Momentum Distribution of an Interacting Many-Boson System at High Density

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The momentum distribution function $n_p$ is obtained for an interacting many-boson system at high density using the Rayleigh-Schrödinger perturbation theory in the scheme of the density and phase operator approach (DPO). The expression obtained has a correct form in the low momentum limit in accord with the condition first given by Gavoret and Nozières. The origin of an unphysical result found by Grest that $n_p$ becomes negative for low wave numbers will be elucidated. Using the expression for $n_p$, the ground-state energy is re-obtained. The result agrees completely with that given by Brueckner and Lee.

§ 1. Introduction

In our three previous papers it has been shown that convergent expressions for the excitation energy $\varepsilon_p$, the ground-state energy $E_0$, the structure factor $S_p$ and the momentum distribution function $n_p$ of an interacting many-boson system can be obtained using the perturbation theory in the scheme of the density and phase operator approach (DPO). In this paper we would like to present a detailed discussion on the momentum distribution obtained previously having an exact expression in the low momentum limit. The ground-state energy is re-obtained using the expressions for $n_p$ and $S_p$. The result agrees precisely with that obtained from the classical Bogoliubov theory (B) re-formulated by Brueckner and Lee. With the aid of the equation for the structure factor, the momentum distribution can be given in terms of the observed values of the structure factor instead of its unperturbed values $\lambda_p$'s. A remark will be made on this expression of $n_p$ in relation to the problem of an unphysical result found by Grest that $n_p$ becomes negative for wave numbers lower than 0.3Å⁻¹ when the experimental data of the x-ray scattering due to Achter and Meyer are substituted for the $S_p$'s included in the expression of $n_p$.

Recently Grest derived an expression for the momentum distribution of a boson system at high density on the basis of B using the perturbation theory. A couple of years ago, Berdahl derived the same expression from B following the adiabatic theorem by regarding the free particle energy as an adiabatic parameter. As is well known, it is assumed in B that a large number of bosons can have zero momentum and the field operators with zero momentum; $a_0^+$ and $a_0$ may
be considered as c-number quantities to be put equal to $n_0^{1/2}$, the square root of the mean occupation number with zero momentum. For a system having only a small number of particles with zero momentum, for example liquid $^4$He, this assumption is not appropriate. At present we have no definite answer, both theoretically and experimentally, to either presence or absence of $n_0$ in liquid $^4$He.\footnote{10}

Using the Bijl-Dingle-Jastrow (BDJ) type of variational wave function, Lee and Wong\footnote{11} obtained the momentum distribution function which agrees in the uniform limit with the first order term given in this paper, but the higher order correction terms to it were not given explicitly in this limit. For the sake of consistency of the theory of collective variables, the momentum distribution should be derived in its own scheme of description. Until now the momentum distribution has not been obtained on the basis of this theory.\footnote{21}

In § 2 and the Appendix, the derivation of the previous result is fully described using a graphic representation of the perturbation terms up to those including a factor $1/N$ where $N$ is the total number of particles. The expression for $n_p$ will be written in terms of vertex functions having familiar forms appeared in the method of correlated basis functions (CBF)\footnote{12} which are related to the previous ones in a quite simple fashion. In § 3, using the equation for the structure factor, the unperturbed values $\lambda_p$'s involved in the expression for $n_p$ are replaced by the observed values $S_p$'s to prepare for the discussion in the next section. In § 4 the origin of the unphysical result found by Grest will be elucidated giving an explicit expression for $n_p$ in the low momentum limit. The failure of this expression in the low momentum region is solely attributed to an unsatisfactory evaluation of the mean occupation number with zero momentum $n_0$. A method will be proposed to make $n_p$ remain positive in the low momentum limit. In § 5 the ground-state energy is re-obtained using $n_p$ and $S_p$. The result is in accord with that given by B in the high density limit. The difference between this result and that given by CBF in the uniform limit will be discussed. In § 6 the meaning of the cutoff wave number introduced in our previous papers will be interpreted so that no misunderstandings about its meaning might be occurred. A brief remark will be made on the relationship to the theory of magnetism.

§ 2. The occupation number operator $N_p$

In the second paper in Ref. 2), the author obtained the momentum distribution $n_p$ by taking the average of the occupation number operator $N_p$ with respect to the perturbed ground-state of DPO. In this section and the Appendix, we would show its derivation in more detail to obtain an apparently convergent expression for $n_p$ by using the Rayleigh-Schrödinger perturbation theory.

