Quantum Statistics of the Distribution Functions*

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A statistical-mechanical theory of evaluating the distribution functions of a many-body system is presented. The theory is a natural extension of the quantum statistical theory of Lee and Yang for the grand partition function and gives a new formalism which is different from that developed recently by Fujita, Isihara, and Montroll. The density matrices are first developed in the Uhlenbeck–de Boer U functions. A diagrammatical consideration separates out nonconnected products from connected products of the U functions, yielding an expansion formula which is simpler than that reported by de Boer some time ago. Application of the resulting expression to free bosons and fermions is made. Then the distribution functions are developed in the binary kernel introduced by Yang and Lee. This expansion is used for the evaluation of the pair distribution function of a hard-sphere Bose gas at the lowest temperature. The results improve upon those reported previously by Lee, Huang, and Yang and others. The normalization and divergence difficulties encountered by Fujita and Hirota are removed. Actually, their interpretation of Lee, Huang, and Yang's results in terms of the chain diagrams is not satisfactory. Instead the chain diagram results may be compared with the more recent results by Wu. Use of the approximate pseudopotential $\phi=8\pi a\delta(r_1-r_2)$ is reflected in insufficiency of the chain diagram approximation. Satisfactory and consistent results are obtained when a new set of diagrams is taken into consideration.

1. INTRODUCTION

THE thermodynamical properties of a many-body system may be derived from the partition function, and there have been published a number of quantum-statistical theories for the partition function.[1] However, it is also important to evaluate the density matrix itself and its diagonal elements—the distribution functions.[2] In particular, the pair distribution function is most important in deriving thermodynamic functions and obtaining information concerning the spatial correlations of particles. Particularly, for a Bose system it is recalled that Feynman attributed the peculiar properties of liquid helium to the energy spectrum via the pair distribution function.[3]

Recently a quantum-statistical method of evaluating the pair distribution function has been presented by Fujita, Isihara, and Montroll.[4] These authors have generalized the theory of Montroll and Ward for the grand partition function of a quantum-mechanical system and have applied their general formalism to an electron gas. However, their method is based on a perturbation expansion in potentials and may not be conveniently applied to the cases where the Fourier transforms of the interaction potentials do not exist. In the present paper, therefore, we aim at developing a new theory of the pair distribution function applicable to such cases.

The theory which will be developed in this paper is a natural extension of the quantum-statistical theory given recently by Yang and Lee for the grand partition function.[5] In a series of papers, these investigators have extended Uhlenbeck and de Boer's U-function method for quantum gases, and applied their formalism to investigating a Bose gas at very low temperatures. Since such a gas may be considered as a model of liquid helium and since the singular hard-sphere potential prohibits the usual perturbation methods, its treatment is of considerable theoretical interest.[6,7]

For this purpose, Lee, Huang, and Yang introduced the pseudopotential and evaluated the ground-state wave function. The wave function was then used for the evaluation of the ground-state energy and the pair distribution function. The ground-state energy thus evaluated involved a divergence due to the approximation made in the pseudopotential. Subtracting the divergent term, they arrived at the correct ground-state energy, which coincided with that obtained by Lee and Yang by the binary kernel method. However, it is to

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[1] M. L. Goldberger and E. N. Adams II, J. Chem. Phys. **20**, 240 (1952); T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955); J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957); N. M. Hugenholtz, Physica **23**, 481 (1957); J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957); **A243**, 336 (1958); **A244**, 199 (1958); M. Shafroth, S. Butler, and J. Blatt, Helv. Phys. Acta **30**, 93 (1957); C. Bloch, Nucl. Phys. **7**, 451 (1958); C. Bloch and C. De Dominicis, *ibid.* **7**, 459 (1958); **10**, 181 (1959); M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 366 (1957); M. Gell-Mann, *ibid.* **106**, 369 (1957); E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).

[2] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, translated by R. A. Silverman (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963); P. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959); A. Klein and R. Prange, *ibid.* **112**, 994 (1958).

[3] R. P. Feynman, Phys. Rev. **97**, 660 (1955).

[4] S. Fujita, A. Isihara, and E. Montroll, Bull. Classe Sci. Acad. Roy. Belg. **44**, 1018 (1958).

[5] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959); **116**, 25 (1959); **117**, 22 (1960).

[6] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 117, 1128 (1957).

[7] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957); K. Huang, C. N. Yang, and J. Luttinger, *ibid.* **105**, 776 (1957); C. De Dominicis and P. C. Martin, *ibid.* **105**, 1417 (1957); T. D. Lee, K. Huang, and C. N. Yang, *ibid.* **106**, 1135 (1957).

be noted that the same wave function was used in deriving the pair distribution function. Thus, one may expect a possible improvement upon their distribution function.

More recently, Fujita and Hirota, using Yang and Lee's approximate pseudopotential, evaluated the pair distribution function of a dilute hard-sphere gas at the lowest temperature by summing the chain diagrams.[8] However, their treatment involved two unfortunate difficulties; one concerned with the normalization, and the other with the divergence in the ground-state energy to which their pair distribution function leads. They could not resolve these difficulties, as mentioned in their paper, but were obliged to remove arbitrarily the undesirable term in their resulting expression to make their results agree with those reported previously by Lee, Huang, and Yang.

In view of these situations it is desirable to try to develop a new theory for the pair distribution function of a hard-sphere Bose gas. We shall show in this article that the interpretation of Lee, Huang, and Yang's result by Fujita and Hirota in terms of the chain diagrams is not correct. Actually, the chain diagrams are important at large distances, and at small distances a new set of diagrams plays a more important role than the chain diagrams. This new set of diagrams may be considered as a special type of chain diagram. We find it convenient to distinguish these diagrams from the chain diagrams because their summation corresponds to introducing an effective two-particle propagator, while the summation over chain diagrams corresponds to an effective interaction potential.

In the next section we shall first express the distribution functions in a series of U functions. We then express the series in the binary kernel introduced by Lee and Yang. Finally, we apply the result to a dilute hard-sphere gas in the ground state. As a result of taking the new set of diagrams into consideration the divergence and normalization difficulties encountered by Fujita and Hirota will be removed. The necessity for considering such diagrams will be elucidated in the discussion section of this article.

Throughout this paper we shall use units such that $\hbar=1$ and $2m=1$, where m is the mass. Also, we shall use β for $1/kT$ and z for the absolute activity.

2. EXPANSION OF THE DISTRIBUTION FUNCTION

We shall start with the density matrix for an N-particle system:

$$\langle \mathbf{r}'^N|W_N{}^\alpha|\mathbf{r}^N\rangle=\sum_k \psi_k(\mathbf{r}'^N)\exp(-\beta\mathfrak{IC}_N)\psi_k{}^*(\mathbf{r}^N), \quad (2.1)$$

where $\mathbf{r}^N=(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_2,\cdots,\mathbf{r}_N)$ and

$$W_N=\exp(-\beta\mathfrak{IC}_N), \quad (2.2)$$

$\mathfrak{IC}$ being the Hamiltonian

$$\mathfrak{IC}_N=-\sum_{i=1}\nabla_i{}^2+\sum_{i<j}\phi_{ij}. \quad (2.3)$$

The ψ_k form an orthonormal complete set of functions. The suffix α to W_N indicates the statistics appropriate to the system. Thus,

$$\langle \mathbf{r}'^N|W_N{}^\alpha|\mathbf{r}^N\rangle=\sum_P C_P\langle \mathbf{r}'^N|W_N|\mathbf{r}^N\rangle. \quad (2.4)$$

The sign function C_P takes on the value $+1$ or -1 for fermions depending on the even or odd permutations P of the particle coordinates, and $+1$ for bosons.

The reduced distribution function for the n particles of coordinates $\mathbf{r}^n$ in this system is given by

$$g_N{}^{(n)}=\frac{1}{(N-n)!}\frac{1}{Z_N}\int\langle \mathbf{r}^N|W_N|\mathbf{r}^N\rangle d\mathbf{r}_{n+1}d\mathbf{r}_{n+2}\cdots d\mathbf{r}_N, \quad (2.5)$$

where Z_N, the partition function, is

$$Z_N=\frac{1}{N!}\int\langle \mathbf{r}^N|\exp(-\beta\mathfrak{IC}_N)|\mathbf{r}^N\rangle d\mathbf{r}^N. \quad (2.6)$$

In treating many-body systems, it is convenient to use the distribution functions defined in the grand canonical ensemble

$$\begin{aligned} g^{(n)}(\mathbf{r}^n)&=\frac{1}{\Xi}\sum_{N\geq n} g_N{}^{(n)}z^N Z_N \\ &=\frac{1}{\Xi}\sum_{N\geq n}\frac{z^N}{(N-n)!}\int\langle \mathbf{r}^N|W_N{}^\alpha|\mathbf{r}^N\rangle d\mathbf{r}_{n+1}\cdots d\mathbf{r}_N, \end{aligned} \quad (2.7)$$

where Ξ is the grand partition function

$$\Xi=\sum z^N Z_N. \quad (2.8)$$

Following de Boer[9] and Lee and Yang,[2] we introduce the U functions by

$$\begin{aligned} &\langle \mathbf{r}_1'|W_1{}^\alpha|\mathbf{r}_1\rangle=\langle \mathbf{r}_1'|U_1{}^\alpha|\mathbf{r}_1\rangle; \\ &\langle \mathbf{r}_1',\mathbf{r}_2'|W_2{}^\alpha|\mathbf{r}_1,\mathbf{r}_2\rangle=\langle \mathbf{r}_1'|U_1{}^\alpha|\mathbf{r}_1\rangle\langle \mathbf{r}_2'|U_1{}^\alpha|\mathbf{r}_2\rangle \\ &\qquad+\langle \mathbf{r}_1',\mathbf{r}_2'|U_2{}^\alpha|\mathbf{r}_1,\mathbf{r}_2\rangle; \\ &\qquad\cdots, \end{aligned} \quad (2.9)$$

and define the cluster integrals by

$$b_l=\frac{1}{l!V}\int\langle \mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|U_l{}^\alpha|\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle d\mathbf{r}^l. \quad (2.10)$$

Then, the grand partition function may be expanded in a cluster series:

$$\ln\Xi=V\sum_l b_l z^l. \quad (2.11)$$

[8] S. Fujita and R. Hirota, Phys. Rev. **118**, 6 (1960).

