{-1}-(2\epsilon)^{-1}\right]$$

$$\xrightarrow[\Omega\to\infty]{}-\xi\Delta^{(0)}-\tfrac{1}{4}W\xi^2-(32/15)(W\xi)(n\xi^3a^3/\pi)^{1/2}=\tfrac{1}{4}W\xi^2\left[1+(272/15)(n\xi a^3/\pi)^{1/2}+O(na^3)+O(na\lambda_T^2)^{-1}\right]. \quad (63)$$

To obtain the first line of Eq. (63) we have used the first-order identity

$$(\epsilon_1+\epsilon_+)(\epsilon_1+\epsilon_-)=\tfrac{1}{4}(W\xi)^2, \quad (64)$$

which can be proved by combining Eqs. (15) and (19). To obtain the last line of Eq. (63), we have used Eq. (38). It should be observed that the functions $N_{\mu,\nu}'$ have not contributed to this final result, which shows once again that the ground state of the Bose and Boltzmann systems are the same.

The fractional occupation ξ of the zero-momentum state, near $T=0$, can now be determined by using Eq. (3′) of MI.

$$(n\beta)^{-1}(\partial f/\partial\xi)=\partial g/\partial\xi, \quad (65)$$

where according to Eqs. (2) and (38)

$$g=\tfrac{1}{2}(W\xi)\left[1+(40/3)(n\xi a^3/\pi)^{1/2}+O(na^3)+O(na\lambda_T^2)^{-1}\right]. \quad (66)$$

One then finds

$$(1-\xi)=(8/3)(na^3/\pi)^{1/2}+O(na^3)+O(na\lambda_T^2)^{-1}. \quad (67)$$

The quantity $(1-\xi)$ is often referred to as the "depletion factor" of the zero-momentum state. At $T=0$, it is due entirely to the particle interactions.

The pressure is given by Eq. (11) in MI as

$$n^{-1}\mathcal{P}=(n\beta)^{-1}f=\tfrac{1}{4}W\left[1+(64/5)(na^3/\pi)^{1/2}+O(na^3)+O(na\lambda_T^2)^{-1}\right], \quad (68)$$

where we have substituted Eq. (67) into Eq. (63) to obtain this result. Notice that the pressure does not vanish at $T=0$ for a Bose gas of hard spheres, as it does when the diameter of the spheres is zero (i.e., when $W\to 0$).

The energy per particle of the dilute Bose gas of hard spheres is found by substituting Eqs. (63) and (66) into Eq. (13′) of MI.

$$\frac{\langle E\rangle}{\langle N\rangle}=g-n^{-1}\frac{\partial f}{\partial\beta}+\beta\frac{\partial g}{\partial\beta}\xrightarrow[T\to0]{}g-(n\beta)^{-1}f$$

$$=\tfrac{1}{4}W\left[1+(128/15)(na^3/\pi)^{1/2}+O(na^3)+O(na\lambda_T^2)^{-1}\right]. \quad (69)$$

This is the well-known result of Lee, Huang, and Yang.[4] In order to check that our assumption (2) is correct. We calculate the thermodynamic potential g thermodynamically by using the relation

$$g=\left.\frac{\partial\langle E\rangle}{\partial\langle N\rangle}\right|_{S,\Omega}=\frac{\langle E\rangle}{\langle N\rangle}+n\frac{\partial}{\partial n}\left(\frac{\langle E\rangle}{\langle N\rangle}\right)_{S,\Omega}, \quad (70)$$

where S is the entropy. At zero temperature, holding the entropy constant is equivalent to holding the temperature constant, and, therefore, Eq. (70) is equivalent to the statement that the pressure is given at $T=0$ by

$$n^{-1}\mathcal{P}\xrightarrow[T\to0]{}n\frac{\partial}{\partial n}\left(\frac{\langle E\rangle}{\langle N\rangle}\right). \quad (71)$$

Rembering that W depends linearly on n, we find that Eqs. (71) and (69) are in agreement with Eq. (68). Therefore, the assumption (2) is shown to be valid in this first-order calculation.

