Correlation Functions in Ring - Diagram Approximation*

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The singlet and pair correlation functions of particles in quantum-mechanical many-body systems are evaluated in ring diagram approximation; thereby consideration is also given to chain diagrams. The results, expressed in terms of the eigenvalues characteristic of the topologically different diagrams which enter the theory, agree with what we expect from Montroll and Ward's results on the grand partition function.

I. INTRODUCTION

Statistical-mechanical theories of the grand partition function of a many-body system have been developed greatly in the past decade. As a result, a linked-cluster expansion of the equation of state or the logarithm of the grand partition function of interacting fermions or bosons has been obtained.[1] Important explicit results have been derived, based on considerations of particular diagrams. For instance, Montroll and Ward[2] showed how the Gell-Mann and Brueckner formula[3] could be obtained by summing ring diagrams which are formed by "torons" characteristic of quantum statistics.

It is the purpose of this article to derive a formula for the pair distribution function (pdf hereafter), extending our previous theories based on chain diagrams.[4] Namely, we shall present a theory for the pdf to ring-diagram approximation. In comparison with the case of a grand-partition function, we must consider more diagrams for the pdf because the diagrams are labeled in terms of two particles. Moreover, chain diagrams should be included in our consideration since these yield contributions of lower order than ring diagrams.

We shall develop our theory for general quantum-mechanical systems, assuming that the potentials allow Fourier transformation. Quantum gases with hard-core potentials have been treated by the binary-kernel method and the pseudopotential method.[5]

In the next section we shall introduce conjugate diagrams which play important roles in developing our theory. These diagrams are classified and treated separately in accordance with the number of interaction lines and the topological structure. Thus, in Section III, discussions will be offered on one-interaction line diagrams. In Section IV, treatments of ring diagrams will be presented, and in Section V a special case of two-line diagrams will be discussed. Throughout this paper, we shall choose the units such that $\hbar = 1$ and $2m = 1$, m being the particle mass.

II. CONJUGATE DIAGRAMS

We shall evaluate the pdf based on the general linked-cluster expansion formula which Fujita, Isihara, and Montroll (hereafter FIM) reported in 1958[4]:

$$\rho_2(r) = \rho_1^{\,2} + \sum\nolimits_{l \geq 2} b_l(\vec{r}_1, \vec{r}_2) z^l , \tag{2.1}$$

$$r = |\vec{r}_2 - \vec{r}_1|$$

where ρ_1 is the singlet distribution function, z is the fugacity, and the b_l are the cluster integrals for l-particle connected graphs labeled by the particles 1 and 2. Using this formula, which is general, FIM obtained a chain-diagram result for an electron gas. They have also considered watermelon-type diagrams, but only for classical cases. We are going to use the general formula (2.1) for quantum-mechanical cases.

Generally, the graphs entering in the evaluation of $b_l(r)$ may be classified in accordance with the number of passes from particle 1 to particle 2 which are provided either with statistical connections (exchanges) or potential forces. Thus there are two possible cases:

I. 1 and 2 are in the same toron.
II. 1 and 2 are in different torons.

Here the first group has an exchange between 1 and 2, letting these particles form a toron graph. In the second case, the toron formed by 1 is separated statistically from that including 2. Of course, these two torons are connected by interaction lines.

Further classification of diagrams may be made in accordance with the number of interaction lines. We shall assume that the Fourier transform $u(\vec{q})$ of the potential $\phi(r)$ exists and is finite:

$$u(q) = \int \phi(r) e^{i\vec{q}\cdot\vec{r}} d\vec{r} . \tag{2.2}$$

An interaction line will be represented by a wavy line. A series of unlabeled toron graphs connected by interaction lines may be summed easily. Therefore it is convenient to introduce a box diagram with an effective line to represent the series as in Fig. 1. Here a toron is illustrated by a circle. The toron can be arbitrary in order.

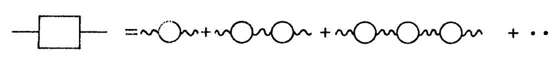

FIG. 1. A box diagram representing a chain of toron graphs.

Since our treatment is in the grand ensemble, a circle may be considered to represent actually an infinite sum of toron graphs.