[9] J. de Boer, Rept. Progr. Phys. **12**, 305 (1948).

Correspondingly, the one-body distribution function may be developed in a series of U functions as follows:

$$g^{(1)}(\mathbf{r}_1)=\frac{1}{\Xi}\sum_{N=1}^{\infty}\frac{z^N}{(N-1)!}\int d\mathbf{r}_2\cdots d\mathbf{r}_N\langle \mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N|\,W_N{}^{\alpha}|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N\rangle$$

$$=\frac{1}{\Xi}\sum_{N=1}^{\infty}\frac{z^N}{(N-1)!}\sum_{l=1}^{N}\frac{(N-1)!}{(l-1)!(N-l)!}\int d\mathbf{r}_2\cdots d\mathbf{r}_l\langle \mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,U_l{}^{\alpha}|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle$$

$$\times\frac{(N-l)!}{2\pi i}\oint\exp\Big[\sum_s x^s(s!)^{-1}\int\langle \mathbf{r}^s|\,U_s{}^{\alpha}|\,\mathbf{r}^s\rangle d\mathbf{r}^s\Big]\frac{dx}{x^{N-l+1}}$$

$$=\frac{1}{\Xi}\frac{1}{2\pi i}\oint\exp\Big[\sum_s x^s(s!)^{-1}\int\langle \mathbf{r}^s|\,U_s{}^{\alpha}|\,\mathbf{r}^s\rangle d\mathbf{r}^s\Big]\frac{dx}{x-z}\sum_l\frac{z^l}{(l-1)!}\int d\mathbf{r}_2d\mathbf{r}_3\cdots d\mathbf{r}_l\langle \mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,U_l{}^{\alpha}|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle$$

$$=\sum_{l=1}^{\infty}\frac{z^l}{(l-1)!}\int\langle \mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,U_l{}^{\alpha}|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle d\mathbf{r}_2\cdots d\mathbf{r}_l. \tag{2.12}$$

Here in the second line the combinatorial factor corresponds to choosing $l-1$ particles out of $N-1$ particles, excluding the first particle with the coordinates $\mathbf{r}_1$. The factor $(N-l)!$ is due to the combinatorial factor of subgrouping $(N-l)$ particles into m_l groups of l particles subject to

$$\sum lm_l=N-l. \tag{2.13}$$

This factor is

$$(N-l)!\sum_{m_l}\prod_l\frac{1}{[m_l!][l!]^{m_l}}.$$

Here the weight factors $\prod 1/[m_l!][l!]^{m_l}$ have been automatically included in the above equation in the expansion of the exponential function. Thus the last expression (2.12) is obtained by simply using the expansion (2.11) for the grand partition function.

The pair distribution function may be expressed in a similar cluster series by remembering that the products of U_l functions which appear in the expansion of $W_N{}^{\alpha}$ can be classified into two groups:

(i) products which involve $\mathbf{r}_1$ and $\mathbf{r}_2$ in separate U functions;
(ii) those in which $\mathbf{r}_1$ and $\mathbf{r}_2$ appear in the same U functions.

The first group has a common structure of the following type:

$$\langle \mathbf{r}_1,\mathbf{r}_3,\cdots,|\,U_l|\,\mathbf{r}_1,\mathbf{r}_3,\cdots\rangle\langle \mathbf{r}_2,\mathbf{r}_4,\cdots|\,U_m|\,\mathbf{r}_2,\mathbf{r}_4,\cdots\rangle$$
$$\times\{\text{sum of products of } U \text{ functions corresponding to the remaining } (N-l-m) \text{ particles}\}.$$

The integrations over the U functions which do not involve 1 or 2 are the same as in Eq. (2.10). Introducing a necessary combinatorial factor, we thus have

$$\frac{(N-2)!}{(l-1)!(N-l-1)!}\frac{(N-l-1)!}{(m-1)!(N-l-m)!}\int\langle \mathbf{r}_1,\mathbf{r}_3,\cdots|\,U_l|\,\mathbf{r}_1,\mathbf{r}_3,\cdots\rangle d\mathbf{r}_3\cdots d\mathbf{r}_l$$
$$\times\int\langle \mathbf{r}_2,\mathbf{r}_4,\cdots|\,U_m|\,\mathbf{r}_2,\mathbf{r}_4,\cdots\rangle d\mathbf{r}_4\cdots d\mathbf{r}_m\frac{(N-l-m)!}{2\pi i}\oint\frac{\exp\Big[\sum x^s(s!)^{-1}\int\langle \mathbf{r}^s|\,U_s|\,\mathbf{r}^s\rangle d\mathbf{r}^s\Big]}{x^{N-l-m+1}}dx.$$

Therefore, multiplying this by $z^N/\Xi(N-2)!=z^lz^mz^{N-l-m}/\Xi(N-2)!$ and summing over all N values starting with $N=2$, we obtain

$$\frac{1}{\Xi}\sum_l\frac{z^l}{(l-1)!}\int\langle \mathbf{r}_1,\mathbf{r}_3,\cdots|\,U_l|\,\mathbf{r}_1,\mathbf{r}_3,\cdots\rangle d\mathbf{r}_3\cdots d\mathbf{r}_l\sum_m\frac{z^m}{(m-1)!}\int\langle \mathbf{r}_2,\mathbf{r}_4,\cdots|\,U_m|\,\mathbf{r}_2,\mathbf{r}_4,\cdots\rangle d\mathbf{r}_4\cdots d\mathbf{r}_m$$
$$\times\frac{1}{2\pi i}\oint\frac{\exp\Big[\sum_s x^s(s!)^{-1}\int\langle \mathbf{r}^s|\,U_s|\,\mathbf{r}^s\rangle d\mathbf{r}^s\Big]}{x-z}dx=g^{(1)}(\mathbf{r}_1)g^{(1)}(\mathbf{r}_2). \tag{2.14}$$

The terms belonging to the second group have the form

$$\langle \mathbf{r}_1,\mathbf{r}_2,\cdots|\,U_l\,|\,\mathbf{r}_1,\mathbf{r}_2,\cdots\rangle\times\text{sum of products of } U \text{ functions which do not involve either } r_1 \text{ or } r_2.$$

The necessary combinatorial factor and the contribution are

$$\frac{(N-2)!}{(l-2)!(N-l)!}(N-l)!\frac{1}{2\pi i}\oint\frac{\exp\left[\sum x^s(s!)^{-1}\int\langle\mathbf{r}^s|\,U_s\,|\,\mathbf{r}^s\rangle d\mathbf{r}^s\right]}{x^{N-l+1}}dx\int\langle\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,U_l\,|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle d\mathbf{r}_3 d\mathbf{r}_4\cdots d\mathbf{r}_l.$$

Multiplying this by $z^N/\Xi(N-2)!$, and performing the summation over N, we end up with

$$\frac{1}{\Xi}\sum_{l=2}\frac{z^l}{(l-2)!}\int\langle\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\cdots,\mathbf{r}_l|\,U_l\,|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle d\mathbf{r}_3\cdots d\mathbf{r}_l\frac{1}{2\pi i}\oint\frac{dx}{x-z}\exp\left[\sum_s x^s(s!)^{-1}\int\langle\mathbf{r}^s|\,U_s\,|\,\mathbf{r}^s\rangle d\mathbf{r}^s\right]$$

$$=\sum_2\frac{z^l}{(l-2)!}\int\langle\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,U_l\,|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle d\mathbf{r}_3\cdots d\mathbf{r}_l. \quad (2.15)$$

Therefore, combining (2.14) and (2.15) we arrive at the formula

$$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=\sum\frac{z^l}{(l-2)!}\int\langle\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,U_l\,|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle d\mathbf{r}_3\cdots d\mathbf{r}_l+g^{(1)}(\mathbf{r}_1)g^{(1)}(\mathbf{r}_2). \quad (2.16)$$

This coincides with the cluster expansion obtained by Fujita, Isihara, and Montroll in terms of the propagators. It is remarked that these authors expanded the pair distribution function in ascending powers of the potentials. We have not expanded the U functions yet, but later shall develop U in the binary kernel introduced by Lee and Yang.

Our graphical considerations enabled us to separate out in Eq. (2.16) those configurations of particles which are not correlated. In this respect, it is more convenient than the expansion reported by de Boer.[9]

3. MOMENTUM-SPACE REPRESENTATION

The pair distribution function may be conveniently represented in momentum space. For this purpose we use the transformation matrix

$$\langle\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_l|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle=(1/\Omega^{l/2})\exp(-i\sum_s\mathbf{k}_s\cdot\mathbf{r}_s). \quad (3.1)$$

Its inverse is

$$\langle\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l|\,\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_l\rangle=(1/\Omega^{l/2})\exp(i\sum_s\mathbf{k}_s\cdot\mathbf{r}_s), \quad (3.2)$$

where Ω represents the volume of the system. We write the matrix element of $U_l{}^\alpha$ in r space as follows:

$$\langle\mathbf{r}_1',\mathbf{r}_2',\cdots,\mathbf{r}_l'|\,U_l{}^\alpha\,|\,\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle=\frac{1}{\Omega^l}\sum_{\mathbf{k}',\mathbf{k}}\langle\mathbf{k}_1',\mathbf{k}_2',\cdots,\mathbf{k}_l'|\,U_l{}^\alpha\,|\,\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_l\rangle\exp(i\sum\mathbf{k}_s'\cdot\mathbf{r}_s'-i\sum\mathbf{k}_s\cdot\mathbf{r}_s). \quad (3.3)$$