By writing the field operator of bosons $a_p$ in terms of the Fourier transform of the number density operator $\rho(r)$ and that of the phase operator $\phi(r)$, in a box of volume $V$, as
The occupation number operator of bosons with the momentum $\hbar p$ is expressed by

$$N_p = a_p^+ a_p = N_p^{(1)} + N_p', \quad N_p^{(1)} = \frac{1}{\sqrt{V}} \int \rho_p \phi_{-p} + \frac{1}{\hbar} \phi_p \phi_{-p} + \frac{i}{2\hbar} (\rho_p \phi_p - \phi_p \rho_p - p),$$

(2.1)

where the normalized Fourier transforms are defined by

$$\rho_p = N^{-1/2} \int \rho(r) \exp(-i\hbar \cdot r) dr, \quad \phi_p = \frac{N^{1/2}}{V} \int \phi(r) \exp(i\hbar \cdot r) dr,$$

(2.2)

and $N_p'$ represents the higher order terms in $\rho_p$ and $\phi_p$ which involve a factor $N^{1-n}$ for an $n$-fold product of $\rho_p$ and $\phi_p$. By introducing the field operators of phonons, $B_p^+$ and $B_p$, the lowest order bilinear terms assumes the form

$$N_p^{(2)} = N_p^{(2,1)} + N_p^{(2,2)} +$$

(2.4)

and $N_p^{(2,1)}$ becomes

$$N_p^{(2,1)} = \frac{1}{4} \left( \lambda_p + \frac{1}{\lambda_p} \right) (B_p^+ B_p + B_{-p}^+ B_{-p}) - \frac{1}{2} (B_p B_p - B_{-p} B_{-p}),$$

(2.5)

$$N_p^{(2,2)} = \frac{1}{4} \left( \lambda_p - \frac{1}{\lambda_p} \right) (B_{-p}^+ B_{-p} + B_p B_p),$$

(2.6)

where $\lambda_p$ is defined by

$$\lambda_p = \left[ \varepsilon_p (\varepsilon_p + 2NV_p) \right]^{1/2}, \quad \varepsilon_p = \hbar p^2 / (2M),$$

(2.7)

and $V_p$ is the Fourier transform of the interaction potential and $M$ is the particle mass.

The first order expectation value of $N_p^{(2,1)}$ becomes

$$n_p^{(1)} = \langle 0 | N_p^{(2,1)} | 0 \rangle = \frac{1}{4\lambda_p} (1 - \lambda_p)^2,$$

(2.8)

for the unperturbed ground state represented by $| 0 \rangle$ where $B_p | 0 \rangle = 0$. The average of each bilinear product included in $N_p^{(2)}$ with respect to $| 0 \rangle$ is given by the contraction at the same time when Wick's theory of the normal product
expansion is employed as follows:

\[ \langle \Phi_0 | \rho_{p} \rho_{-p} | \Phi_0 \rangle = \rho_{p} \rho_{-p} = \lambda_p, \quad \langle \Phi_0 | \phi_{p} \phi_{-p} | \Phi_0 \rangle = \phi_{p} \phi_{-p} = \frac{\hbar^2}{4 \lambda_p}, \]

\[ \langle \Phi_0 | \rho_{p} \phi_{p} | \Phi_0 \rangle = \rho_{p} \phi_{p} = -\phi_{p} \rho_{p} = -\langle \Phi_0 | \phi_{p} \rho_{p} | \Phi_0 \rangle = \frac{i \hbar}{2}. \]  

(2.9)

These results will be used in the Appendix to obtain the expectation values of the quaternary terms in \( \rho_{p} \) and \( \phi_{p} \). The perturbation calculation for the operators \( N_{p}^{\omega} \) and \( N_{p}' \) will be shown graphically in the Appendix. The momentum distribution given there as the expectation values of \( N_{p} \) for the perturbed ground state represented by \( | \Psi_{0} \rangle \) up to the terms including explicitly a factor \( 1/N \), i.e., up to the quaternary terms, has the following form:

\[ n_{p} = \frac{1}{4 \lambda_p} (1 - \lambda_p^2) + \frac{1}{16N} \sum_{q,r} \delta_{p+q+r,0} \left\{ (1 + \lambda_p^2) \lambda_q \lambda_r \frac{\alpha(p, q, r)^2}{b(p, q, r)^2} \right\} \]

\[ - (1 - \lambda_p^2) \frac{\alpha(p, q, r) \gamma(p, q, r)}{p^2 b(p, q, r)} + 2 \left[ (1 - \lambda_q \lambda_r) \frac{1}{\lambda_p} \right] \]

\[ - (1 - \lambda_q \lambda_r) \frac{\alpha(p, q, r)}{b(p, q, r)} \left[ \frac{(1 - \lambda_p^2)}{2 \lambda_p} \left( \frac{1}{\lambda_q} - 4 + \lambda_q + \lambda_r \right) \right] \]

\[ + (1 - \lambda_p^2) \left( 1 - \lambda_q \right) \left( 1 - \lambda_r \right) \frac{2}{1 + \lambda_p} \left[ -\lambda_p (p^2 + q^2 + r^2)/p^2 \right] \]

\[ + (1 - \lambda_q)^2 (1 - \lambda_r)^2/(2 \lambda_q \lambda_r), \]  

(2.10)

where \( \alpha(p, q, r) \) and \( \gamma(p, q, r) \) are the vertex functions used in CBF and related to \( a(p, q, r) \) and \( c(p, q, r) \) used in the second paper in Ref. 2) by

\[ \alpha(p, q, r) = a(p, q, r) + b(p, q, r) \]

\[ = p \cdot q \lambda_r (1 - \lambda_p)(1 - \lambda_q) + q \cdot r \lambda_p (1 - \lambda_q) (1 - \lambda_r) + r \cdot p \lambda_q (1 - \lambda_r) (1 - \lambda_p), \]