6. DISTRIBUTION FUNCTIONS

In this section we shall begin by determining a first-order expression for the momentum distribution, valid for all T. The zero-temperature limit of this expression will then provide us with an independent means for checking the expression (67) for the depletion factor $(1-\xi)$. Finally, we shall write down a first-order expression for the pair-distribution function.

According to Eq. (103) in MII, the momentum distribution is given by

$$\langle n(\mathbf{p})\rangle=\zeta^{-1}(\beta,\mathbf{p})N_{1,1}'(\mathbf{p})-1, \quad (72)$$

where we have used Eq. (2) and set $B(\mathbf{p})=0$. The first-order expression for the momentum distribution is obtained by substituting Eqs. (33) and (36) into (72):

$$\langle n(\mathbf{p})\rangle=\{\nu'(\mathbf{p})+[1+\nu'(\mathbf{p})]^2[K_{0,2}'(\mathbf{p})]^2\}\times\{1-[1+\nu'(\mathbf{p})]^2[K_{0,2}'(\mathbf{p})]^2\}^{-1}. \quad (73)$$

Now, in the very-low-temperature region of (52), the function $\zeta(\beta,\mathbf{p})$ of Eq. (23) is exponentially small for $\mathbf{p}\neq0$. Therefore, when $na\lambda_T^2\gg1$, the quantity $\nu'(\mathbf{p})$ in (73) can be set equal to zero, and the expression for the momentum distribution becomes

$$\langle n(\mathbf{p})\rangle\xrightarrow[T\to0]{}\alpha_{\mathrm{p}}^2(1-\alpha_{\mathrm{p}}^2)^{-1}, \quad (74)$$

where we have used the explicit expression (31) for $K_{0,2}'(\mathbf{p})$, and defined

$$\alpha_{\mathrm{p}}\equiv\tfrac{1}{2}(W\xi)(\epsilon_++\epsilon_1)^{-1}=(\tfrac{1}{2}W\xi)^{-1}(\epsilon_-+\epsilon_1). \quad (75)$$

The second line of Eq. (75) follows from the identity (64).

Equation (74) has been previously obtained by Lee, Huang, and Yang.[4] It is not correct, however, when $\beta\omega_{\mathrm{p}}\ll(na\lambda_T^2)^{-1}\ll1$. In this case the inequality (52) is not valid, and one obtains instead of (74) the expression

$$\langle n(\mathbf{p})\rangle \cong (4\beta\omega_{\mathrm{p}})^{-1}, \quad \beta\omega_{\mathrm{p}} \ll (na\lambda_T^2)^{-1} \ll 1. \qquad (74')$$

The result shows that the momentum distribution diverges as p^{-2} when $\mathbf{p}\to 0$, contrary to the prediction of (74).

The momentum region governed by (74′) is vanishing small in the low-temperature region $(na\lambda_T^2)\gg 1$. Therefore, we may use only Eq. (74) to compute the depletion factor, by the equation

$$(1-\xi)=(n\Omega)^{-1}\sum_{\mathbf{p}}\langle n(\mathbf{p})\rangle \underset{\Omega\to\infty}{\longrightarrow} (8/3)(n\xi^3a^3/\pi)^{1/2}. \qquad (76)$$

Equation (76) is in agreement with the result (67), because we may set $\xi=1$ on the right-hand side of (76) to first approximation.

We next investigate the pair-distribution function, $D(r)$. An exact expression for this quantity is given by Eq. (100) of MI. To first order, this expression is

$$D(r)\cong 1+2\xi[F_{1,1}(r)+F_{0,2}(r)] +[F_{1,1}(r)]^2+[F_{0,2}(r)]^2, \qquad (77)$$

where the functions $F_{1,1}(r)$ and $F_{0,2}(r)$ (in the limit $\Omega\to\infty$) are given by Eqs. (98) in MI as

$$F_{1,1}(r)=n^{-1}(2\pi)^{-3}\int d^3p e^{i\mathbf{p}\cdot\mathbf{r}}\langle n(\mathbf{p})\rangle, \qquad (78)$$

$$F_{0,2}(r)=n^{-1}(2\pi)^{-3}\int d^3p e^{i\mathbf{p}\cdot\mathbf{r}}N_{0,2}(\mathbf{p}) \times\exp\beta(\omega_{\mathrm{p}}+\omega_{-\mathrm{p}}-2g) =n^{-1}(2\pi)^{-3}\int d^3p e^{i\mathbf{p}\cdot\mathbf{r}}N_{2,0}'(\mathbf{p}). \qquad (79)$$