Thus, by putting $\mathbf{r}_1'=\mathbf{r}_1$, $\mathbf{r}_2'=\mathbf{r}_2$, $\cdots$, and integrating over $\mathbf{r}_3$, $\mathbf{r}_4$, $\cdots$, $\mathbf{r}_l$ we get

$$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)\sim\frac{1}{\Omega^2}\sum_{\mathbf{k}_1'\mathbf{k}_2',\mathbf{k}_1\mathbf{k}_2}\exp[i(\mathbf{k}_1'-\mathbf{k}_1)\cdot\mathbf{r}_1+i(\mathbf{k}_2'-\mathbf{k}_2)\cdot\mathbf{r}_2]\sum_{\mathbf{k}_3\cdots\mathbf{k}_l}\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\cdots,\mathbf{k}_l|\,U_l{}^\alpha\,|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\cdots,\mathbf{k}_l\rangle. \quad (3.4)$$

For the sake of simplicity, we shall define the momentum-space pair correlation matrix $N(\mathbf{k}_1',\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2)$ by

$$N(\mathbf{k}_1',\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2)=\sum_{l=2}\frac{z^l}{(l-2)!}\sum_{k_2\cdots k_l}\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\cdots,\mathbf{k}_l|\,U_l{}^\alpha\,|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\cdots,\mathbf{k}_l\rangle. \quad (3.5)$$

Then, using Eq. (2.16) $g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ can be expressed in a more compact form as follows:

$$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\Omega^2}\sum_{\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_1,\mathbf{k}_2}N(\mathbf{k}_1',\mathbf{k}_2';\,\mathbf{k}_1,\mathbf{k}_2)\exp[i(\mathbf{k}_1'-\mathbf{k}_1)\cdot\mathbf{r}_1+i(\mathbf{k}_2'-\mathbf{k}_2)\cdot\mathbf{r}_2]+[g^{(1)}]^2. \quad (3.6)$$

The pair distribution function may be defined in an infinite volume, and correspondingly, the summation over the k's may be replaced by integration. In the case where the system is homogeneous, $g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ depends only on the relative distance $|\mathbf{r}_2-\mathbf{r}_1|$. Also $(1/\Omega)\sum_k \rightarrow (1/8\pi^3)\int$. Thus, performing the integration over the total momentum, we arrive at a single expression

$$g^{(2)}(|\mathbf{r}_2-\mathbf{r}_1|)=(8\pi^3)^{-2}\int d\mathbf{q} \times\exp[2i\mathbf{q}\cdot(\mathbf{r}_2-\mathbf{r}_1)]N(\mathbf{q})+[g^{(1)}]^2, \quad (3.7)$$

where

$$\mathbf{q}=\tfrac{1}{2}[(\mathbf{k}_1-\mathbf{k}_2)-(\mathbf{k}_1'-\mathbf{k}_2')]. \quad (3.8)$$

The function $N(q)$ appearing in the integrand of Eq. (3.7) may be evaluated by a diagram method. For this purpose we return to the original function $N(\mathbf{k}_1',\mathbf{k}_2';\mathbf{k}_1,\mathbf{k}_2)$. This involves arguments which are not necessary in the evaluation of $g^{(2)}(|\mathbf{r}_2-\mathbf{r}_1|)$. Use of the conservation laws removes them.

The matrix element $\langle\mathbf{r}_1',\mathbf{r}_2',\cdots,\mathbf{r}_l'|U_l^{\alpha}|\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle$ may be expanded in a series of products of lower order U functions. The expansion may be obtained by considering all possible subgrouping of l integers and considering all permutations of the integers thus subgrouped. However, no term in the series shall be split into terms corresponding to completely separate number groups. For instance, in the case of U_2^s, the term $\langle\mathbf{r}_1'|U_2|\mathbf{r}_1\rangle\langle\mathbf{r}_2'|U_1|\mathbf{r}_2\rangle$ should be excluded. Thus, we have

$$\langle\mathbf{r}_1',\mathbf{r}_2'|U_2^{\alpha}|\mathbf{r}_1,\mathbf{r}_2\rangle=\pm\langle\mathbf{r}_1'|U_1|\mathbf{r}_2\rangle\langle\mathbf{r}_2'|U_1|\mathbf{r}_1\rangle +\langle\mathbf{r}_1',\mathbf{r}_2'|U_2|\mathbf{r}_1,\mathbf{r}_2\rangle\pm\langle\mathbf{r}_2',\mathbf{r}_1'|U_2|\mathbf{r}_1,\mathbf{r}_2\rangle,$$

where $+$ and $-$ signs in the first and the last terms correspond to bosons and fermions, respectively. As in this example, we have in the right-hand side of such an expansion those terms which correspond to all the even and odd permutations. Thus, if an l integer is partitioned so that m_t groups of t integers appear in accordance with the relation

$$\sum tm_t=l,$$

we will have in the right-hand side of the expansion a group of terms

$$\sum_P C_P'\langle\mathbf{r}_1',\mathbf{r}_2',\cdots,\mathbf{r}_t'|U_t|\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_t\rangle =\langle\mathbf{r}_1',\mathbf{r}_2',\cdots,\mathbf{r}_t'|\Gamma_t^s|\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_t\rangle. \quad (3.9)$$

Here Γ_t^s represents the total of the left-hand side. Thus, if the expansion is expressed in the most general way, we have

$$\langle\mathbf{r}_1',\mathbf{r}_2',\cdots,\mathbf{r}_l'|U_l^s|\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_l\rangle =\sum\{\langle\mathbf{r}_C'|\Gamma_1^s|\mathbf{r}_A\rangle\langle\mathbf{r}_D'|\Gamma_1^s|\mathbf{r}_B\rangle\cdots\} \times\{\langle\mathbf{r}_G',\mathbf{r}_A'|\Gamma_2^s|\mathbf{r}_E,\mathbf{r}_F\rangle\cdots\}. \quad (3.10)$$

In this expression, the first curly bracket involves products of Γ_1's, the second curly bracket involves the products of Γ_2^s's, and so on. Γ_1 is identical with U_1^s:

$$\langle\mathbf{k}'|U_1^s|\mathbf{k}\rangle\approx\langle\mathbf{k}'|\Gamma_1^s|\mathbf{k}\rangle =\langle\mathbf{k}'|U_1|\mathbf{k}\rangle =\delta_{\mathbf{k}\mathbf{k}'}\exp(-\beta k^2). \quad (3.11)$$

Correspondingly, in k space we expect the following expansion:

$$\langle\mathbf{k}_1',\mathbf{k}_2',\cdots,\mathbf{k}_l'|U_l^s|\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_l\rangle =\sum\{\langle\mathbf{k}_C'|\Gamma_1^s|\mathbf{k}_A\rangle\langle\mathbf{k}_D'|\Gamma_1^s|\mathbf{k}_B\rangle\cdots\} \times\{\langle\mathbf{k}_G',\mathbf{k}_H'|\Gamma_2^s|\mathbf{k}_E,\mathbf{k}_F\rangle\cdots\}. \quad (3.12)$$

In Eqs. (3.10) and (3.11), the coordinates of the terms in different brackets must be correlated with each other. For instance $\mathbf{k}_G$ might coincide with $\mathbf{k}_B$ and $\mathbf{k}_D'$ with $\mathbf{k}_A$.

The terms appearing in the right-hand side of Eq. (3.12) may be represented by diagrams similar to those introduced by Lee and Yang. The general rules of such a graphical representation, which is suitable to the evaluation of $N^{(2)}$, are as follows:

(1) Each n vertex represents Γ_n of a matrix element such as:

$$\langle\mathbf{k}_{B_1}',\mathbf{k}_{B_2}',\cdots,\mathbf{k}_{B_n}'|\Gamma_n^s|\mathbf{k}_{A_1},\mathbf{k}_{A_2},\cdots,\mathbf{k}_{A_n}\rangle.$$

(2) The coordinates $\mathbf{k}_{A_i}$ in a ket are represented by incoming lines of momenta $\mathbf{k}_{A_i}$, while those in a bra are represented by outgoing lines of momenta $\mathbf{k}_{B_i}'$.

(3) All the $\mathbf{k}_i'$ are connected to $\mathbf{k}_i$. The number of loops going out of each vertex will represent the order of Γ.

(4) A factor z is assigned to each internal line.

(5) A factor S^{-1} is introduced, where S represents the total number of permutations that leave a graph topologically unchanged.

(6) A contracted graph generated by Γ_s represents the sum of all the graphs generated by various orders of Γ_s. We represent the contracted graphs by dotted graphs. For example, a single dotted circle represents

$$\langle\mathbf{k}_i'|\Gamma_1|\mathbf{k}_i\rangle+\langle\mathbf{k}_i'|\Gamma_1|\mathbf{k}_j\rangle\langle\mathbf{k}_j'|\Gamma_1|\mathbf{k}_i\rangle+\cdots,$$

which is illustrated in Fig. 1. The contracted diagram generated by Γ_2 is illustrated in Fig. 2.

(7) A factor $m(\mathbf{k}_i)$ is assigned to the ith internal line of a contracted graph, where $\mathbf{k}_i\neq\mathbf{k}_1$ or $\mathbf{k}_2$ and

$$m(\mathbf{k}_i)=\frac{z}{1-z\exp(-\beta k_i^2)}.$$

In applying the rules a few remarks may be helpful. First, it is noted that

$$\langle\mathbf{r}_1'|U_1^s|\mathbf{r}_1\rangle=\lambda^{-3}\exp[-(\mathbf{r}_1-\mathbf{r}_1')^2/4\beta]; \quad \lambda=(4\pi\beta)^{1/2}. \quad (3.13)$$

λ is the thermal de Broglie wavelength. In momentum space, $\langle \mathbf{k}_1' | U_1 | \mathbf{k}_1 \rangle$ is given by Eq. (3.11). It is represented by a straight line $\mathbf{k}_1\mathbf{k}_1'$ of a single vertex representing Γ_1.