(2.11)

\[ \gamma(p, q, r) = c(p, q, r) + d(p, q, r) \]

\[ = p \cdot q \lambda_r (1 + \lambda_p)(-1 + \lambda_q) + q \cdot r \lambda_p (1 - \lambda_q)(1 - \lambda_r) + r \cdot p \lambda_q (-1 + \lambda_r)(1 + \lambda_p), \]

(2.12)

where \( b(p, q, r) = \lambda_q \lambda_r p^2 + \lambda_p \lambda_r q^2 + \lambda_q \lambda_p r^2 \) and \( d(p, q, r) = -\lambda_q \lambda_r p^2 + \lambda_p \lambda_q q^2 + \lambda_p \lambda_r r^2 \). This expression has an apparently convergent form which vanishes identically by putting \( \lambda_p = \lambda_q = \lambda_r = 1 \). We can readily see that the previous expression is re-obtained by substituting (2.11) and (2.12) in (2.10). The Rayleigh-Schrödinger perturbation theory is not the unique method to reach this expression. A more sophisticated method, for example, the adiabatic perturbation theory or the new
Sunakawa theory (the YKS theory)\textsuperscript{19} may be used to confirm this result.\textsuperscript{*1, **1}

§ 3. The structure factor

The structure factor $S_p$ is obtained as the average of $\rho_{p0-\rho/2}/N$ with respect to the ground state represented by $|\Psi_0\rangle$ (see Appendix, Eq. (A·6)). Using the field operators of phonons we have

$$S_p = \langle \Psi_0 | \rho_{p0-\rho/2} | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle$$

$$= \lambda_p \langle \Psi_0 | (B_p + B_p^+)(B_p + B_p^+)^+ | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle = \lambda_p + \Delta \lambda_p,$$  \hspace{1cm} (3·1)

$$\Delta \lambda_p = \sum_{q,r} \delta \lambda_p (\lambda_p, \lambda_q, \lambda_r) \delta_{p+q+r,0},$$  \hspace{1cm} (3·2)

where

$$\delta \lambda_p (\lambda_p, \lambda_q, \lambda_r) = \frac{1}{4N} \left[ \frac{\lambda_p^2 \lambda_q \lambda_r}{b(p,q,r)} \right] + \frac{\alpha(p,q,r)^2}{b(p,q,r) \lambda_p^2} \right].$$  \hspace{1cm} (3·2')

This expression corresponds to the structure factor obtained experimentally from the neutron scattering or the x-ray scattering. In a previous paper\textsuperscript{10} we evaluated the structure factor by following the same method, although the contribution coming from the quaternary Hamiltonian $H'$ was ignored. In obtaining the excitation energy by a renormalized perturbation theory this contribution from $H'$ is not necessary as mentioned in another previous paper.\textsuperscript{10} By solving $\lambda_p$ inversely in terms of the $S_p$'s from (3·1) we can write

$$\lambda_p = S_p - \sum_{q,r} \delta \lambda_p (S_p, S_q, S_r) \delta_{p+q+r,0},$$  \hspace{1cm} (3·3)

which includes the higher order perturbation terms beyond of order $1/N$. Using this equation we can express the momentum distribution in terms of the $S_p$'s which are furnished by the experimental data. This kind of treatment was proposed by the author\textsuperscript{11} and later by Tsuzuki\textsuperscript{16} and Grest and Rajagopal\textsuperscript{16} in obtaining the excitation energy.

From (2·10) and (3·3) we find

$$n_p = (1/4S_p) (1 - S_p)^2 + (1/8N) \sum_{q,r} \delta_{p+q+r,0} \left( S_q S_r \alpha'(p,q,r)^2 \right.$$  \hspace{1cm} (3·3')

\[ \sum_p E_{\theta}(p+k)(1-\lambda_{p+k}^2)(1-\lambda_p)(1+\lambda_{p+k}^2) / (\lambda_{p+k}^4 + k^2 + k) \].
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\[ \alpha'(p, q, r) = (1 - S_p)(1 - S_q)(1 - S_r) + \frac{1}{4}(1 - S_q)^3(1 - S_r)^3/(S_q S_r) \]

\[ \beta'(p, q, r) = \left( \frac{1 - S_p}{S_p} \right) \cdot \left( \frac{1 - S_q}{S_q} \right) \cdot \left( \frac{1 - S_r}{S_r} \right) \]

where \( \alpha'(p, q, r) \) and \( \beta'(p, q, r) \) are given by \( \alpha(p, q, r) \) and \( \beta(p, q, r) \) by replacing \( \lambda_p's \) by the \( S_p's \) in these factors. Gresel\(^7\) derived a formula corresponding to this on the basis of B and found an unphysical result that the momentum distribution becomes negative for wave numbers lower than 0.3A\(^{-1}\). The origin of this failure will be elucidated in the next section.