To obtain the second line of Eq. (79), we have used the second of Eqs. (87) and (97) in MII. In the low-temperature limit (52), the expression for $F_{0,2}(r)$ can be written as

$$F_{0,2}(r)\underset{T\to 0}{\longrightarrow} -n^{-1}(2\pi)^{-3}\int d^3p e^{i\mathbf{p}\cdot\mathbf{r}}\alpha_{\mathrm{p}}(1-\alpha_{\mathrm{p}}^2)^{-1}, \qquad (80)$$

where we have again used the explicit expression (31) for $K_{0,2}'(\mathbf{p})$ along with the definition (75). When Eqs. (78) and (80) are substituted into Eq. (77), then one finds, once again a result previously derived by Lee, Huang, and Yang.[4,10] We observe that the $F_{1,1}^2$ and $F_{0,2}^2$ terms are really second-order terms, according to our convention, and that a neglected term $F_{1,2}(r)$ in Eq. (100) of MI can be the same order of magnitude as these terms for certain regions of r. We have not pursued this investigation any further, at present.

7. ATTRACTIVE INTERACTIONS

It is of considerable interest to determine the generalization of the expressions which we have derived in Secs. 2–6, to the case when on attractive potential is added to the hard-sphere repulsions. This problem has previously been examined by Huang[11] for a long-range attraction, with the aid of the pseudopotential method. In this section, we shall approach the question from a general point of view, in order to indicate how a microscopic theory of liquid helium II might be developed. In this approach, we shall retain the general convention regarding the orders of graphs, defined at the beginning of Sec. 2. Our principal modification will be to abandon the approximations (12) and (12′) for the pair functions, and we shall then derive general first-order expressions for the energies $\epsilon_+(\mathbf{k})$ and $\epsilon_-(\mathbf{k})$.

Suppose now, that the general expression (38) in MII for the primed pair functions is substituted into Eqs. (3)–(5), and that these equations are, in turn, substituted into the first line of Eq. (17). In this case, the two identities which one obtains instead of (20), are

$$\sum_{i=+,-} i\exp[t_2\epsilon_i(\mathbf{k})]P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right) \times[A_i^{(>)}(t_2,\mathbf{k})-A_i^{(<)}(t_2,\mathbf{k})]G_i(t_2,\mathbf{k})=0,$$
$$\sum_{i=+,-} iP\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right)A_i^{(>)}(t_2,\mathbf{k}) \times g_{i,1}(\mathbf{k}-\mathbf{k}|00)=0, \qquad (81)$$

where

$$G_i(t_2,\mathbf{k}) =g_{0,0}(00|\mathbf{k}-\mathbf{k})+\sum_{\mathbf{k}_5\mathbf{k}_6} f_2(\mathbf{k}-\mathbf{k}|\mathbf{k}_5\mathbf{k}_6|00) \times\exp[-t_2(\epsilon(\mathbf{k}_5)+\epsilon(\mathbf{k}_6))] \times\left[P\left(\frac{1}{\epsilon(\mathbf{k}_5)+\epsilon(\mathbf{k}_6)-\epsilon_i(\mathbf{k})-\epsilon_1(-\mathbf{k})}\right) -P\left(\frac{1}{\epsilon(\mathbf{k}_5)+\epsilon(\mathbf{k}_6)}\right)\right]. \qquad (82)$$

The function $g_{i,j}(\mathbf{k}_1\mathbf{k}_2|\mathbf{k}_3\mathbf{k}_4)$ is defined by Eq. (39) in MII, and the function $f_2(\mathbf{k}_1\mathbf{k}_2|\mathbf{k}_5\mathbf{k}_6|\mathbf{k}_3\mathbf{k}_4)$ is determined by comparing Eq. (6) in MII with an explicit expression for the untransformed pair function.[12] Equations (81) and (82) are valid even for the mathematical idealization of an infinite repulsive core interaction. That is to say, they are the completely general first-order identities which replace the approximations (20). It is convenient, however, to assume that the repulsive interaction is *not* infinite, in which case the various $B(\mathbf{k})$ functions are identically zero. Then, both of the identities (21) are

[10] See also L. S. Garcia-Colin, J. Math. Phys. **1**, 87 (1960).