Box diagrams may be connected together. However, a linear array of box diagrams does not make much sense, because the result is a box diagram. A tree of box diagrams may have branches or articulation points as shown in Fig. 2.

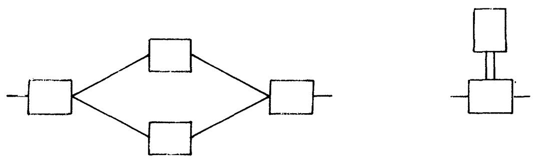

FIG. 2. Simple connection of box diagrams.

In what follows we shall consider diagrams of lower order in an effective line. Figure 3 illustrates diagrams to two effective lines. The diagrams in the same row will be called *conjugate* to each other in the sense that they have the same effective interaction lines, except that an exchange of 1 and 2 takes place in one or the other diagram of a conjugate pair depending on whether it belongs to the group I or II. In the figure, the separated graphs A_S and $A_S{}^2$ appear not in the evaluation of $b_l(r)$ but instead in that of ρ_1. They are illustrated to indicate how the diagrams contributing to ρ_1 are coupled with those for $b_l(r)$.

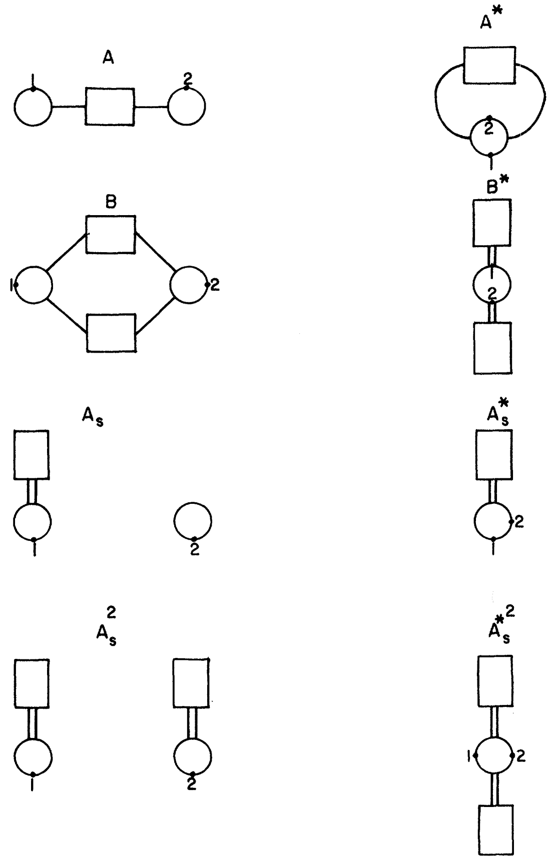

FIG. 3. Conjugate diagrams necessary for the pdf in the ring-diagram approximation.

It is remarked that in the momentum representation of the propagators of these graphs the coordinates of 1 are combined with those for 2 and appear only in the exponential functions. Namely, these coordinates yield a phase factor to each propagator. Thus, except for a phase factor, conjugate diagrams have the same structure for their propagators.

The rules to construct a propagator for fermions are, briefly, as follows. The cases of bosons follow easily from fermion expressions.

1. For the propagation of 1 or 2 we put

$$f(\vec{p}_i) \quad (i=1,2)\ ,$$

where $f(p) = ze^{-\beta p^2}/(1+ze^{-\beta p^2})$.

The corresponding phase factor is of the following form

$$\exp i\vec{p}_i \cdot \vec{r}_i\ .$$

2. For the propagation of an unlabeled particle with an absorption line of momentum $\vec{q}$ we write

$$-u(q)[1-f(\vec{p}+\vec{q})]\ .$$

3. For the propagation of an unlabeled particle with an emission of momentum $\vec{q}\,'$ which follows the absorption of $\vec{q}$, we give

$$-u(q')[1-f(\vec{p}+\vec{q}-\vec{q}\,')]\ .$$

4. The positions in the reciprocal temperature space of these interaction lines $\vec{q}$ or $\vec{q}\,'$ enter in the Boltzmann factors.

5. If the interaction lines with $\vec{q}$ and $\vec{q}\,'$ are connected to an unlabeled box diagram the momentum conservation $\vec{q}=\vec{q}\,'$ holds.

These rules will be understood clearly when applied to explicit cases. We shall develop our theory along the lines mentioned in the introduction.