For the next simplest case of $l=2$, we have

$$\langle \mathbf{k}_1',\mathbf{k}_2' | U_2{}^s | \mathbf{k}_1,\mathbf{k}_2 \rangle = \langle \mathbf{k}_2' | U_1 | \mathbf{k}_1 \rangle \langle \mathbf{k}_1' | U_1 | \mathbf{k}_2 \rangle + \langle \mathbf{k}_1',\mathbf{k}_2' | \Gamma_2{}^s | \mathbf{k}_1,\mathbf{k}_2 \rangle . \quad (3.14)$$

Accordingly, we have the two diagrams such as illustrated in Fig. 3. Here Fig. 3(a) represents the first term and Fig. 3(b) the second term of Eq. (3.14). These diagrams reduce to toron-type diagrams introduced by Montroll and Ward [Figs. 3(a'), 3(b')] if the end points of the straight lines are connected. The series appearing in the right-hand side of Eq. (3.12) may then be rearranged in accordance with the number of toron loops. In particular, U_l involves a term which consists of l Γ_1's. It may be represented by l-toron diagrams since all the Γ_1's must be connected with each other through their arguments.

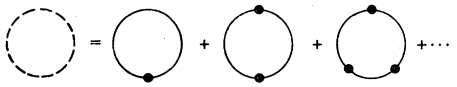

FIG. 1. A contracted graph (dotted circle) generated by Γ_1.

4. FREE PARTICLE

We shall now compute N_0 for a system of noninteracting bosons applying the above rules. In this special case, all U_l for $l \geq 2$ vanish. Thus, corresponding to Fig. 4 we have

$$\begin{aligned} N_0 &= \delta_{\mathbf{k}_2'\mathbf{k}_1}\delta_{\mathbf{k}_1'\mathbf{k}_2}\{z^2 \exp(-\beta k_1{}^2 - \beta k_2{}^2) + z^3 \exp(-\beta k_1{}^2) \\ &\quad \times \exp(-2\beta k_2{}^2) + z^3 \exp(-2\beta k_1{}^2) \exp(-\beta k_2{}^2) + \cdots\} \\ &= \delta_{\mathbf{k}_2'\mathbf{k}_1}\delta_{\mathbf{k}_1'\mathbf{k}_2} \exp(-\beta k_1{}^2 - \beta k_2{}^2) m(\mathbf{k}_1) m(\mathbf{k}_2) , \end{aligned} \quad (4.1)$$

where

$$m(\mathbf{k}) = \frac{z}{1 - z \exp(-\beta k^2)} , \quad (4.2)$$

By substituting Eq. (4.1) into Eq. (3.6), we get

$$\begin{aligned} g_0{}^{(2)}(\mathbf{r}_1,\mathbf{r}_2) &= \frac{1}{\Omega^2} \sum_{\mathbf{k}_1,\mathbf{k}_2} \exp(-\beta k_1{}^2 - \beta k_2{}^2) m(\mathbf{k}_1) m(\mathbf{k}_2) \\ &\quad \times \exp\{i\mathbf{k}_1 \cdot (\mathbf{r}_2 - \mathbf{r}_1) - i\mathbf{k}_2 \cdot (\mathbf{r}_2 - \mathbf{r}_1)\} + [g_0{}^{(1)}]^2 \\ &= n^2 + \left| \frac{1}{\Omega} \sum_{k} \exp(-\beta k^2) m(\mathbf{k}) \right. \\ &\quad \left. \times \exp[-i\mathbf{k} \cdot (\mathbf{r}_2 - \mathbf{r}_1)] \right|^2 , \end{aligned} \quad (4.3)$$

where we have identified $g_0{}^{(1)}$ as the number density n.

We have derived the above formula for free bosons.

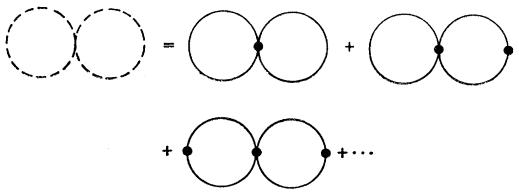

FIG. 2. A contracted graph (dotted circle) generated by Γ_2.

For free fermions we need only to use

$$m(\mathbf{k}) = \frac{z}{1 + z \exp(-\beta k^2)} , \quad (4.4)$$

and a minus sign for the second term in Eq. (4.3).

Equation (4.3) is in agreement with the expression derived by Fujita, Isihara, and Montroll by summing toron diagrams.[10] The labor of evaluation is more or less the same.

It may be interesting to check the normalization of Eq. (4.3). Upon integrating over $\mathbf{r}_1$ and $\mathbf{r}_2$ we find

$$\int g_0{}^{(2)}(\mathbf{r}_1,\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 = \langle N \rangle^2 + \sum_k e^{-2\beta k^2} m^2(k) .$$

Using the grand ensemble relations,

$$\begin{aligned} \langle N \rangle &= \sum_k m(k) e^{-\beta k^2} , \\ \langle N^2 \rangle - \langle N \rangle^2 &= \sum_k m(k) e^{-\beta k^2} + \sum_k m^2(k) e^{-2\beta k^2} , \end{aligned} \quad (4.5)$$

we end up with

$$\int g_0{}^{(2)}(\mathbf{r}_1,\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 = \langle N(N-1) \rangle . \quad (4.6)$$

5. THE BINARY KERNEL

Further reduction of Eq. (2.16) may be achieved by expanding U_l in powers of the interaction potential, since the operator W_N defined by Eq. (2.2) may be

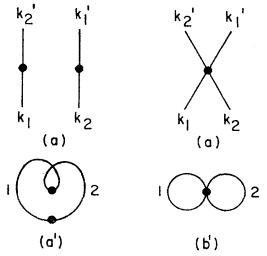

FIG. 3. Diagrams for $U_2{}^s$.

[10] S. Fujita, A. Isihara, and E. W. Montroll, Ref. 4. See also, F. London, J. Chem. Phys. 11, 203 (1943) and G. Placzek, Proc. 2nd Berkeley Symp. Math. Stat. and Prob. 581, 1950 (unpublished).

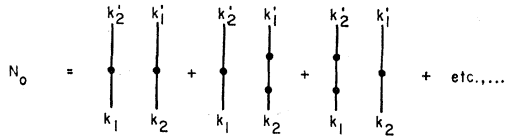

FIG. 4. Diagrams for a free-particle system.

expanded in the following well-known perturbation series:

$$W_N(\beta)=W_N{}^0(\beta)+\int_0^\beta W_N{}^0(\beta-\beta')(-\Phi_N)W_N{}^0(\beta')d\beta'$$
$$+\int_0^\beta d\beta'\int_0^{\beta'} d\beta'' W_N{}^0(\beta-\beta')(-\Phi_N)$$
$$\times W_N{}^0(\beta'-\beta'')(-\Phi_N)W_N{}^0(\beta'')+\cdots, \quad (5.1)$$

where it is assumed that the potential $\Phi_N=\sum\phi_{ij}$ is finite and the series converges. Also

$$W_N{}^0(\beta)=\prod_{i=1}^N w(\beta;i);$$
$$w(\beta;i)=\exp(\beta\nabla_i{}^2). \quad (5.2)$$

The right-hand side of Eq. (5.1) may be represented by diagrams. For this purpose, $w(\beta-\beta';i)$ shall be represented by a vertical line segment ii' of length $\beta-\beta'$, the position of i' corresponding to an interaction, say $-\phi(|r_i'-r_j'|)$, which takes place at an intermediate temperature β' and is represented by a horizontal line at β'. The horizontal lines in a diagram are placed such that the lower lines represent the interaction potentials which appear further to the right in the perturbation series. Then $W_N(\beta)$ is represented by connected and unconnected diagrams. On the other hand, U_l is expressed only in terms of connected diagrams of l particles.

The diagrams for the operator W_N or U_l are simpler than those introduced by Montroll and Ward for the propagators. This is because no complication due to statistics comes in here. However, when one tries to evaluate the matrix element of W_N or U_l, toron-type diagrams may be introduced in accordance with the symmetry of the function operated by W_N or U_l.

The general structure of our diagram representation is simple, and no elaborate discussion seems to be necessary. Instead, it seems advisable to add comments on the binary kernel[11] $B(\beta)$ and the corresponding diagrams.

Lee and Yang introduced the binary kernel by

$$B(\beta;1,2)=-\phi_{12}\exp(-\beta H_2), \quad (5.3)$$

where B is related to U_2 by the differential equation

$$B(\beta;1,2)=(\partial U_2/\partial\beta)-(\nabla_1{}^2+\nabla_2{}^2)U_2(\beta). \quad (5.4)$$

The binary kernel is determined by two particles and is dependent only implicitly on the potential function. It may, therefore, be used even for the cases where the potential is divergent.

We shall represent the binary kernel as in Fig. 5.

In terms of the binary kernel the first few U_l are expressed as follows:

$$U_2=\int_0^\beta d\beta' w(\beta-\beta';1)w(\beta-\beta';2)B(\beta';1,2);$$

$$U_3=\int_0^\beta d\beta'\int_0^{\beta'} d\beta'' w(\beta-\beta'';1)w(\beta-\beta';2)w(\beta-\beta';3)$$
$$\times B(\beta'-\beta'';2,3)B(\beta'';1,2)w(\beta'';3)$$
$$+\int_0^\beta d\beta'\int_0^{\beta'} d\beta'' w(\beta-\beta';1)w(\beta-\beta';2)w(\beta-\beta'';3)$$
$$\times B(\beta'-\beta'';1,2)B(\beta'';2,3)w(\beta'';1)+\cdots. \quad (5.5)$$

The corresponding diagrams are given in Fig. 6.

The binary kernel for hard spheres has been evaluated by Lee and Yang. In the next section we shall use the expansion of B in the hard-sphere diameter a:

$$B=B_1+B_2+\cdots;$$
$$B_1=-a\pi^{-2}\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_1'-\mathbf{k}_2')\exp[-\beta(k_1{}^2+k_2{}^2)];$$
$$B_2=\pi^{-5/2}a^2\delta(\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1'-\mathbf{k}_2')\exp[-\beta(k_1{}^2+k_2{}^2)]$$
$$\times\Big[|\mathbf{k}_1-\mathbf{k}_2|\int_0^{(2\beta)^{1/2}|\mathbf{k}_1-\mathbf{k}_2|} dx\exp(x^2)-(2\beta)^{-1/2}$$
$$\times\exp[2\beta(\mathbf{k}_1-\mathbf{k}_2)^2]\Big]. \quad (5.6)$$

6. CHAIN-DIAGRAM APPROXIMATION

In this section we shall evaluate the pair distribution function for a dilute Bose gas at absolute zero temperature in the chain-diagram approximation. The chain diagrams are obtained by connecting 1 and 2 by a linear array of the other particles linked together by binary kernels as shown in Fig. 7. The calculations may be made for a Boltzmann gas because at absolute zero the

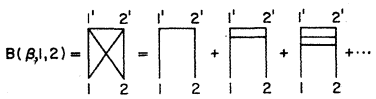

FIG. 5. The binary kernel.