[11] Kerson Huang, Phys. Rev. **115**, 765 (1959); **119**, 1129 (1960).

[12] F. Mohling, Phys. Rev. **124**, 583 (1961), gives explicit expressions, in terms of two-particle reaction matrices, for the functions f_1 and f_2 which determine $g_{i,j}(\mathbf{k}_1\mathbf{k}_2|\mathbf{k}_3\mathbf{k}_4)$. Section V also shows how all three of these functions can be related to matrix elements of scattering operators. Equations (30) and (66) of this reference are required in order to obtain the form (82) of the function $G_i(t_2,\mathbf{k})$.

also correct, and we have four equations for the determination of the four $A_i^{(<)}$ and $A_i^{(>)}$. It is important to observe that the coefficients of the $A_i^{(<)}$ and $A_i^{(>)}$ in Eqs. (81) have a different form *after* the Λ transformation from the form (20) which they had before the Λ transformation. On the other hand, Eqs. (21) are unchanged by the Λ transformation. This point has been discussed in detail in MII. We shall not consider these equations further, as their solution is not required in the present calculations.

The calculation of $\mathcal{P}'(t_2,t_1,\mathbf{k})$ just described, starting from the first line of Eq. (17), also yields terms of the form (18) for $\Lambda(t_2,t_1,\mathbf{k})$. By identifying these terms with $\Lambda(t_2,t_1,\mathbf{k})$ one finds a general first-order expression for $\Delta_i(\mathbf{k})$, which replaces Eq. (19),

$$\Delta_i(\mathbf{k})=(x\Omega)g_{i,0}(\mathbf{k}0|\mathbf{k}0)+\tfrac{1}{4}(x\Omega)^2[g_{0,0}(00|\mathbf{k}-\mathbf{k})]^2P\left(\frac{1}{\epsilon_i(\mathbf{k})+\epsilon_1(-\mathbf{k})}\right). \quad (83)$$

In a similar manner one can show that the general first-order expression for $\Delta^{(1)}(-\mathbf{k})$ is

$$\Delta^{(1)}(-\mathbf{k})=(x\Omega)g_{1,0}(-\mathbf{k}0|-\mathbf{k}0). \quad (84)$$

This expression replaces Eq. (15), and Eq. (16) is replaced by the expression

$$K_{1,1}^{(1)\prime}(t_2,t_1,-\mathbf{k})=(x\Omega)\theta(t_2-t_1)\sum_{\mathbf{k}_5\mathbf{k}_6}f_2(-\mathbf{k}0|\mathbf{k}_5\mathbf{k}_6|-\mathbf{k}0)\times P\left(\frac{1}{\epsilon_1(-\mathbf{k})-\epsilon(\mathbf{k}_5)-\epsilon(\mathbf{k}_6)}\right)\times\exp(t_2-t_1)[\epsilon_1(-\mathbf{k})-\epsilon(\mathbf{k}_5)-\epsilon(\mathbf{k}_6)]. \quad (85)$$

It is only to the extent that this last expression can be neglected that one is entitled to use the first line of Eq. (17) to calculate $\mathcal{P}'(t_2,t_1,\mathbf{k})$, as we have done. We shall not write down the corresponding first-order expression for $P'(t_2,t_1,\mathbf{k})$, Eq. (27).