III. ONE-LINE DIAGRAMS

A circle diagram, which is the sum of torons of all orders with an absorption and an emission line, may be represented by a propagator constructed in accordance with the rules presented in the previous section. As a result we find the following expression for the propagator:

$$G(\vec{q},\alpha) = (2\pi)^{-3}\int f(\vec{p})[1-f(\vec{p}+\vec{q})]e^{-\alpha[(\vec{p}+\vec{q})^2-\vec{p}^2]}d\vec{p}\,, \tag{3.1}$$

where $\alpha = |\beta'' - \beta'|$, β'' and β' being the locations of the interaction lines. It is convenient to consider the propagator in terms of eigenvalues determined by the eigenvalue problem

$$\int G(\vec{q}, |\beta'' - \beta'|)\psi_j(\beta')d\beta' = \lambda_j \psi_j(\beta'') . \quad (3.2)$$

For this problem we assume a periodicity

$$G(\vec{q}, \alpha) = G(\vec{q}, \alpha + \beta) \quad (3.3)$$

so that

$$\psi_j(\beta') = \beta^{-1/2} \exp(-2\pi i j \beta'/\beta) . \quad (3.4)$$

The eigenvalues are given by

$$\lambda_j(\vec{q}) = (2\pi)^{-3} \int d\vec{p}[z(e^{-\beta\vec{p}^2} - e^{-\beta(\vec{p}+\vec{q})^2})][(\vec{p}+\vec{q})^2 - \vec{p}^2 - 2\pi i j/\beta]^{-1}[1-f(\vec{p})][1-f(\vec{p}+\vec{q})] . \quad (3.5)$$

In terms of the eigenvalues, an effective interaction represented by a box diagram is

$$-u(q)/[1 + u(q)\lambda_j], \quad (3.6)$$

where the minus sign is due to the perturbation expansion of the density matrix in powers of the potential.

Using these results, let us investigate the contributions from the one-effective-interaction-line diagrams illustrated in Fig. 1. For this purpose, it is convenient to treat the conjugate diagrams A and A^* at the same time. As mentioned before, they differ only in the phase factor. First, from the rule 1 of the previous section we find a factor

$$f \text{ factor} = [1-f(\vec{p}_1)]f(\vec{p}_1 + \vec{q})[1-f(\vec{p}_2)]f(\vec{p}_2 + \vec{q}) .$$

We are considering a propagation of momentum $\vec{p}_1$ from 0 to β' and that of $(\vec{p}_1 + \vec{q})$ for the rest of a period $(\beta - \beta')$. Since the factor $\exp[-\beta(\vec{p}_1 + \vec{q})^2]$ has been taken in $f(\vec{p}_1 + \vec{q})$, the energy factor determined from the rule 4 is

$$\text{energy factor} = \exp[-\beta'\vec{p}_1^{\,2} + \beta'(\vec{p}_1 + \vec{q})^2 + \beta''\vec{p}_2^{\,2} - \beta''(\vec{p}_2 + \vec{q})^2] .$$

The particle 2 propagates with $(\vec{p}_2 + \vec{q})$ from 0 to β'' where $\vec{q}$ is emitted, and then with $\vec{p}$ for the rest $(\beta - \beta'')$ of a period. The corresponding energy factor is $-\beta''(\vec{p}_2 + \vec{q})^2 - (\beta - \beta'')\vec{p}_2^{\,2}$, but again $-\beta(\vec{p}_2 + \vec{q})^2$ is included in the function $f(\vec{p}_2 + \vec{q})$ so that we arrive at the above expression. With these propagations, the phase factor becomes

$$\text{phase factor} = e^{i\vec{q}\cdot\vec{r}} - e^{i\vec{r}\cdot(\vec{p}_2 - \vec{p}_1)} .$$

An effective interaction line has been expressed in Eq. (3.6). Thus, the whole contribution to $\sum b_l(r)z^l$ from A and A^* assumes the structure:

$$A(r) + A^*(r) = \sum_j (2\pi)^{-9} \int [-u(q)/(1 + u(q)\lambda_j)] \times (f \text{ factor}) \times (\text{energy factor}) \times (\text{phase factor}) \times \psi_j^*(\beta')\psi_j(\beta'')$$
$$\times d\vec{p}_1 d\vec{p}_2 d\vec{q} d\beta' d\beta'' . \quad (3.7)$$