The expression (3·1) and (3·2) can be obtained from the expression for the ground-state energy following the adiabatic theorem by regarding the Fourier transform of the interaction potential \( V_p \) as the adiabatic parameter and by noticing that

\[ S_p = 1 + \langle \mathcal{F}_0 | \frac{\partial H}{\partial (N V_p)} | \mathcal{F}_0 \rangle / \langle \mathcal{F}_0 | \mathcal{F}_0 \rangle, \quad (3·5) \]

and

\[ \frac{\partial \lambda_p}{\partial (N V_p)} = -\lambda_p^3/\phi_p^{(g)}. \quad (3·6) \]

Berdahl\(^9\) obtained the structure factor from the ground-state energy of the Bogoliubov-Zubarev theory (BZ).\(^{10}\) So far as the structure factor is concerned, we can obtain the same exact result for the one-dimensional model of Lieb and Liniger,\(^{18}\) whichever collective variable theory one follows, in contrast with the case of the ground-state energy,\(^8\) because we can safely neglect a one-dimensional sum of the form

\[ \sum_{q, r} \partial_{p+q, r} \left[ p \cdot q \cdot (1 - \lambda_q) + p \cdot r (1 - \lambda_r) \right], \quad (3·7) \]

while a similar double summation appeared in the expression for the ground-state energy is by no means negligible.

\[ \mathsection 4. \text{The low momentum limit for the case of liquid } ^4\text{He} \]

We consider that the unperturbed structure factor \( \lambda_p \) approaches zero linearly in \( p \) as the wave number decreases, as in the case with the three-dimensional soft-core interaction or the one-dimensional \( \delta \)-function interaction. In the low-momentum limit we obtain

\[ \alpha(p, q, -p - q) \rightarrow \gamma(p, q, -p - q) \rightarrow -\lambda_p q^2 (1 - \lambda_q)^2, \]

\[ b(p, q, -p - q) \rightarrow 2\lambda_p \lambda_q q^2. \quad (4·1) \]
From (3·2) and (4·1), we find that the structure factor approaches the form

\[ S_p = \lambda_p + \frac{1}{8N} p^{-2} \lambda_p^3 \sum_q q^2 (1 - \lambda_q)^2 / \lambda_q, \tag{4·2} \]

and, by neglecting the terms of order higher than \(1/N^{3/2}\) the momentum distribution can be expressed as

\[ n_p = \frac{1}{4N \lambda_p} \left[ N - \frac{1}{4} \sum_q (1 - \lambda_q)^2 / \lambda_q \right] - \frac{1}{32N} p^{-1} \lambda_p \sum_q q^2 (1 - \lambda_q)^2 / \lambda_q, \tag{4·3} \]

\[ = \frac{1}{4NS_p} n_{q^{(0)}}, \tag{4·4} \]

where \(n_{q^{(0)}}\) stands for the unperturbed value of the number of bosons having zero momentum and is defined by

\[ n_{q^{(0)}} = N - \sum_q (1 - \lambda_q)^2 / (4\lambda_q) = N - \sum_q n_{q^{(0)}}, \tag{4·5} \]

which should remain positive.

From (3·4), in place of (4·3), we have

\[ n_p = \frac{1}{4NS_p} n_{q^{(0)}}, \quad n_{q^{(0)}} = N - \sum_q (1 - S_q)^2 / (4S_q). \tag{4·6} \]

Using the experimental data of the x-ray scattering due to Achter and Meyer, \(n_{q^{(0)}}\) was estimated by Grest as \(-0.27N\). From (4·6), as \(p \to 0\), we have

\[ n_p = -0.14(MC/hp), \tag{4·7} \]

where \(C\) is the sound velocity of liquid \(4\)He. Here we would like to estimate the next higher order term of order \(p^0\) from (3·4) and (4·1) obtaining

\[ n_p = \frac{1}{4NS_p} n_{q^{(0)}} + \frac{1}{32N} \sum_q \left[ (1 - S_q)^2 + (1 - S_q')^2 / S_q^2 \right]. \tag{4·8} \]

The correction term to (4·7) amounts to 0.23. Thus we can see that (4·8) becomes negative for sufficiently low wave numbers \(p = 0.1A^{-1}\). This result can be confirmed by a numerical computation of (3·4). By the above discussion it has been elucidated why Grest found an unphysical result that \(n_p\) becomes negative below \(p = 0.3A^{-1}\).

In order to improve this result we have to take account of the higher order perturbation terms beyond those of order \(1/N\). Here we would propose a simplest way to prevent the unphysical result by rewriting (3·4) in the form

\[ n_p = n_p^{(0)} \left( 1 - \frac{1}{N} \sum_q n_{q^{(0)}} \right) + n_p^{''}, \tag{4·9} \]

where \(n_p^{(0)} = (1 - S_p)^2 / (4S_p)\) and \(n_p^{''}\) represents the residual terms in (3·4) and \(n_p^{''} \to 0.23\) as \(p \to 0\). When \(n_{q^{(0)}}\) in the bracket of (4·9) is replaced by \(n_p^{(0)}\), (4·9) may be considered as an equation to solve \(n = \sum_q n_q = N - n_q\), i.e., the number of
Particles with non-zero momenta in the ground state. Since $\sum_n n^\prime_n$ is estimated as $0.96N$, we have $n^\prime = 0.98N$ or $n_0 = 0.02N$, therefore $n_p$ can remain positive for low wave numbers. Using this value for $n_0$ in place of $n_p^{(0)}$ in (4.8), in the low momentum limit, we have

$$n_p = 0.01(MC/\hbar p) + 0.23.$$  \hfill (4.10)

Although, in view of the Gavoret-Nozières condition, the procedure made for (4.9) to replace $n_p^{(0)}$, by $n_p$ seems to be reasonable at the present stage of the problem, we have, of course, to take account of the higher order corrections to the both expressions (2.10) and (3.4) and also the corresponding correction to $n_p^{(0)}$ in (4.9), in order to have a definite answer to presence or absence of the number of condensed particles $n_0$ in liquid 4He which is not at so high a density.