The expression (83), for the determination of the Δ_i, has coefficients (the $g_{i,j}$) that result in a solution which differs in several ways from the solution (25) to Eq. (19). As with Eqs. (81), this difference is due to the Λ transformation. Thus, one can solve Eq. (83) algebraically to find for[13] $\epsilon_i(\mathbf{k})$

$$\epsilon_i(\mathbf{k})=\tfrac{1}{2}(x\Omega)[g_{1,0}(-\mathbf{k}0|-\mathbf{k}0)-g_{i,0}(\mathbf{k}0|\mathbf{k}0)]+i\{[\omega(\mathbf{k})+\Delta^{(0)}-\tfrac{1}{2}(x\Omega)\times(g_{1,0}(-\mathbf{k}0|-\mathbf{k}0)+g_{i,0}(\mathbf{k}0|\mathbf{k}0))]^2-\tfrac{1}{4}(x\Omega)^2[g_{0,0}(00|\mathbf{k}-\mathbf{k})]^2\}^{1/2}, \quad (86)$$

where to first approximation $\Delta^{(0)}$ is given by

$$\Delta^{(0)}=\tfrac{1}{2}(x\Omega)g_{0,0}(00|00). \quad (87)$$

There are two significant differences between the solutions (86) and (25). One is that $\epsilon_+(\mathbf{k})$ and $\epsilon_-(\mathbf{k})$ no longer differ only by a minus sign. The second difference is that Eq. (86) is actually an integral equation for the determination of $\Delta_i(\mathbf{k})$, because $g_{i,0}$ depends functionally on $\Delta_i(\mathbf{k})$. In fact, in a higher order calculation one would find that Eqs. (81) also become integral equations.

It is not our purpose to pursue the analysis of a general Bose system any further in this paper. Rather, we shall consider the specific example of a weak, short-range, attractive square well of depth $V_0=(\hbar^2\mu^2/M)$ and diameter b outside of the repulsive core of diameter a. For such a problem the first thought which might come to mind is to merely replace the quantity a in Eq. (25) by the scattering length

$$a_s=a-(b-a)(y^{-1}\tan y-1)\underset{y\ll 1}{\longrightarrow}a-\tfrac{1}{3}(b-a)y^2+O(y^4), \quad (88)$$

where $y=\mu(b-a)$. Clearly, for a weak, short-range attraction ($y\ll 1$) the scattering length cannot be negative.

The proper way to consider this problem is to write down the general expression for $g_{i,j}(\mathbf{k}_1\mathbf{k}_2|\mathbf{k}_3\mathbf{k}_4)$, and then to take the limit $\mathbf{k}_i\to 0$ [see Eq. (10′)]. In Ref. 14, we have written down the exact expression for the S-wave part of $g_{i,j}(\mathbf{k}_1\mathbf{k}_2|\mathbf{k}_3\mathbf{k}_4)$ for this problem, which is the only part which survives in the zero-momentum limit. If one examines the zero-momentum limit of this expression for a weak, short-range attraction (outside of a repulsive core), then one finds the limiting expression for $y\ll 1$:

$$g_{i,j}(00|00)=-\Omega^{-1}(8\pi\hbar^2/M)[a_s+\epsilon_{i,j}^{1/2}a_s^2\theta(\epsilon_{i,j})+O(\epsilon_{i,j}a_s^3)], \quad (89)$$

where $\theta(z)$ is a step function and

$$\epsilon_{i,j}(\mathbf{k}_1,\mathbf{k}_2)=-k_{12}^2+(M/\hbar^2)[\Delta_i(\mathbf{k}_1)+\Delta_j(\mathbf{k}_2)], \quad (90)$$
$$\mathbf{k}_{12}=\tfrac{1}{2}(\mathbf{k}_2-\mathbf{k}_1).$$

Therefore, since $\epsilon_{i,j}$ will be $\sim -na$ for weak attractions, the guess (88) is essentially correct to the order which we are calculating.

We finally consider the possibility that the parameters of the attractive interaction give a negative scattering length ($a_s<0$). In this case, the energies $\epsilon_i(\mathbf{k})$, as given by Eq. (25) with $a\to a_s$, would become complex. Such a result should not occur for a real problem when using the methods of equilibrium quantum statistics. Moreover, the consideration of the second term in (89) does not alleviate this difficulty, even though it has the correct sign, because it is much smaller than the first term when $n|a_s|^3\ll 1$.