The contribution from A_S^* of order u^2 and higher is found by combining the three cases: the case in which the absorption line enters in the diagram first, that in which the emission line takes place first, and that in which the absorption and emission appear in a propagator of an unlabeled particle at the same time. The last case is a special type of the former two cases. In this case it does not matter which line enters first in the graph because of the integrations over β' and β''. These three cases are expressed in the f factors as follows:

$$f(\vec{p}_1)[1-f(\vec{p}_1)]f(\vec{p}_1 + \vec{q})f(\vec{p}_2) + f(\vec{p}_1)f(\vec{p}_1 + \vec{q})[1-f(\vec{p}_1 + \vec{q})]f(\vec{p}_2 + \vec{q}) - f(\vec{p}_1)[1-f(\vec{p}_1)]f(\vec{p}_2)$$
$$= -\frac{\partial}{\partial \ln z}\{f(\vec{p}_1)[1-f(\vec{p}_1 + \vec{q})]\} f(\vec{p}_2) + f(\vec{p}_1)f(\vec{p}_1 + \vec{q})[1-f(\vec{p}_1 + \vec{q})][f(\vec{p}_2 + \vec{q}) - f(\vec{p}_2)], \quad (3.8)$$

where in the right-hand side we have introduced a derivative with respect to z for our later convenience.

The diagrams A_S^* which are first order in $u(q)$ correspond to torons with a self-interaction. In contrast to the cases considered for Eq. (3.8) no exchange of absorption and emission lines take place for this case. Also, a self-interaction of the same particle should be prohibited.

Thus, we end up with

$$A_s^*(r) = (2\pi)^{-9}\int\{[-2\beta u(\vec{q})]f(\vec{p}_1)f(\vec{p}_1+\vec{q})[1-f(\vec{p}_1)]f(\vec{p}_2)e^{i(\vec{p}_2-\vec{p}_1)\cdot\vec{r}}\}d\vec{p}_1 d\vec{p}_2 d\vec{q} + \sum_j \frac{1}{(2\pi)^9}\int\left(\frac{u^2(q)\lambda_j}{1+u(q)\lambda_j}\right)$$

$$\times\left[\left(-\frac{\partial}{\partial \ln z}f(\vec{p}_1)[1-f(\vec{p}_1+\vec{q})]\right)f(\vec{p}_2)+f(\vec{p}_1)f(\vec{p}_1+\vec{q})[1-f(\vec{p}_1+\vec{q})][f(\vec{p}_2+\vec{q})-f(\vec{p}_2)]\right]e^{i(\vec{p}_2-\vec{p}_1)\cdot\vec{r}}$$

$$\times\exp\{(\beta''-\beta')[\vec{p}_1^{\,2}-(\vec{p}_1+\vec{q})^2]\}\psi_j^*(\beta')\psi_j(\beta'')d\beta' d\beta'' d\vec{p}_1 d\vec{p}_2 d\vec{q}. \tag{3.9}$$

Here it is remarked that the momentum of the particle 2 is chosen sometimes to be $\vec{p}_2+\vec{q}$ instead of simply $\vec{p}_2$. This corresponds to the use of the same phase factor and yields the momentum conservation $\vec{p}_1=\vec{p}_2$ when the term including such a momentum is integrated over $\vec{r}$. In this connection, it is further remarked that the two integrals

$$\int\exp[-(\beta''-\beta')g(p)]\psi_j^*(\beta')\psi_j(\beta'')d\beta' d\beta'' \quad\text{and}\quad \int\exp[(\beta''-\beta')g(p)]\psi_j^*(\beta')\psi_j(\beta'')d\beta' d\beta''$$

yield the same real part. In Eq. (3.9) a weight factor due to the exchange between 1 and 2 is added. However, the second term, characterized by a factor $-u^2(q)\lambda_j[1+u(q)\lambda_j]$, does not have such a factor because of another factor $\frac{1}{2}$ due to ring formation.

