Ground-state energy density of a dilute Bose gas in the canonical transformation

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A ground state energy density of an interacting dilute Bose gas system is studied in the canonical transformation scheme. It is shown that the transformation scheme enables us to calculate a higher order correction of order \( n a^3 \) in the particle depletion and ground state energy density of a dilute Bose gas system, which corresponds to the density fluctuation contribution from the excited states. Considering two-body interaction only, the coefficient of \( n a^3 \) term is shown to be \( 2(\pi - 8/3) \) for the particle depletion, and \( 16(\pi - 8/3) \) for the ground state energy density.

Keywords: canonical transformation; homogeneous Bose system; ground state energy density.

I. INTRODUCTION

Investigation of an interacting dilute Bose gas has a long history beginning with the seminal works of Bogoliubov, Beliaev, Lee, Huang and Yang, Hugenholtz and Pines. This topic has been amply discussed in standard text books.1,2,3 Despite the successful demonstration of Bose-Einstein condensation (BEC) in inhomogeneous system of dilute alkali gases during the last decade, the dilute interacting Bose fluids in homogeneous system is one of the fundamental interests still in statistical physics.

The ground state energy density of the dilute system is expressed in the following general form:4

\[
\frac{E_g}{V} = \frac{2\pi \hbar^2 a^2}{m} \sum_{i=0}^{\infty} \sum_{j=0}^{[i/2]} C_{ij} (n a^3)^{i/2} \{ \ln(n a^3) \}^j, \tag{1}
\]

where \( n = N/V \) is the particle density. Since unconfined BEC occurs for a two-body repulsive interaction, the s-wave scattering length \( a \) is positive. \([i/2]\) is the Gauss number which takes the integer part of \( i/2 \), and \( C_{ij} \) are the coefficients in the expansion. Through elaborate calculations, it is known that:5

\[
\frac{E_g}{V} = \frac{2\pi \hbar^2 a^2}{m} \left[ 1 + \frac{128}{15\sqrt{\pi}} (n a^3)^{1/2} + \left\{ \frac{8(4\pi - 3\sqrt{3})}{3} \ln(n a^3) + \kappa \right\} n a^3 + \ldots \right]. \tag{2}
\]

Comparing Eq. (1) with Eq. (2), we find the coefficients as \( C_{00} = 1 \), \( C_{10} = 128/15\sqrt{\pi} \), and \( C_{21} = 8(4\pi - 3\sqrt{3})/3 \). Nevertheless, the coefficient of \( C_{21} \) was calculated early in 1950’s.4,6,7 the constant \( \kappa = C_{20} \) and other higher order terms did not receive much attention.

Hugenholtz and Pines mentioned that the expansion is not a simple power series, rather it involves the logarithm of expansion parameter \( na^3 \). Although Fetter and Walecka gave a rough estimate on the fluctuation contribution from the condensate in the order of \( na^3 \), they stated that the coefficient \( C_{20} \) has never been determined.8 In order to get a deeper understanding of the ground state over the mean field results, it is necessary to calculate corrections from the quantum fluctuations. Earlier derivation of rigorous upper and lower bounds had been given by Dyson.8 Also an improved calculation on the lower bounds has been carried by Lieb and Yngvason.8

Some practical calculations of the coefficient \( C_{20} \) were carried out very recently by two groups. Our group obtained \( C_{20} \) from the fluctuation contribution by using the functional Schrödinger picture approach of two-body interaction.9,10 The Schrödinger picture for many particle systems or relativistic quantum field theory is an infinite dimensional extension of quantum mechanics and leads into a functional formulation.11,12,13 However, the result has not been confirmed using a separate independent method. Another contribution by three-body interaction has been calculated by Braaten et al. In their calculation the core potential is necessary to find \( C_{20} \), and they calculated \( C_{20} \) as a function of an effective potential parameter \( r_s \). Therefore, the two results for \( C_{20} \) are independent.

In this paper, we consider the contribution from the condensate fluctuation, which is independent on the details of the potential and two-body interaction only. We show that the result obtained by the Schrödinger picture can be obtained by a more standard canonical transformation method. In the process we obtain the fluctuation correction

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to the particle depletion, and $C_{10}$ in Eq. (11) from second order ground state expansion. Also, we will consider the fluctuation contribution from the condensate, and then calculate the coefficients $C_{20}$ and $C_{30}$. On the other hand $C_{21}$ which come from three-body interaction will not be touched.