[13] It is interesting to compare Eq. (86) with Eq. (4.7) in S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. 34, 433 (1958) [English transl.: Soviet Phys.—JETP 7, 299 (1958)]. Thus, $\epsilon_+(\mathbf{k})$ reduces to Beliaev's $\epsilon(\mathbf{k})$ when the $g_{i,j}$'s are all replaced by free-particle scattering amplitudes.

[14] F. Mohling, Phys. Rev. 128, 1365 (1962).

The only conclusion which can be drawn from the preceding paragraph is that the low-density Bose gas near $T=0$ does not exist when $a_s<0$. That is to say, a Bose gas having short-range interactions with $a_s<0$ will collapse to densities such that the low-density approximations (10) and (10′) are not valid. For a Bose gas with weak long-range attractions, the calculation of Huang[11] has shown that the low-density approximations (10) and (10′) may remain valid in certain circumstances even though $a_s<0$. To show this, Huang considers a nonlocal, or velocity-dependent, two-particle interaction, which is equivalent in this case to considering a very-low-momentum variation of $g_{i,j}$ in the approximation (89).

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Silicon-Crystal Determination of the Absolute Scale of X-Ray Wavelengths*†

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In a recent evaluation of the atomic constants, the value of Avogadro's number is $N=6.02252\times10^{23}$ (g mole)$^{-1}\pm11$ ppm (probable error). Measurements on the atomic weight of silicon give $A=28.0857$ ±10 ppm. Precision measurements of the density of silicon combined with the above values in the Bragg equation $a=(fA/\rho N)^{1/3}$ result in an absolute grating constant of high precision. X-ray diffraction measurements with the same crystal yield the grating constant in x units; thus the conversion factor from x units to cm can be evaluated. X-ray and density measurements have been made on 17 selected silicon crystals from four different sources. The statistical error in the measurement of the densities of the 17 crystals was ±0.4 ppm. To obtain the absolute density error, a 3 ppm probable error in the density of water must be added, giving a total error of ±3.1 ppm. The measured densities of two of the 17 crystals differed from the average by more than 3 σ, probably indicating a difference in the density of the crystals. The x-ray diffraction measurements were made with a double-crystal spectrometer using the copper $K\alpha_1$ and $K\alpha_2$ lines. The wavelengths in angstroms were evaluated from the Bragg law for each of the 17 crystals and for the α_1 and α_2 lines. The average wavelengths were Cu $K\alpha_1=1.540563$ Å±5 ppm, and Cu $K\alpha_2=1.544390$ Å±5 ppm. Taking the *peak* wavelength values of 1537.400 xu±1 ppm for the Cu$K\alpha_1$ and 1541.219 xu±6.5 ppm for the Cu $K\alpha_2$ lines yields a wavelength conversion factor from angstrom to thousand x units of $\Lambda=1.002057$ Å/kxu±5ppm. Recalculation of the best measurements in the literature with current values of the atomic weights gave values which agree with the present work within probable errors. Plane-ruled-grating measurements of x-ray wavelengths yield a value of $\Lambda=1.00203\pm30$ ppm, which is lower than the above values, but the probable errors overlap.

INTRODUCTION

THE absolute (cm or Å) scale of x-ray wavelengths has been established primarily by the ruled grating measurements[1–4] of a few x-ray lines which gave the correction factor[5] 1.00203 for converting wavelengths in x units to mÅ. The impossibility of accurately correcting Tyrén's concave grating measurements for the Lamb shift,[6] DuMond and Kirkpatrick's[7] difficulties in repeating Tyrén's measurements, theoretical questions,[8] and the experimental problems involved in attempting to improve the plane grating measurements by the use of crystals for separating the α_1, α_2 lines, emphasize the importance of establishing the x-ray wavelength scale by other methods. Actually only one set of plane grating measurements[1] is free of serious errors, and this has a probable error of 30 ppm.

Bragg[9] was the first to calculate the grating constant

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