We shall now attempt rewriting Eq. (3.9) as a simpler expression. For this purpose, and in view of Eqs. (3.2) and (3.8), we introduce the eigenvalues defined by

$$\lambda_j(\vec{q},\vec{r},z) = (2\pi)^{-3}\int f(\vec{p})[1-f(\vec{p}+\vec{q})]\exp\alpha[\vec{p}^2-(\vec{p}+\vec{q})^2]\exp(-i\vec{p}\cdot\vec{r}+2\pi ij\alpha/\beta)d\alpha d\vec{p};$$

$$\mu_j(\vec{q},\vec{r},z) = (2\pi)^{-3}\int f(\vec{p})f(\vec{p}+\vec{q})[1-f(\vec{p}+\vec{q})]\exp\alpha[\vec{p}^2-(\vec{p}+\vec{q})^2]\exp(-i\vec{p}\cdot\vec{r}+2\pi ij\alpha/\beta)d\alpha d\vec{p}. \tag{3.10}$$

In particular, we observe

$$\lambda_j(q,0,z) = \lambda_j(q). \tag{3.11}$$

We introduce also

$$\rho_1^{(0)}(r) = 1/(2\pi)^3\int f(\vec{p})e^{i\vec{p}\cdot\vec{r}}d\vec{p}; \quad \rho_1^{(1)}(r) = \beta/(2\pi)^6\int f(\vec{p})f(\vec{p}+\vec{q})[1-f(\vec{p})]u(q)e^{i\vec{p}\cdot\vec{r}}d\vec{p}d\vec{q}. \tag{3.12}$$

These latter quantities are related to the singlet distribution function (sdf hereafter) ρ_1. As in the case of the pdf, the diagrams for the sdf may be classified in terms of the numbers of interaction lines. Correspondingly, we write

$$\rho_1 = \rho_1^{(0)}+\rho_1^{(1)}+\rho_1^{(2)}+\dots. \tag{3.13}$$

The evaluation of the terms in the right-hand side of this equation is similar to that of the pdf. Omitting the details, we give the results for first few terms:

$$\rho_1^{(0)} = 1/(2\pi)^3\int f(\vec{p})d\vec{p}; \quad \rho_1^{(1)} = \beta/(2\pi)^6\int f(\vec{p})f(\vec{p}+\vec{q})[1-f(\vec{p})]u(\vec{q})d\vec{p}d\vec{q};$$

$$\rho_1^{(2)} = \sum_j\frac{1}{2(2\pi)^3}\int\frac{\partial\lambda_j}{\partial\ln z}\frac{\lambda_j u^2(q)}{1+\lambda_j u(q)}d\vec{q}; \quad \rho_1^{(0)}(0)=\rho_1^{(0)}; \quad \rho_1^{(1)}(0)=\rho_1^{(1)};\dots. \tag{3.14}$$

Thus, returning to the pdf, we have the expression

$$\rho_2(r)-\rho_1^2 = \sum_{l\geq 2}^{\infty} z^l(b_l^{\mathrm{I}}(r)+b_l^{\mathrm{II}}(r)+\cdots), \tag{3.15}$$

where the right-hand side includes the contributions from one-effective-line diagrams, two-line diagrams, etc. We have arrived at

$$\sum_l z^l b_l^{\mathrm{I}}(r) = A(r)+A^*(r)+A_s^*(r) \tag{3.16}$$

where $A(r)+A^*(r) = \dfrac{1}{(2\pi)^3\beta}\sum_j\int\left(\dfrac{u(q)}{1+\lambda_j u(q)}\right)[\lambda_j^{\,2}l^{-i\vec{q}\cdot\vec{r}}-\lambda_j^{\,2}(\vec{q},r,z)]d\vec{q};$

$$A_S^*(r) = -2\rho_1^{(1)}(r)\rho_1^{(0)}(r) + \frac{\rho_1^{(0)}(r)}{(2\pi)^3}\sum_j\int\left(-\frac{u^2(q)\lambda_j}{1+\lambda_j u(q)}\right)\left(-\frac{\partial\lambda_j(q,r,z)}{\partial\ln z} + \mu_j(q,r,z)(e^{-i\vec{q}\cdot\vec{r}}-1)\right)d\vec{q}. \quad (3.17)$$