In case of a charged Bose gas at high density, no unphysical result appears and $n_0^{(0)}$ given by (4.5) and $n_p^{(0)}$ given by (4.6) remain positive in the high-density limit.

## § 5. The ground-state energy

Using the expression for the momentum distribution (2.10) the mean kinetic energy with respect to the ground state is given by

$$\langle T \rangle_0 = \langle \mathcal{W}_0 | T | \mathcal{W}_0 \rangle / \langle \mathcal{W}_0 | \mathcal{W}_0 \rangle = \sum_p \varepsilon_p^{(0)} \langle \mathcal{W}_0 | n_p | \mathcal{W}_0 \rangle / \langle \mathcal{W}_0 | \mathcal{W}_0 \rangle = \sum_p \varepsilon_p^{(0)} n_p + \delta n_p,$$  \hfill (5.1)

where $\delta n_p$ is the correction to the first order expectation value given by (2.10). Using the expression for the structure factor (3.1), the mean potential energy can be written in the form

$$\langle V \rangle_0 = \langle \mathcal{W}_0 | V | \mathcal{W}_0 \rangle / \langle \mathcal{W}_0 | \mathcal{W}_0 \rangle = \frac{N}{2} \sum_p V_p (S_p - 1).$$  \hfill (5.2)

From (2.7) we can write $NV_p$ in terms of $\varepsilon_p^{(0)}$ and $\lambda_p$ as

$$NV_p = \varepsilon_p^{(0)} \left( \frac{1}{\lambda_p^2} - 1 \right),$$  \hfill (5.3)

and since we know that $S_0 = N$ by the definition we can obtain

$$\langle V \rangle_0 = \frac{N^2}{2} V_0 - \frac{1}{4} \sum_p \varepsilon_p^{(0)} \left[ \left( \frac{1}{\lambda_p} \right)^2 (1 + \lambda_p) + \left( \frac{1}{\lambda_p^2} \right) \delta \lambda_p \right].$$  \hfill (5.4)

From (2.10) and (3.2) the ground-state energy $E_0$ can be expressed as

$$E_0 = \langle T \rangle_0 + \langle V \rangle_0 = E_0^{(0)} + \Delta E_0,$$  \hfill (5.5)

where $E_0^{(0)}$ is the unperturbed ground-state energy of DPO given by (A.7) and the correction term $\Delta E_0$ has the form
\[
\Delta E_0 = \sum_p \varepsilon_p \left[ \Delta n_p + \frac{1}{4} \left( \frac{1}{\lambda_p^2} - 1 \right) \Delta \lambda_p \right]
\]
\[
= \frac{1}{8N} \sum_{p,q,r} \partial_{p+q+r,0} \varepsilon_p \left[ \frac{\alpha(p, q, r)^2}{b(p, q, r)} \right] \lambda_q \lambda_r
\]
\[
+ (\lambda_q + \lambda_r - \lambda_p - 2\lambda_q \lambda_r + \lambda_p \lambda_q \lambda_r) \frac{\alpha(p, q, r)}{b(p, q, r)}
\]
\[
+ \frac{1}{4} \left( 1 - \lambda_p \right)^2 (1 - \lambda_q)^2 (1 - \lambda_r)^2 / (\lambda_p \lambda_q)
\]
\[
- \frac{1}{4} \left( 1 - \lambda_p \right)^2 (1 - \lambda_q)^2 / (\lambda_p \lambda_q) + \frac{1}{4} (1 - \lambda_q)^2 (1 - \lambda_r)^2 / (\lambda_q \lambda_r).
\]

(5.6)

Considering that \(\alpha(p, q, r)\) and \(b(p, q, r)\) are symmetric with respect to \(p, q\) and \(r\) we obtain

\[
E_0 = E_0^a + E_0^b + E_0^c,
\]
\[
E_0^a = - \frac{\hbar^2}{48MN} \sum_{p, q, r} \partial_{p+q+r,0} \varepsilon_p \frac{\alpha(p, q, r)^2}{b(p, q, r)},
\]
(5.7)
\[
E_0^b = \frac{\hbar^2}{16MN} \sum_{p, q, r} \partial_{p+q+r,0} \varepsilon_p (1 - \lambda_p) (1 - \lambda_q) (1 - \lambda_r),
\]
(5.8)
\[
E_0^c = \frac{\hbar^2}{96MN} \sum_{p, q, r} \partial_{p+q+r,0} [p \cdot q (1 - \lambda_p)^2 (1 - \lambda_q)^2 / (\lambda_p \lambda_q)
\]
\[
+ q \cdot r (1 - \lambda_q)^2 (1 - \lambda_r)^2 / (\lambda_q \lambda_r) + r \cdot p (1 - \lambda_r)^2 (1 - \lambda_p)^2 / (\lambda_r \lambda_p)].
\]
(5.9)