[11] A. J. F. Siegert and E. Teramoto, Phys. Rev. 110, 1232 (1958); T. D. Lee and C. N. Yang, *ibid.* 113, 1165 (1959).

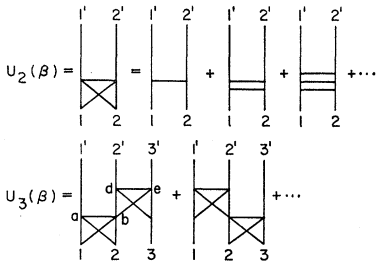

FIG. 6. Diagrams representing U_2 and U_3 in terms of the binary kernel.

result can also be used for a Bose gas.

We start with

$$U_2(\beta)=\int_0^\beta d\beta' w(\beta-\beta';1)w(\beta-\beta';2)B(\beta';1,2). \quad (6.1)$$

In coordinate representation, this matrix element is [see Fig. 7(a)]

$$\langle \mathbf{r}_1',\mathbf{r}_2'|\,U_2(\beta)\,|\,\mathbf{r}_1,\mathbf{r}_2\rangle=\int_0^\beta d\beta'\int d\mathbf{r}_a d\mathbf{r}_b\langle \mathbf{r}_1'|\,w(\beta-\beta')\,|\,\mathbf{r}_a\rangle$$
$$\times\langle \mathbf{r}_2'|\,w(\beta-\beta')\,|\,\mathbf{r}_b\rangle\langle \mathbf{r}_a,\mathbf{r}_b|\,B(\mathbf{r}')\,|\,\mathbf{r}_1\mathbf{r}_2\rangle, \quad (6.2)$$

where

$$\langle \mathbf{r}'|\,w(\beta)\,|\,\mathbf{r}\rangle=(8\pi^3)^{-1}\int d\mathbf{k}\,\exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')-\beta k^2]. \quad (6.3)$$

The transformation to momentum-space representation is achieved by using

$$\langle \mathbf{r}|\,\mathbf{k}\rangle=(8\pi^3)^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r}). \quad (6.4)$$

The result is

$$\langle \mathbf{k}_1',\mathbf{k}_2'|\,U_2(\beta)\,|\,\mathbf{k}_1,\mathbf{k}_2\rangle=\int\langle \mathbf{k}_1'|\,\mathbf{r}_1'\rangle\langle \mathbf{k}_2'|\,\mathbf{r}_2'\rangle\langle \mathbf{r}_1|\,\mathbf{k}_1\rangle\langle \mathbf{r}_2|\,\mathbf{k}_2\rangle$$
$$\times\langle \mathbf{r}_1',\mathbf{r}_2'|\,U_2(\beta)\,|\,\mathbf{r}_1,\mathbf{r}_2\rangle d\mathbf{r}_1'd\mathbf{r}_2'd\mathbf{r}_1d\mathbf{r}_2. \quad (6.5)$$

Introducing Eqs. (6.2) and (6.3) into Eq. (6.5) and carrying out the $\mathbf{r}_1'$ and $\mathbf{r}_2'$ integrations, we obtain

$$\langle \mathbf{k}_1',\mathbf{k}_2'|\,U_2(\beta)\,|\,\mathbf{k}_1,\mathbf{k}_2\rangle$$
$$=\int_0^\beta d\beta'\exp\{-(\beta-\beta')k_1'^2-(\beta-\beta')k_2'^2\}$$
$$\times\langle \mathbf{k}_1',\mathbf{k}_2'|\,B(\beta')\,|\,\mathbf{k}_1,\mathbf{k}_2\rangle. \quad (6.6)$$

This is an exact result. We now make an attempt at evaluating U_2 approximately to order a, replacing B by B_1 given by Eq. (5.6). The result is

$$\langle \mathbf{k}_1',\mathbf{k}_2'|\,U_2(\beta)\,|\,\mathbf{k}_1,\mathbf{k}_2\rangle=-a\pi^{-2}\int_0^\beta d\beta'\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_1'-\mathbf{k}_2')$$
$$\times\exp\{-(\beta-\beta')(k_1'^2+k_2'^2)-\beta'(k_1^2+k_2^2)\}. \quad (6.7)$$

This expression may be simplified by remembering that by definition $g^{(2)}$ is a function only of relative coordinates if the system is homogeneous. Thus, we introduce the relative momenta and the center-of-gravity momenta as follows:

$$\begin{aligned}&\mathbf{k}=\tfrac{1}{2}(\mathbf{k}_1-\mathbf{k}_2), \quad \mathbf{k}'=\tfrac{1}{2}(\mathbf{k}_1'-\mathbf{k}_2'),\\ &\mathbf{K}=\mathbf{k}_1+\mathbf{k}_2, \quad \mathbf{K}'=\mathbf{k}_1'+\mathbf{k}_2'.\end{aligned} \quad (6.8)$$

Using Eq. (6.8) in Eq. (6.7) and integrating over $\mathbf{K}$ and $\mathbf{K}'$, we obtain

$$\langle \mathbf{k}'|\,U_2|\,\mathbf{k}\rangle=-\left(\frac{2\pi}{\beta}\right)^{3/2}a\pi^{-2}\int_0^\beta d\beta'$$
$$\times\exp\{-2\beta(k'^2-2\beta'(k^2-k'^2)\}. \quad (6.9)$$

Further simplification may be achieved by introducing the next transformation of variables:

$$\begin{aligned}&\mathbf{q}=\tfrac{1}{2}(\mathbf{k}-\mathbf{k}');\\ &\mathbf{Q}=\mathbf{k}+\mathbf{k}'.\end{aligned} \quad (6.10)$$

Using Eq. (6.10) in Eq. (6.9) and integrating over Q, we arrive at a simple function of q which we may denote by $u_2(q)$:

$$u_2(q)=-\left(\frac{2\pi}{\beta}\right)^3(a\pi^{-2})\int_0^\beta d\beta'\exp\left\{-4(\beta-\beta')q^2\right.$$
$$\left.+\frac{4}{\beta}(\beta-\beta')^2q^2-4\beta'q^2+\frac{4\beta'^2}{\beta}q^2\right\}. \quad (6.11)$$

The right-hand side may be rewritten as follows:

$$u_2(q)=-\left(\frac{2\pi}{\beta}\right)^3(a\pi^{-2})\int_0^\beta d\beta' K(q;\beta-\beta')K(q;\beta'), \quad (6.12)$$

where

$$K(q,|x-y|)=\exp\{-4|x-y|q^2+4\beta^{-1}(x-y)^2q^2\}. \quad (6.13)$$

Before attempting to simplify U_2 further, we may consider the chain diagrams for U_4 as shown in Fig. 7(c).

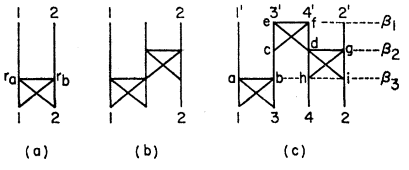

FIG. 7. First three chain diagrams.

Correspondingly we have

$$\langle \mathbf{r}_1',\mathbf{r}_2',\mathbf{r}_3',\mathbf{r}_4'|\,U_4|\,\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4\rangle$$
$$=\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_2}d\beta_3 d\mathbf{r}_a d\mathbf{r}_b d\mathbf{r}_c d\mathbf{r}_d\cdots d\mathbf{r}_i\langle \mathbf{r}_3'|\,w_1(\beta-\beta_1)|\,\mathbf{r}_e\rangle\langle \mathbf{r}_4'|\,w_1(\beta-\beta_1)|\,\mathbf{r}_f\rangle\langle \mathbf{r}_e,\mathbf{r}_f|\,B(\beta_1-\beta_2)|\,\mathbf{r}_c,\mathbf{r}_d\rangle$$
$$\times\langle \mathbf{r}_2'|\,w_1(\beta-\beta_2)|\,\mathbf{r}_g\rangle\langle \mathbf{r}_d,\mathbf{r}_g|\,B(\beta_1-\beta_2)|\,\mathbf{r}_h,\mathbf{r}_i\rangle\langle \mathbf{r}_i|\,w_1(\beta_3)|\,\mathbf{r}_2\rangle\langle \mathbf{r}_h|\,w_1(\beta_3)|\,\mathbf{r}_4\rangle\langle \mathbf{r}_1'|\,w_1(\beta-\beta_3)|\,\mathbf{r}_a\rangle$$
$$\times\langle \mathbf{r}_c|\,w_1(\beta_2-\beta_3)|\,\mathbf{r}_b\rangle\langle \mathbf{r}_a,\mathbf{r}_b|\,B(\beta_3)|\,\mathbf{r}_1,\mathbf{r}_3\rangle+\text{similar terms}. \quad (6.14)$$

Here it is assumed that

$$\beta>\beta_1>\beta_2>\beta_3.$$

The corresponding momentum-space representation is

$$\langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3',\mathbf{k}_4'|\,U_4|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle$$
$$=\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_2}d\beta_3 d\mathbf{k}_c d\mathbf{k}_d\exp\{-(\beta-\beta_1)(k_3'^2+k_4'^2)\}\langle \mathbf{k}_3',\mathbf{k}_4'|\,B(\beta_1-\beta_2)|\,\mathbf{k}_c,\mathbf{k}_d\rangle$$
$$\times\exp\{-(\beta-\beta_2)k_2'^2\}\langle \mathbf{k}_2',\mathbf{k}_d|\,B(\beta_2-\beta_3)|\,\mathbf{k}_2,\mathbf{k}_4\rangle\exp\{-\beta_3(k_2^2+k_4^2)\}\exp\{-(\beta_2-\beta_3)k_c^2\}$$
$$\times\exp\{-(\beta-\beta_3)k_1'^2\}\langle \mathbf{k}_1',\mathbf{k}_c|\,B(\beta_3)|\,\mathbf{k}_1,\mathbf{k}_3\rangle+\text{similar terms}. \quad (6.15)$$