IV. RING-DIAGRAM APPROXIMATION

The diagrams of the types B and B^* of Fig. 3 are of two effective interaction lines. We shall call them two-line diagrams. The two interaction lines will be represented by the momenta $\vec{q}$ and $\vec{q}\,'$. The product of the effective interactions which enter is

$$u(q')u(q)/[1+\lambda_j u(q')][1+\lambda_l u(q)].$$

To express the propagator, it is convenient to introduce the notation

$$E_{jl}(\beta',\beta'';\vec{q},\vec{q}\,') = \exp[-\beta'\vec{p}^2-(\beta''-\beta')(\vec{p}+\vec{q})^2+\beta''(\vec{p}+\vec{q}+\vec{q}\,')^2]\,\psi_j^*(\beta')\psi_l(\beta''). \quad (4.2)$$

Then we find the following three terms

$$[1-f(\vec{p})][1-f(\vec{p}+\vec{q})]f(\vec{p}+\vec{q}+\vec{q}\,')E_{jl}(\beta',\beta'';\vec{q},\vec{q}\,') + [1-f(\vec{p})][1-f(p+q')]f(\vec{p}+\vec{q}+\vec{q}\,')E_{lj}(\beta'',\beta';\vec{q}\,',\vec{q})$$
$$-[1-f(\vec{p})]f(\vec{p}+\vec{q}+\vec{q}\,')E_{lj}(\beta'',\beta';\vec{q}\,',\vec{q})$$

corresponding to the cases where the interaction lines q and q′ are interchanged, the last term compensating a double counting when the two lines appear in the same toron.

Therefore we introduce the eigenvalues defined by

$$\nu_{jl}(\mathrm{r},\vec{q},\vec{q}\,') = (1/2\pi^3\beta)\int\{(1-f(\vec{p})[1-f(\vec{p}+\vec{q})]f(\vec{p}+\vec{q}+\vec{q}\,')E_{jl}(\beta',\beta'';\vec{q},\vec{q}\,') + [1-f(\vec{p})][1-f(\vec{p}+\vec{q}\,')]f(\vec{p}+\vec{q}+\vec{q}\,')$$
$$\times E_{lj}(\beta'',\beta';\vec{q}\,',\vec{q}) - [1-f(\vec{p})]f(\vec{p}+\vec{q}+\vec{q}\,')E_{lj}(\beta'',\beta';\vec{q}\,',\vec{q})\}d\beta'd\beta''d\vec{p}. \quad (4.3)$$

We note, then, that the diagrams B correspond to

$$e^{i\vec{r}\cdot(\vec{q}+\vec{q}\,')}\nu_{jl}(0,\vec{q},\vec{q}\,')\nu_{jl}^*(0,\vec{q},\vec{q}\,')$$

while the B^* correspond to

$$-e^{i\vec{r}\cdot(\vec{q}+\vec{q}\,')}\nu_{jl}(\vec{r},\vec{q},\vec{q}\,')\nu_{jl}^*(\vec{r},\vec{q},\vec{q}\,'),$$

where $\vec{r}=\vec{r}_2-\vec{r}_1$ as before. Summing these two contributions, we arrive at

$$\sum_l z^l b_l^{\mathrm{II}}(r) = \frac{1}{2(2\pi)^6}\sum_{jl}\int d\vec{q}d\vec{q}\,'\frac{u(q)u(q')}{[1+\lambda_j u(q)][1+\lambda_l u(q')]}e^{i\vec{r}\cdot(\vec{q}+\vec{q}\,')}$$
$$\times[\nu_{jl}(0,\vec{q},\vec{q}\,')\nu_{jl}^*(0,\vec{q},\vec{q}\,')-\nu_{jl}(\vec{r},\vec{q},\vec{q}\,')\nu_{jl}^*(\vec{r},\vec{q},\vec{q}\,')]. \quad (4.4)$$