The first two expressions \(E_0^a\) and \(E_0^b\) have the same forms as obtained by Lee\(^6\) in the uniform limit of CBF and by the author using DPO.\(^7\) The additional term denoted by \(E_0^c\) is nothing but the difference between the ground-state energy of the Bogoliubov theory re-formulated by Brueckner\(^9\) and Lee\(^6\) denoted by \(E_0^{BB}\) and that of CBF denoted by \(E_0^{CBF}\) and

\[
E_0 = E_0^{BB} = E_0^{CBF} + E_0^c.
\]
(5.10)

Following the adiabatic theorem, one can derive the momentum distribution (2.9) from the expression \(E_0\) regarding \(\varepsilon_p^{(0)}\) as an adiabatic parameter and writing

\[
(h^2 / M) p \cdot q = \varepsilon_p^{(0)} - \varepsilon_q^{(0)} - \varepsilon_p^{(0)}.
\]

Giving the momentum distribution in the form

\[
n_p = \langle \Psi_0 | \partial H / \partial \varepsilon_p^{(0)} | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle,
\]
(5.11)

and using the identity

\[
\frac{\partial \lambda_p}{\partial \varepsilon_p^{(0)}} = \frac{1}{2} (\lambda_p / \varepsilon_p^{(0)}) (1 - \lambda_p^2),
\]
(5.12)

we are led to the correct result given by (2.10). Berdahl obtained the momentum distribution using the expression \(E_0^{BB}\). So far as one follows the adiabatic theorem, neither \(E_0^{CBF}\) nor \(E_0^{BZ}\) given by the Bogoliubov-Zubarev theory\(^9\) or by Berdahl\(^9\)
and Grest and Rajagopal\textsuperscript{29} yields the correct expression for $n_p$. In this meaning, $E_0^a$ is indispensable in obtaining the momentum distribution. The value of the ground-state energy itself, however, is solely determined by $E_0^a$ and $E_0^b$ alone, as long as $\lambda_p$ is a well-behaving function. Indeed, as shown by Lee\textsuperscript{20} and Takahashi,\textsuperscript{21} for the one-dimensional problem of Lieb and Liniger, $E_0^a$ and $E_0^b$ are sufficient to obtain the exact value of the energy in the high density limit.

Recently Hiroike\textsuperscript{22} has derived the same expression as $E_0^{\text{CBF}}$ from his own theory which is considered as a reformulation of the Bogoliubov-Zubarev theory dealing with a cutoff wave number $k_c$.

§ 6. Remarks

In a previous paper\textsuperscript{23} the author proposed a method of collective description introducing a cutoff wave number $q_0$. In this paper the density fluctuations and the Fourier transforms of the phase operator having wave numbers lower than $q_0$ are given by DPO, while those having the higher wave numbers are considered as given by B. This theory is successfully applied to the theory of liquid $^4$He. We know that DPO is exact in the high density limit as shown explicitly for the one-dimensional model of Lieb and Liniger. So far as the problems in the high density limit are concerned, the results obtained by this theory should be independent of the cutoff, because DPO and B lead to the same exact results by letting $q_0$ tend to infinity or tend to zero, respectively. This situation is not always true in the region of intermediate densities. For example, liquid $^4$He is not at so high a density that the $1/N$-expansion method of DPO does not prevail without restriction. This is the reason why the author introduced a cutoff wave number. In this intermediate region, DPO will be pertinent to describe phenomena associated with long wave lengths, while B will be suitable for those associated with short wave lengths.

The DPO theory resembles the Holstein-Primakoff theory\textsuperscript{24} of spin waves in the theory of magnetism. It has been shown\textsuperscript{25} that the Hamiltonian of an interacting many-boson system is obtained by taking the continuum limit for the Hamiltonian of a quantum lattice model, in which a number of bosons are allowed to occupy the same lattice point. When a repulsive interaction is introduced in this model and the coupling parameter of this interaction tends to infinity, this model becomes equivalent to the Matsubara-Matsuda model\textsuperscript{26} of the quantum lattice gas whose algebra is completely equivalent to the $X$-$Y$ model\textsuperscript{27} in the theory of magnetism. It is a distinguished feature of the problem that the exact expression for the ground-state energy of the one-dimensional model of Lieb and Liniger\textsuperscript{18} approaches, in the low density and the strong coupling limit, that obtained in the continuum limit of the Matsubara-Matsuda model. The value of this ground state energy is nothing but the mean Fermi energy of the one-dimensional problem, i.e., $E_0 = [(\pi n)^2/(6M)]N$, where $n = N/L$ and $L$ is the length of the box.
The theory of collective variables does not work better in the low density limit than the Holstein-Primakoff theory does for a ferromagnet in the low spin-quantum-number limit. It is worth while making efforts to investigate the region of intermediate densities of a many-boson system by extending both the theory of collective variables and the continuum-limit theory of the Matsubara-Matsuda model.

From our point of view, the cutoff-dependent theory is useful in this intermediate region and expected to serve as a bridge leading to a more sophisticated renormalization theory.