Replacing B by B_1 and putting $\mathbf{k}_i'=\mathbf{k}_i$ for all i, we obtain

$$\langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\mathbf{k}_4|\,U_4|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle$$
$$=(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_2}d\beta_3\int dk_c dk_d\exp\{-(\beta-\beta_1)(k_3^2+k_4^2)\}\delta(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_c-\mathbf{k}_d)\exp\{-(\beta_1-\beta_2)(k_c^2+k_d^2)\}$$
$$\times\exp\{-(\beta-\beta_2)k_2'^2\}\delta(\mathbf{k}_d+\mathbf{k}_2'-\mathbf{k}_2-\mathbf{k}_4)\exp\{-(\beta_2-\beta_3)(k_2^2+k_4^2)\}\exp\{-\beta_3(k_2^2+k_4^2)\}\exp\{-(\beta_2-\beta_3)k_c^2)\}$$
$$\times\exp\{-(\beta-\beta_3)k_1'^2\}\delta(k_1'+k_c-k_1-k_3)\{\exp-\beta_3(k_1^2+k_3^2)\}+\text{similar terms}. \quad (6.16)$$

We integrate the right-hand side over the momenta of intermediate states and introduce u_4 by

$$\langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\mathbf{k}_4|\,U_4|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle=\delta(\mathbf{k}_1'+\mathbf{k}_2'-\mathbf{k}_1-\mathbf{k}_2)$$
$$\times\langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\mathbf{k}_4|\,u_4|\,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle. \quad (6.17)$$

We then integrate u_4 over the momenta $\mathbf{k}_3$ and $\mathbf{k}_4$. In view of the δ function we may put $2\mathbf{q}=\mathbf{k}_1-\mathbf{k}_1'=-(\mathbf{k}_2-\mathbf{k}_2')$. Also, we change variables so that

$$\begin{aligned}&\mathbf{k}_1=\tfrac{1}{2}\mathbf{K}+\mathbf{k};\quad \mathbf{k}_1'=\mathbf{k}_1-2\mathbf{q},\\ &\mathbf{k}_2=\tfrac{1}{2}\mathbf{K}-\mathbf{k};\quad \mathbf{k}_2'=\mathbf{k}_2+2\mathbf{q},\\ &2\mathbf{q}=\mathbf{k}_1-\mathbf{k}_1'=-(\mathbf{k}_2-\mathbf{k}_2'),\end{aligned} \quad (6.18)$$

and as in the case of u_2, we perform integrations over the momenta K and k. The result is a simple function of q which may be expressed as follows:

$$u_4(q)=\left(\frac{2\pi}{\beta}\right)^3\left(\frac{\pi}{\beta}\right)^3(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_3}d\beta_3$$
$$\times K(q;\beta-\beta_3)K(q,\beta_1-\beta_2)K(q,\beta_1-\beta_3)K(q,\beta_2)$$
$$+\text{similar terms}. \quad (6.19)$$

Removing the condition on the β's we may rewrite Eq. (6.19) as

$$u_4(q)=\left(\frac{2\pi}{\beta}\right)^3\left(\frac{\pi}{\beta}\right)^3(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_3}d\beta_3$$
$$\times K(q,|\beta-\beta_3|)K(q,|\beta_3-\beta_1|)K(q,|\beta_1-\beta_2|)$$
$$\times K(q,\beta_2)+\text{similar terms}. \quad (6.20)$$

It is remarked that there are altogether six similar chain diagrams for u_4. These differ from each other only in "time ordering." Therefore, using the Dyson theorem, their total contribution is

$$u_4(q)=2\left(\frac{2\pi}{\beta}\right)^3\left(\frac{\pi}{\beta}\right)^3(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta}d\beta_2\int_0^{\beta}d\beta_3$$
$$\times K(q,|\beta-\beta_1|)K(q,|\beta_1-\beta_2|)$$
$$\times K(q,|\beta_2-\beta_3|)K(q,|\beta_3|), \quad (6.21)$$

where the domain of integration is from 0 to β. The factor 2 is due to the interchange of the particles 3 and 4.

The generalization of the above results of Eqs. (6.12)

and (6.21) is not difficult. We end up with the following chain-diagram contribution to u_l:

$$u_l=(l-2)!(-a\pi^{-2})^{l-1}\left(\frac{2\pi}{\beta}\right)^3\left(\frac{\pi}{\beta}\right)^{3(l-2)/2}\times\int_0^\beta d\beta_1\int_0^\beta d\beta_2\cdots\int_0^\beta d\beta_{l-1}K(q,|\beta-\beta_1|)\times K(q,|\beta_1-\beta_2|)\cdots K(q,|\beta_{l-1}|). \quad (6.22)$$

It is convenient to change the scale of all the time variables by using the variable x_i defined by

$$x_i=\beta_i/\beta.$$

Accordingly, Eq. (6.22) assumes the form

$$u_l=(l-2)!(-a\pi^{-2})(2\pi/\beta)^3(\pi/\beta)^{3(l-2)/2}\beta^{l-1}\times\int_0^1 dx_1\int_0^1 dx_2\cdots\int_0^1 dx_{l-1}K(q,|1-x_1|)\times K(q,|x_1-x_2|)K(q,|x_2-x_3|)\cdots K(q,x_{l-1}). \quad (6.23)$$

We may consider that the function K is cyclic in x so that the eigenfunctions are $\exp(2\pi imx)$, m being a plus or minus integer or zero.

Thus, the mth eigenvalue of K is given by

$$\Lambda_m=\int_0^1\int_0^1 K(q,|x-y|)\psi_m{}^*(x)\psi_m(y)dxdy; \quad (6.24)$$

namely,

$$\Lambda_m=\int_0^1 \exp(-gu+gu^2)\exp(2\pi imu)du, \quad (6.25)$$

where we have used the abbreviation

$$g=4\beta q^2. \quad (6.26)$$

Λ_m should be real. Thus, Eq. (6.25) may be rewritten as

$$\Lambda_m=\int_0^1 du[\cos 2\pi mu]\exp(-gu+gu^2). \quad (6.27)$$

We are interested in the low-temperature limit of Λ_m. Taking the limit of g going to infinity we find that

$$\Lambda_m\to 2g/(g^2+4\pi^2m^2). \quad (6.28)$$

The multiple integrations in Eq. (6.23) are now performed in terms of the above eigenfunctions and eigenvalues.

We first note that if

$$K_l(q;1-0)=\int_0^1 dx_1\int_0^1 dx_2\cdots\int_0^1 dx_{l-1}K(q,1-x_1)\times K(q,|x_1-x_2|)\cdots K(q,|x_{l-1}-0|) \quad (6.29)$$

and if

$$\Lambda\psi(x)=\int_0^1 K(q,|x-y|)\psi(y)dy, \quad (6.30)$$

then, since $\psi(1)=\psi(0)=1$, we have

$$K_l(q,1-0)=\sum_m \Lambda_m{}^l\psi(1)\psi^*(0)=\sum_m \Lambda_m{}^l. \quad (6.31)$$

Therefore, we arrive at

$$u_l=(l-2)!(-a\pi^{-2})^{l-1}\left(\frac{2\pi}{\beta}\right)^3\left(\frac{\pi}{\beta}\right)^{3(l-2)/2}\beta^{l-1}\sum_{m=-\infty}^{\infty}\Lambda_m{}^l. \quad (6.32)$$

Expressing this result in terms of $\lambda=(4\pi\beta)^{1/2}$, the thermal wavelength, we find

$$u_l{}^c(q)=-32(l-2)!\pi^3a^{-1}\lambda^{-2}\sum_{m=-\infty}^{\infty}(-2a\lambda^{-1}\Lambda_m)^l, \quad (6.33)$$

where we have added the superscript c to show the chain-diagram contribution. Therefore, the Fourier transform $N(q)$ of the correlation function which has been introduced by Eqs. (3.5) and (3.7) is given by

$$N(q)=-32\pi^3a^{-1}\lambda^{-2}\sum_{l=2}^{\infty}\sum_m(-)^l(2az\lambda^{-1}\Lambda_m)^l=-128\pi^3az^2\lambda^{-4}\sum_{m=-\infty}^{\infty}\Lambda_m[\Lambda_m{}^{-1}+2az\lambda^{-1}]^{-1}. \quad (6.34)$$

Substitution of Λ_m from Eq. (6.28) gives

$$N(q)=-512\pi^5az^2\lambda^{-3}\sum_{m=-\infty}^{\infty}q^4[q^4+4\pi^4m^2\lambda^{-4}]^{-1}\times[q^4+4\pi az\lambda^{-3}q^2+4\pi^4m^2\lambda^{-4}]^{-1}. \quad (6.35)$$

For a dilute system the activity z may be replaced by z_0, the value for the noninteracting case:

$$z_0=n\lambda^3. \quad (6.36)$$

In the limit $\lambda\to\infty$, we may consider $x=2\pi^2m/\lambda$ as a continuous variable and replace the summation by integration. Thus,

$$N(q)=-256\pi^3an^2\int_{-\infty}^{\infty}q^4[q^4+x^2]^{-1}[q^4+4\pi anq^2+x^2]^{-1}dx=-\frac{256\pi^4an^2}{\gamma}\left[1-\left(1+\frac{\gamma}{q^2}\right)^{-1/2}\right], \quad (6.37)$$

where

$$\gamma=4\pi an. \quad (6.38)$$

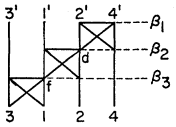

FIG. 8. Tick-tack-toe diagram.