It is remarked that at $\vec{r}=0$ the right-hand side vanishes. Also, if $\vec{q}=-\vec{q}\,'$ and $\vec{r}=0$

$$\nu_{jl}(0,\vec{q},\vec{q}\,') = (2\pi)^{-3}\int d\vec{p}f(\vec{p})[1-f(\vec{p}+\vec{q})][1-f(\vec{p})-f(\vec{p}+\vec{q})]\int_0^\beta \exp\alpha[p^2-(p+q)^2]\int_0^\beta\psi_j^*(\beta')\psi_l(\beta')d\beta'$$
$$\times\psi_l(\beta'')\psi_l^*(\beta')d(\beta''-\beta') = (\partial\lambda_j/\partial\ln z)\delta_{jl}, \quad (4.5)$$

where we have used

$$\psi_l^*(\beta')\psi_l(\beta') = 1/\beta.$$

In the diagrams $A_S{}^{*2}$, one finds a doubling of the structure of $A_S{}^*$ in which the interaction lines are absorbed and emitted at the same time. We define

$$\gamma(\vec{q}, \vec{r}) = \sum_j \frac{1}{(2\pi)^3} \int \frac{u^2(q)\lambda_j}{1+u(q)\lambda_j} \{f(\vec{p})[1-f(\vec{p})]f(\vec{p}+\vec{q}) + f(\vec{p})f(\vec{p}+\vec{q})[1-f(\vec{p}+\vec{q})]\, e^{-i\vec{q}\cdot\vec{r}} - f(\vec{p})[1-f(\vec{p})]\}$$

$$\times \exp\alpha[\vec{p}^2-(\vec{p}+\vec{q})^2]\exp(-i\vec{r}\cdot\vec{p})\psi_j{}^*(\beta')\psi_j(\beta'')d\beta' d\beta'' d\vec{p}\,. \tag{4.6}$$

Then by a similar consideration to that for $A_S{}^*$, we find the $A_S{}^{*2}$ contributions to be given by

$$\sum_l z^l b_l{}^S(r) = -\{[1/2(2\pi)^3]\int \gamma(\vec{q}, \vec{r})d\vec{q}\}^2 \tag{4.7}$$

In particular, at $r = 0$

$$\gamma(\vec{q}, 0) = -\sum_i \{u^2(q)\lambda_j/[1+u(q)\lambda_j]\}(\partial\lambda_j/\partial \ln z)\,. \tag{4.8}$$

V. CONCLUDING REMARKS

The results which we have obtained will be examined in this section. First, let us investigate the behavior of the pdf at $r = 0$. It is clear from Eqs. (3.17) that

$$A(0) + A^*(0) = 0\,,$$

$$A_S{}^*(0) = [\rho_1{}^{(0)}/(2\pi)^3\beta]\sum_j \int \{u^2(q)\lambda_j/[1+u(q)\lambda_j]\}(\partial\lambda_j/\partial \ln z)d\vec{q} = -2\rho_1{}^{(0)}(\rho_1{}^{(1)} + \rho_1{}^{(2)})\,. \tag{5.1}$$

The right-hand side of Eq. (4.4) vanishes at $r = 0$, and from Eqs. (4.7) and (4.8) we find

$$\sum b_l{}^S(0)z^l = -[\rho_1{}^{(1)}]^2\,. \tag{5.2}$$

From Eqs. (2.1), (5.1), and (5.2), we find

$$\rho_2(0) - \rho_1{}^2 = -(\rho_1{}^{(0)})^2 + A_S{}^*(0) + \sum z^l b_l{}^S(0)\,; \tag{5.3}$$

where $-(\rho_1{}^{(0)})^2$ in the right-hand side is due to a term $-[\rho_1{}^{(0)}(r)]^2$ in the pdf of an ideal fermion gas:

$$\rho_2{}^{(0)}(r) = (\rho_1{}^{(0)})^2 - [\rho_1{}^{(0)}(r)]^2$$

Thus, for fermions we have the expected result,

$$\rho_2{}^{(0)} = 0\,. \tag{5.4}$$

The pdf gives directly the internal energy and the equation of state. Montroll and Ward reported theoretical expressions for these quantities evaluated in a ring-diagram approximation from the grand partition function. Let us therefore examine whether our results agree with theirs.