Appendix

— A Graphic Representation of the Perturbation Calculation —

By using Eq. (2·1) the higher order terms in $N_p$ denoted by $N_p'$ in (2·2) can be expressed in terms of the Fourier transforms $\rho_p$ and $\phi_p$. Among these higher order terms, first we would calculate the first order averages of the quaternary terms having an explicit factor $1/N$ with respect to the unperturbed ground state represented by $|\Phi_0\rangle$. These averages are given by two products of contractions of Wick's expansion theory introduced by (2·8). For example, we obtain

$$
\langle \Phi_0 | \sum_{q,q'} \rho_{p|p-q|q'} \phi_{q|q'} | \Phi_0 \rangle = \sum_{q,q'} (\rho_{p|p-q|q'} \phi_{q|q'})
$$

$$
+ \rho_{p|p-q|q'} \phi_{q|q'} + \rho_{p|p-q|q'} \phi_{q|q'} = i \frac{3}{8\lambda_q}.
$$

(A·1)

After some simple manipulations, the average of the following quaternary terms,

$$
N_p^{(4)} = \frac{1}{N} \sum_{q,q'} \frac{1}{164} (\rho_{p|p-q|q'} \phi_{q|q'})
$$

$$
+ \frac{i}{16\hbar} (\rho_{p|p-q|q'} \phi_{q|q'} - \rho_{p|p-q|q'} \phi_{q|q'})
$$

$$
- \rho_{p|p-q|q'} \phi_{q|q'} + \phi_{p|p-q|q'} \phi_{q|q'}
$$

$$
+ \rho_{p|p-q|q'} \phi_{q|q'} - \rho_{p|p-q|q'} \phi_{q|q'}
$$

$$
+ \frac{1}{16\hbar} (4\rho_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'} - 2\rho_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'})
$$

$$
- 2\phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'} - 2\phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'}
$$

$$
+ 3\rho_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'}
$$

$$
- \phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'}
$$

$$
+ \frac{1}{12\hbar} (3\rho_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'} - 3\phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'})
$$

$$
- \phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'}
$$

$$
+ \frac{1}{12\hbar} (3\phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'} - 4\phi_{p|p-q|q'} \phi_{q|q'} \phi_{q|q'})
$$

(A·2)
reads

\[ n_p^{(0)} = \frac{1}{16N} \sum_q [2 + 4\lambda_p(\lambda_q - 1) + (1 - \lambda_q)^2(1 - \lambda_{p-q})^2/(2\lambda_q\lambda_{p-q}) \]

\[ - (1 - \lambda_p)^2(1 - \lambda_q)^2/(\lambda_p\lambda_q) \].

This average value should be considered together with the contribution coming from the second order perturbation terms given in the following. The non-diagonal terms denoted by \( N_p^{(2,\beta)} \) in (2.6) and those involved in \( N_p^{\gamma} \) denoted by \( N_p^{(\omega)} \) which are necessary to calculate the second order correction to the momentum distribution \( n_p \) have the form

\[ N_p^{(2,\beta)} = \frac{1}{4} \left( \lambda_p - \frac{1}{\lambda_p} \right) (B^+pB^+p + B_pB_{-p}) \],

\[ N_p^{(\gamma)} = -\frac{1}{8} \sum_{q,r} \delta_{p+q+r,0} (\lambda_p\lambda_q\lambda_r/N)^{1/2} \left( 1 + \frac{1}{\lambda_p\lambda_q} - \frac{1}{\lambda_q\lambda_r} + \frac{1}{\lambda_r\lambda_p} \right) \]

\[ \times (B^+pB^+qB^+r + B_pB_qB_r) \].

The average values are obtained for the perturbed ground state given by

\[ |\Phi_0\rangle = \left[ 1 + \frac{Q}{E_0 - H_0} H' + \frac{Q}{E_0 - H_0} H' - \frac{Q}{E_0 - H_0} H' \right] |\Phi_0\rangle \],

where \( Q \) is a projection operator defined by \( Q = 1 - |\Phi_0\rangle\langle\Phi_0| \) and \( E_0^{(0)} \) is the unperturbed ground-state energy of DPO given by

\[ E_0^{(0)} = \frac{1}{2} N^2 V_0 - \frac{\hbar^2}{8M} \sum_p \left( 1 - \frac{1}{\lambda_p} \right)^2 \],

and as shown in Ref. 2) the Hamiltonians \( H_0 \) and \( H' \) have the form

\[ H_0 = \sum_p \hbar^2 p^2/(2M\lambda_p) B^+_pB_p + E_0^{(0)} \sum_p (\hbar^2 p^2/2M) n_p^{(0)} \],

\[ H' = H'_a + H'_b + H'_c \],

\[ H'_a = \sum_{p,q} \delta_{p+q+r,0} \Gamma_a(p, q, r) B^+_pB^+_qB^+_r + \text{h.c.} \],

\[ H'_b = \sum_{p,q} \delta_{p+q+r,0} \Gamma_b(p, q, r) B^+_pB_qB_r + \text{h.c.} \],

\[ H'_c = \hbar^2/(8MN) \sum_{p,q} \left[ (p^2 + q^2) \lambda_p\lambda_q - p^2\lambda_p \right] B^+_pB^+_q + \text{h.c.} \],

where the vertex functions \( \Gamma_a(p, q, r) \) and \( \Gamma_c(p, q, r) \) are given by