Thus, using Eq. (3.7) we obtain

$$g^{(2)}(r)=-4\pi^{-2}\gamma^{-1}an^2 \times\int dq e^{2i\mathbf{q}\cdot\mathbf{r}}\left\{1-\left(1+\frac{\gamma}{q^2}\right)^{-1/2}\right\}+n^2. \quad (6.39)$$

The evaluation of the right-hand-side integral has not been achieved. However, for small and large distances we have

$$\begin{aligned} g^{(2)}(r)&=n^2(1-2a/r), && (r\ll r_c)\\ &=n^2(1-(4\pi^{5/2}a^{1/2}n^{3/2})^{-1}r^{-4}); && (r\gg r_c), \end{aligned} \quad (6.40)$$

where

$$r_c=(16\pi an)^{-1/2}. \quad (6.41)$$

These results coincide with those obtained by Fujita and Hirota by using the pseudopotential. These authors compared their results with those obtained by Lee, Huang, and Yang. As we shall see in the next section, caution is necessary in such a comparison.

7. THE TICK-TACK-TOE DIAGRAMS

In addition to the chain diagrams, another infinite set of diagrams plays an important role in the evaluation of the pair distribution function. Some of the diagrams which belong to this category are shown in Fig. 8. These are the diagrams which involve only one cross in each column, determined by a pair of neighboring vertical lines, and in each row, determined by the cross itself, the cross 1–2 existing always. In view of their appearance, these diagrams may be called the tick-tack-toe diagrams. These diagrams are in a sense chain diagrams, but may be named differently because they have never been considered before, and also because their effective role is different from that of the chain diagrams, as we shall discuss later.

It is convenient to start with a special case. Let us evaluate the matrix element corresponding to Fig. 8:

$$\begin{aligned}&\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3',\mathbf{k}_4'|U_4|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle\\ &=(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_2}d\beta_3 dk_f dk_d\exp\{-(\beta-\beta_1)(k_2'^2+k_4'^2)\}\delta(\mathbf{k}_d+\mathbf{k}_4-\mathbf{k}_2'-\mathbf{k}_4')\exp\{-(\beta_1-\beta_2)(k_d^2+k_4^2)\}\\ &\quad\times\exp(-\beta_2k_4^2)\exp(-(\beta-\beta_2)k_1'^2)\delta(\mathbf{k}_f+\mathbf{k}_2-\mathbf{k}_1'-\mathbf{k}_d)\exp\{-(\beta_2-\beta_3)(k_f^2+k_2^2)\}\\ &\quad\times\exp(-\beta_3k_2^2)\exp\{-(\beta-\beta_3)k_3'^2\}\delta(\mathbf{k}_3+\mathbf{k}_1-\mathbf{k}_3'-\mathbf{k}_f)\exp\{-\beta_3(k_1^2+k_3^2)\}. \end{aligned} \quad (7.1)$$

Setting $\mathbf{k}_3=\mathbf{k}_3'$, $\mathbf{k}_4=\mathbf{k}_4'$, integrating over $\mathbf{k}_f$ and $\mathbf{k}_d$, and using the notation u_4 for the matrix element thus obtained,

$$\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\mathbf{k}_4|U_4|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle=\delta(\mathbf{k}_1'+\mathbf{k}_2'-\mathbf{k}_1-\mathbf{k}_2)\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3',\mathbf{k}_4|u_4|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle,$$

we get

$$\begin{aligned}&\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3,\mathbf{k}_4|u_4|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4\rangle\\ &=(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_2}d\beta_3\exp\{-\beta(k_1'^2+k_2'^2+k_3^2+k_4^2)\}\exp\{-\beta_2(k_1^2+k_2^2-k_1'^2-k_2'^2)\}. \end{aligned} \quad (7.2)$$

We may integrate this over $\mathbf{k}_3$ and $\mathbf{k}_4$ to obtain

$$\langle\mathbf{k}_1',\mathbf{k}_2'|u_4|\mathbf{k}_1,\mathbf{k}_2\rangle=\left(\frac{\pi}{\beta}\right)^2(-a\pi^{-2})^3\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\int_0^{\beta_2}d\beta_3\exp\{-\beta(k_1'^2+k_2'^2)-\beta_3(k_1^2+k_2^2-k_1'^2-k_2'^2)\}. \quad (7.3)$$

Changing the domain of integration and summing over all 3! similar diagrams we end up with

$$\begin{aligned}\langle\mathbf{k}_1',\mathbf{k}_2'|u_4|\mathbf{k}_1,\mathbf{k}_2\rangle&=\left(\frac{\pi}{\beta}\right)^2(-a\pi^{-2})^3\beta^2\int_0^{\beta}d\beta'\exp\{-\beta(k_1'^2+k_2'^2)-\beta'(k_1^2+k_2^2-k_1'^2-k_2'^2)\}\\ &=\left(\frac{\pi}{\beta}\right)^3(-a\pi^{-2})^3\beta^3\int_0^1 dx\exp\{-\beta(k_1'^2+k_2'^2)-\beta x(k_1^2+k_2^2-k_1'^2-k_2'^2)\}. \end{aligned} \quad (7.4)$$

As in the case of the previous section, one may change the momentum variables twice, and integrate over the total momentum. The resulting function of a single variable is given by

$$u_4(q)=(2\pi/\beta)^3(\pi/\beta)^3(-a\pi^{-2})^3\beta^3\Lambda_0(\beta;q), \quad (7.5)$$

where

$$\Lambda_0(\beta;q)=\int_0^1 dx\exp\{-8x\beta q^2(1-8x\beta q^2)\}. \quad (7.6)$$

The generalization of the above calculation for the case of u_l is straightforward. We end up with

$$u_l(q)=(2\pi/\beta)^3(\pi/\beta)^{3(l-2)/2}(-a\pi^{-2})^{l-1}\beta^{l-1}\Lambda_0(\beta;q). \quad (7.7)$$

In the limit $\beta\to\infty$,

$$\Lambda_0(\beta;q)\to 1/4\beta q^2. \quad (7.8)$$

Thus,

$$u_l(q)=\frac{1}{4q^2}\left(\frac{2\pi}{\beta}\right)^3\left(\frac{\pi}{\beta}\right)^{3(l-2)/2}(-a\pi^{-2})^{l-1}\beta^{l-2}. \quad (7.9)$$

In terms of the thermal wavelength λ, Eq. (7.9) becomes

$$u_l(q)=-32\pi^4a^{-1}\lambda^{-4}(-2a\lambda^{-1})^l q^{-2}. \quad (7.10)$$

Therefore, at finite $z\lambda^{-1}$ one gets for $N(q)$ the following:

$$N(q)=-32\pi^4a^{-1}\lambda^{-4}q^{-2}\sum_{l=3}^{\infty}(-)^l(2az\lambda^{-1})^l. \quad (7.11)$$

The summation begins with $l=3$ because the case $l=2$ has been treated as a chain diagram. Finally, one obtains

$$N(q)=128\pi^4an^2q^{-2}/(1+2az\lambda^{-1}). \quad (7.12)$$

Taking the limit of low temperature and density

$$\lambda\to\infty, \quad z\lambda^{-1}\to\infty$$

in Eq. (7.12), we find that $N(q)$ approaches the following:

$$N(q)=128\pi^4an^2q^{-2}. \quad (7.13)$$

Thus, the contribution of the tick-tack-toe diagrams to the pair distribution function is

$$g_t^{(2)}(r)-n^2=\frac{128\pi^4an^2}{(8\pi^3)^2}\int\exp(2i\mathbf{q}\cdot\mathbf{r})/q^2d\mathbf{q}$$
$$=2an^2/r. \quad (7.14)$$

It is to be remarked that in the above calculation we have taken into consideration only a special type of the tick-tack-toe diagrams which has a structure such that the vertical lines $1-1'$ and $2-2'$ are nearest neighbors. Only such diagrams give a contribution of order a to the distribution function.

8. RESULTS AND CONCLUDING REMARKS

Our final expression for the pair distribution function is obtained by combining the chain-diagram pair distribution function with the tick-tack-toe diagram distribution function. Thus, to first order in a one arrives at

$$g^{(2)}(r)=g_c^{(2)}+g_t^{(2)}$$
$$=n^2; \quad (r\ll r_c) \quad (8.1a)$$
$$=n^2[1-(4\pi^{5/2}a^{1/2}n^{3/2})^{-1}r^{-4}], \quad (r\gg r_c) \quad (8.1b)$$

with

$$r_c=(16\pi an)^{1/2}.$$

This pair distribution function is nearly constant for small r and approaches n^2 in proportion to r^{-4} for large r from lower values.

In Eq. (8.1b), a term which is proportional to $2a/r$ has been omitted because for large distances we have

$$2a/r\ll 2a/r_c$$

or

$$2a/r\ll(16\pi a^3n)^{1/2} \quad (r\gg r_c) \quad (8.2)$$

and the term is negligible.

The pair distribution function thus obtained may be compared with the expression obtained by Lee, Huang, and Yang (LHY) by the method of pseudopotential and the result reported recently by Wu.[12]

According to the calculation of LHY the pair distribution function is given by

$$g_{\mathrm{LHY}}^{(2)}(r)=n^2[\{1+G(r)\}^2+\{1+F(r)\}^2-1-2f\{G(r)+F(r)\}], \quad (8.3)$$

where

$$f=(8/3\pi^{1/2})(na^3)^{1/2}.$$

The functions $F(r)$ and $G(r)$ approach the following forms for small and large distances:

$$F(r)\to 1/\pi^2nr_0r^2,$$
$$G(r)\to -1/\pi^2nr_0r^2, \quad (r\gg r_0) \quad (8.4)$$

and

$$F(r)\to f=(8/3\pi^{1/2})(na^3)^{1/2};$$
$$G(r)\to -(a/r)+(8/\pi^{1/2})(na^3)^{1/2}, \quad (r\ll r_0) \quad (8.5)$$

where

$$r_0=(8\pi an)^{-1/2}=2^{1/2}r_c. \quad (8.6)$$

Thus, the limiting forms of $g_{\mathrm{LHY}}^{(2)}(r)$ are

$$g_{\mathrm{LHY}}^{(2)}(r)=n^2[1-(a/r)]^2+O(a/r_0); \quad (r\ll r_0) \quad (8.7a)$$
$$=n^2[1+(16a/\pi^3nr^4)]; \quad (r\gg r_0). \quad (8.7b)$$

The above expression for small distances may be derived from U_2:

$$z^2\langle r_1,r_2|U_2|r_1,r_2\rangle=z^2(2\pi\lambda^4r^2)^{-1}$$
$$\times\left\{\exp\left[-\frac{r^2}{2\beta}\right]-\exp\left[-\frac{(r-a)^2}{2\beta}\right]\right\}; \quad (r>a). \quad (8.8)$$

Expanding the right-hand side in powers of r and sub-

[12] Tai Tsun Wu, Phys. Rev. **115**, 1390 (1959).

stituting $z=n\lambda^3$ we arrive at

$$g^{(2)}(r)\cong n^2+z^2U_2 = n^2[1-a/r]^2, \quad a<r\leq r_c \tag{8.9}$$

in the zero-temperature limit.