To evaluate the internal energy in a ring-diagram approximation we start with our result based on chain diagrams:

$$A(r) = [1/(2\pi)^3\beta]\sum_j \int d\vec{q}\{-u(q)\lambda_j{}^2/[1+u(q)\lambda_j]\}e^{-i\mathbf{q}\cdot\mathbf{r}}d\vec{q}\,. \tag{5.5}$$

Equation (5.5), when multiplied by ϕ and integrated over r, is supposed to yield a ring-diagram result. The internal energy is obtained by[6]

$$U = -(\partial/\partial\rho)\ln\left(\mathrm{tr}\,e^{-\beta H}\right)\!. \tag{5.6}$$

We make use of a Hamiltonian with a coupling parameter g,

$$H = H_0 + gH_1, \tag{5.7}$$

and observe $\partial U(g)/\partial g = -(\partial/\partial\beta)(\partial/\partial g)(\ln \operatorname{tr} e^{-\beta H}) = \frac{1}{2}V(\partial/\partial\beta)[\beta\int \phi(r)\rho_2(r,g)d\vec{r}]$. (5.8)

Thus integrating over g from 0 to 1, we arrive at

$$U = U_0 + \sum_j [V/2(2\pi)^3](\partial/\partial\beta)\int [(u(q)\lambda_j)^{-1}\ln[1+gu(q)\lambda_j] - g]_0^1 \lambda_j u(q)d\vec{q}$$

$$= U_0 - \tfrac{1}{2}V(2\pi)^{-3}\sum_j \int \{u^2(q)\lambda_j\lambda_j'/[1+u(q)\lambda_j]\}d\vec{q}, \tag{5.9}$$

in agreement with Eq. (5.28) of Montroll and Ward. Here, $\lambda' = \partial\lambda/\partial\beta$.

The normalization of the pdf should be in conformity with the cluster expansion of the grand partition function Ξ. In ring-diagram approximation, our expression for the pdf is supposed to yield

$$\sum V\int z^l b_l(r)\, d\vec{r} = \frac{1}{2}\frac{V}{(2\pi)^3}\sum_j \int d\vec{q}\left[\frac{u^2(q)}{[1+u(q)\lambda_j]^2}\left(\frac{\partial\lambda_j}{\partial \ln z}\right)^2 + \frac{u^2(q)\lambda_j}{1+u(q)\lambda_j}\left(\frac{\partial^2\lambda_j}{(\partial\ln z)^2} - \frac{\partial\lambda_j}{\partial\ln z}\right)\right], \tag{5.10}$$

since[2,3] $\ln\Xi = \ln\Xi^0 + [V/2(2\pi)^3]\sum_j \int \{u(q)\lambda_j - \ln[1+u(q)\lambda_j]\}d\vec{q}$. (5.11)

On the other hand, we have

$$\partial\lambda_j/\partial\ln z = (2\pi)^{-3}\int f(\vec{p})[1+f(\vec{p}+\vec{q})][1-f(\vec{p})-f(\vec{p}+\vec{q})]\exp\alpha[p^2-(\vec{p}+\vec{q})^2]\exp(2\pi ij\alpha/\beta)d\alpha d\vec{p}, \tag{5.12}$$

and
$$\frac{\partial^2\lambda_j}{(\partial\ln z)^2} - \frac{\partial\lambda_j}{\partial\ln z} = -\frac{1}{(2\pi)^3}\int 2f(\vec{p})[1-f(\vec{p}+\vec{q})]\{f(\vec{p})[1-f(\vec{p})] + f(\vec{p}+\vec{q})[1-f(\vec{p}+\vec{q})] - f(\vec{p})f(\vec{p}+\vec{q})\}$$

$$\times \exp\alpha[p^2-(\vec{p}+\vec{q})^2]\exp(2\pi ij\alpha/\beta)\,d\alpha d\vec{p}. \tag{5.13}$$

Therefore, we can express the integrals of the pdf involved in the normalization as follows:

$$V\sum_l \int z^l b_l{}^*(r)d\vec{r} = \frac{V}{2(2\pi)^3}\sum_j \int \frac{u^2(q)\lambda_j}{1+u(q)\lambda_j}\left(\frac{\partial^2\lambda_j}{(\partial\ln z)^2} - \frac{\partial\lambda_j}{\partial\ln z}\right)d\vec{q}; \tag{5.14}$$

$$V\sum \int z^l b_l{}^{\mathrm{II}}(r)d\vec{r} = \frac{V}{2(2\pi)^3}\sum_j \int \left(\frac{\partial\lambda_j}{\partial\ln z}\right)^2 \frac{u^2(q)}{[1+u(q)\lambda_j]^2}\, d\vec{q}, \tag{5.15}$$

which, when combined, yield Eq. (5.10). Thus, we have confirmed that our expression gives the correct expression (5.11) for the grand partition function in ring-diagram approximation.

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