\[ \Gamma_a(p, q, r) = \frac{\hbar^2 N^{-1/2}}{24M} (\lambda_p\lambda_q\lambda_r)^{-1/2} a(p, q, r) \],

\[ \Gamma_c(p, q, r) = \frac{\hbar^2 N^{-1/2}}{8M} (\lambda_p\lambda_q\lambda_r)^{-1/2} c(p, q, r) \].
The contribution to the correction of $n_p^{(0)}$ denoted by $\Delta n_p$ are divided into the following five classes of the averages of the perturbation terms which are given by a sum of products of contractions defined for the field operators of phonons. Each class of the averages corresponds to a set of graphs. Each graph in a set has a certain multiplicity dependent on the structure of the operators included in the averages of this class. The first two kinds of averages belonging to Class A and Class B include one occupation number operator and one kind of Hamiltonian. The third and the fourth kinds of averages belonging to Class C and Class D include one occupation number operator and two kinds of Hamiltonians. The last average belonging to Class E includes only the quaternary occupation number operator given by $(A \cdot 2)$.

The graphs and the types of averages of these classes are shown in the following together with the multiplicity of each graph.

<table>
<thead>
<tr>
<th>Class</th>
<th>Type</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B.</td>
<td></td>
<td>6.</td>
</tr>
<tr>
<td>C.</td>
<td></td>
<td>18.</td>
</tr>
</tbody>
</table>

Fig. A. The white circles stand for $N_p^{(2,3)}$ and the black circles for $H'_s$.

$$
\langle \Phi_0 | N_p^{(2,3)} \frac{Q}{E_p^{(0)} - H_0} H'_s + \text{h.c.} | \Phi_0 \rangle = \frac{1}{8N} \sum_q \lambda_p (1 - \lambda_p^2) [\lambda_q^2 (1 + q^2/p^2) - 1].
$$

Fig. B. The white circles stand for $N_p^{(2)}$ and the black circles for $H'_a$.

$$
\langle \Phi_0 | N_p^{(2)} \frac{Q}{E_p^{(0)} - H_0} H'_a + \text{h.c.} | \Phi_0 \rangle = \frac{1}{8N} \sum_q (\lambda_q^2 + \lambda_p^2 - \lambda_p^4 + \lambda_p^2 \lambda_q^2 \lambda_{p+q}) \frac{a(p, q, p-q)}{b(p, q, p-q)}.
$$

Fig. C. The white circle stands for $N_p^{(2)} - n_p^{(0)}$ and the black circles for $H'_a$.

$$
\langle \Phi_0 | H'_a \frac{Q}{E_p^{(0)} - H_0} (N_p^{(2)} - n_p^{(0)}) \frac{Q}{E_p^{(0)} - H_0} H'_a | \Phi_0 \rangle = \frac{1}{16N} \sum_q \lambda_q \lambda_{p+q} (1 + \lambda_p^2) \frac{a(p, q, p-q)}{b(p, q, p-q)^2}.
$$
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Fig. D. The white circles stand for $N_{p}^{(\alpha)}$, the black circles in the upper middle of two figures for $H_0 \rho$ and the black circles in the ends of the figures for $H_0 \sigma$.

$$
\langle \phi_{\alpha} | N_{p}^{(\alpha)} \frac{Q}{E_{0}^{(\alpha)} - H_0} \frac{Q}{E_{0}^{(\alpha)} - H_0} H_0' + h.c. | \phi_{\alpha} \rangle = -\frac{1}{16N} \sum_{q} (1 - \lambda_\rho^{-1}) a(p, q, -p - q) c(p, q, -p - q) \cdot p^2 b(p, q, -p - q).
$$

Fig. E. The white circle stands for $N_{p}^{(\alpha)}$.

$$
\langle \phi_{\alpha} | N_{p}^{(\alpha)} | \phi_{\alpha} \rangle = n_{p}^{(\alpha)} \quad (\text{see A.3}).
$$

In Class E, as seen from (A.2), there appear five subclasses. The contribution from each member of a subclass is given by a sum of products of two contractions as shown by (A.1).

The solid line in the figures shows a contraction at the same time. The white circle stands for an occupation number operator and the black circle stands for an interaction Hamiltonian.

The expression for the structure factor (3·2') can be derived in a similar way.

References

6) K. A. Brueckner, Phys. Rev. 156 (1967), 204.
T. Nishiyama

22) K. Hiroike, Prog. Theor. Phys. 54 (1975), 308.

**Note added in proof:**

1) The Hamiltonian $H_2'$ given by (A-12) has been driven from (A-2) by separating a trivial Hamiltonian of the form

$$H_2'' = -\left( \hbar^2/32MN \right) \sum_{p,q} \left[ (p+q)^2 - p^2 - q^2 \right] \left( 1 - \lambda_p \right) \left( 1 - \lambda_q \right) \lambda_{p+q} B_p B_q^* + \text{h.c.},$$

which contributes nothing to the expectation values in the uniform high-density limit.

2) Missprints occurred in signs of Eq. (4·1) in the first paper of Ref. 2) which should read

$$T_1' = -\left( \hbar^2/8MN \right) \sum_{k,l} k \cdot l \left[ 1 - \langle 2/N \rangle \rho_{0,l} \right]. \quad (4\cdot1)$$