Our pair distribution function at large distances is characterized by the term proportional to r^{-4}. Fujita and Hirota concluded that the pair distribution function g_c in the chain-diagram approximation is identical with Eq. (8.7b), the result obtained by LHY. However, Eq. (8.7b) differs from Eq. (8.1b) not only in magnitude but also in sign. Definitely, their interpretation of LHY's result in terms of chain diagrams is not correct.

This conclusion may be confirmed if we compare our result with the recent improved result reported by Wu. His expression for the pair distribution function at small distances is

$$g_W^{(2)}(r)=n^2\left[1-\frac{r_0^4}{r^4}\left(16\left(\frac{a^3n}{\pi}\right)^{1/2}\right)\times\left\{1-\left(16\pi+\frac{80}{3}\right)\left(\frac{a^3n}{\pi}\right)^{1/2}\right\}\right] \quad (r\gg r_0). \tag{8.10a}$$

This may be written

$$g_W^{(2)}(r)=n^2\{1+(4\pi+20/3)a(\pi^3ar^4)^{-1} -(4\pi^{5/2}a^{1/2}n^{3/2})^{-1}r^{-4}\} \quad (r\gg r_0). \tag{8.10b}$$

Here, in the right-hand side the second term is small compared to the third term for large distances and may be neglected. Thus, $g_W^{(2)}$ reduces to our expression given by Eq. (8.1b) which is essentially due to chain diagrams.

Thus we can say that for large distances the chain-diagram approximation is good. This is because the chain diagrams correspond to collective interaction of the particles.

Because of this situation, the $g_c^{(2)}$ may be used to evaluate the phonon spectrum. As a matter of fact, if we use $g_c^{(2)}(r)$ in the Feynman-Bijl[13] relation for the phonon spectrum:

$$E_k-E_0=k^2/S(k), \tag{8.11}$$

we end up with

$$S(k)=1+n^{-1}\int g_c^{(2)}(r)e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r} =k(k^2+16\pi an)^{-1/2}, \quad (k\neq 0) \tag{8.12}$$

which is in agreement with the result obtained by Lee, Huang, and Yang.

In other words, we can say that the elementary excitation spectrum in a Bose gas is phonon-like for small values of k. Thus, the pair distribution function which yields the excitation spectrum should correspond to large distances. On the other hand, it is not hard to see that the tick-tack-toe diagrams contribute to the pair distribution function only at small distances.

Compared to Eq. (8.7a), our resulting expression for the pair distribution function for small distances is characterized by lack of a term proportional to $1/r$, and is almost constant to first order in a.

This is because the tick-tack-toe diagrams cancel exactly the $1/r$ term in $g^{(2)}(r)$ which the chain diagrams give, as can be seen from Eqs. (7.14) and Eq. (6.40). The $1/r$ singularity causes, actually, the divergence in the ground-state energy and is not desirable. What follows is further discussion of this point.

The first approximate hard-sphere potential is

$$\phi=8\pi a\delta(r_1-r_2). \tag{8.13}$$

In contrast, the correct pseudopotential is given by

$$\phi=8\pi a\delta(r_1-r_2)(\partial/\partial r)r, \tag{8.14}$$

and includes the operator $(\partial/\partial r)r$. As has been pointed out elsewhere, this operator plays the role of removing the $1/r$ singularity in the ground-state energy. As a matter of fact, according to Lee, Huang, and Yang, if we use the correct pseudopotential the ground-state energy in the second-order perturbation is convergent. Namely, we have

$$E_0^{(2)}=-8\pi a\left(\frac{4\pi a}{\Omega}\right)\frac{N(N-1)}{2}\int\frac{d\mathbf{r}}{\Omega}\delta(r)\frac{\partial}{\partial r}\{rF(r)\} =2.37(a/\Omega^{1/3})(4\pi anN). \tag{8.15}$$

Here, since

$$F(r)=\sum_{k\neq 0}\frac{\exp i\mathbf{k}\cdot\mathbf{r}}{k^2} \rightarrow\frac{\Omega}{4\pi}\left(\frac{1}{r}-\frac{2.37}{\Omega^{1/3}}\right), \tag{8.16}$$

we see that $E_0^{(2)}\rightarrow 0$ for $\Omega\rightarrow\infty$.

On the other hand, use of Eq. (8.13) leads to

$$E_0=4\pi arN-\sum\{P_0^2+p^2-p(p^2+2P_0^2)^{1/2}\}, \tag{8.17}$$

where

$$P_0^2=8\pi an. \tag{8.18}$$

This is, however, divergent. As has been discussed by Lee and Yang, in order to obtain the correct convergent energy it is necessary to add to Eq. (8.17) the term

$$\tfrac{1}{2}(P_0^4/2p^2). \tag{8.19}$$

The same ground-state energy may be derived by using the pair distribution functions. If, however, we use only chain diagrams, the resulting pair distribution function $g_c^{(2)}$ will give rise to a divergence in the ground-state energy. Since the pair distribution function has a

[13] R. P. Feynman, *Progress in Low Temperature Physics*, edited by C. Gorter (North-Holland Publishing Company, Amsterdam, 1955), Vol. 1, Chap. II, p. 36; A. Bijl, Physica **7**, 869 (1940); R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).

physical meaning of its own, this indicates that $g_c^{(2)}$ may not be considered the correct distribution function and that improvements upon the chain-diagram approximation are necessary.

This is indeed achieved by taking the tick-tack-toe diagrams into consideration as we have done in the previous section. It is not hard to obtain the tick-tack-toe diagram contribution to the ground-state energy. We end up with

$$E_T=\tfrac{1}{2}\sum P_0^4/2p^2. \tag{8.20}$$

This is exactly what we needed to add to E_0 of Eq. (8.1) to remove the divergence. Thus, if we use the correct distribution function we get

$$E=4\pi aN-\tfrac{1}{2}\sum\{P_0^2+p^2-p(p^2+2P_0^2)^{1/2}-P_0^4/2p^2\}$$
$$=4\pi anN\{1+(128/15\pi^{1/2})(a^3n)^{1/2}\}, \tag{8.21}$$

which is the result first obtained by Lee and Yang by the binary-kernel method.

It is remarked that the divergence in the ground-state energy is due to the appearance of a term proportional to $1/r$ at short distances. Thus, the correct pair distribution function should not contain $1/r$, in conformity with our result.

Summarizing, we may describe the situation as follows: the operator $(\partial/\partial r)r$ in the pseudopotential requires taking diagrams other than chain diagrams into consideration.

The above observation justifies our result at least for both small and large distances. The behavior of $g^{(2)}(r)$ for the intermediate range requires a numerical evaluation. However, it is interesting to observe that $g^{(2)}(r)$ is less than n^2 at large distances. Thus, in a certain intermediate range the $g^{(2)}(r)$ curve might possibly come out above the n^2 line.

Note added in proof. The authors thank Professor Garcia-Colin for informing them of the following important articles: L. Colin and J. Peretti, Compt. Rend. **248**, 1625 (1959); J. Math. Phys. **1**, 97 (1960); L. Colin, *ibid.* **1**, 87 (1960). The discussions of these articles will be given in a later article.

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Quantum-Mechanical Effects in Stimulated Optical Emission. II

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The existence of multiple-quantum transitions in optically pumped lasers, along with splitting of the laser line due to the modulation of the wave function at an angular frequency determined by the rate of pumping, is demonstrated for a certain class of incoherent broad-band sources pumping large pump bands in crystals. The source consists of a large number of stationary elements emitting wave fields continuously at various arbitrary frequencies and arbitrary phases. The distribution of frequencies and phases among the various elements is random. The pump band belongs to the class found in laser crystals of the ionic type. The analysis shows that such sources pumping such bands act like narrow-line sources pumping narrow lines. The effective linewidth is directly related to the pump rate.

THE existence of multiple-quantum transitions in optically pumped lasers and splitting of the laser line due to the modulation of the wave function at an angular frequency determined by the rate of pumping was shown theoretically by the author in "Quantum Mechanical Effects in Stimulated Optical Emission,"[1,2] hereinafter called "QMESOE I."

The theory set forth in that article showed that the splitting would become manifest at threshold when there are a large number of transitions occurring between the pump band and metastable level along with a high pump rate. Since the splitting is dependent upon the pump rate, it increases directly with the magnitude of the electric intensity of the pump field. In addition to this, it was also shown that at high pump powers most of the emitted power would be due to two-photon transitions.

It was not shown in that article if such splittings and multiple photon transitions would occur if both the source and the pump were broad bands instead of being monochromatic lines. Since the source in QMESOE I was chosen to be a coherent monochromatic source, it is not evident that incoherent broad-band sources pumping broad-pump bands will produce the same effect as coherent monochromatic sources pumping narrow-pump bands.

This question will be examined in this paper and it will be shown that indeed certain classes of incoherent broad-band sources pumping broad-pump bands do

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[1] R. C. Williams, Phys. Rev. **126**, 1011 (1962).
[2] R. C. Williams, Appl. Opt. Suppl. **1**, 63 (1962), reprinted from Phys. Rev. **126**, 1011 (1962).