This paper is organized as follows: In Section II, the interacting Hamiltonian of the dilute Bose system is expanded up to the terms of our interest. In Section III, the canonical transformations are applied twice to diagonalize the Hamiltonian. In Section IV, the particle depletion appearing in the diagonalized Hamiltonian is obtained. In Section V, the fluctuation correction to the ground state energy density is obtained as a series of $n a^3$. In Section VI, we summarise and discuss our results.

II. MANY-BODY DILUTE BOSE GAS SYSTEM

We start with the standard model Hamiltonian for an interacting Bose gas given by:

$$\hat{H} = \sum_{k} \hbar^2 k^2 / 2m a_{k}^\dagger a_k + \frac{g}{2V} \sum_{k_1 k_2 k_3 k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2,k_3+k_4}. \quad (3)$$

Here, the constant matrix element $g$ should be determined by requiring that $\hat{H}$ produces the two-body scattering properties in vacuum. Since the system is dilute enough, we assume that the $s$-wave scattering length $a$ is much less than the inter-particle spacing $n^{1/3}$. As a result of the $n a^3 \ll 1$, this satisfies to be a small expansion parameter. Under this assumption the zero momentum operators $a_0, a_0^\dagger$ become nearly classical due to occurrence of a condensate.

In two-body interaction the interacting part of the Hamiltonian in Eq. (3) is expanded to keep the terms up to order of $N_0^2, N_0$, and $\sqrt{N_0} n a_{10,15}$. We introduce a new variable $\gamma_k$

$$\gamma_k = \sum_{q \neq 0} a_{k+q}^\dagger a_q. \quad (5)$$

Replacing the operators $a_0, a_0^\dagger$ by $\sqrt{N_0}$, and applying the number operator relation $N_0 = \hat{N} - \sum_{k \neq 0} (a_k^\dagger a_k + a_{-k}^\dagger a_{-k})/2$ to Eq. (11), we rewrite the model Hamiltonian as

$$\hat{H} = \frac{1}{2} n^2 V g$$

$$+ \frac{1}{2} \sum_{k \neq 0} \left[ \epsilon_k^0 + n g (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + n g (a_k^\dagger a_{-k} + a_k a_{-k}) \right]$$

$$+ \frac{n g}{\sqrt{N_0}} \sum_{k \neq 0} \gamma_k (a_k + a_{-k}^\dagger), \quad (6)$$

where $\epsilon_k^0 = \hbar^2 k^2 / 2m$. The ground state properties of the above Hamiltonian is to be calculated using a canonical transformation method.
III. CANONICAL TRANSFORMATION METHOD

To diagonalize the above Hamiltonian, we apply the Bogoliubov transformation of the new the operators $a_k$ and $a_k^\dagger$ as follows:

$$
\begin{align*}
a_k &= \frac{1}{\sqrt{1 - A_k^2}} (b_k + A_k b_k^\dagger), \\
a_k^\dagger &= \frac{1}{\sqrt{1 - A_k^2}} (b_k^\dagger + A_k b_{-k}).
\end{align*}
$$

Then, the Hamiltonian in Eq. \((6)\) becomes

$$
\begin{align*}
\hat{H} &= \frac{1}{2} n^2 V g + \sum_{k \neq 0} \frac{1}{1 - A_k^2} [(\epsilon_k^0 + n g) A_k^2 + n g A_k] \\
&+ \frac{1}{2} \sum_{k \neq 0} \frac{1}{1 - A_k^2} [(\epsilon_k^0 + n g)(1 + A_k^2) + 2 n g A_k] (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) \\
&+ \frac{1}{2} \sum_{k \neq 0} \frac{1}{1 - A_k^2} [2(\epsilon_k^0 + n g) A_k + n g (1 + A_k^2)] (b_k^\dagger b_{-k}^\dagger + b_{-k} b_{-k}) \\
&+ \frac{n g}{\sqrt{N}} \sum_{k \neq 0} \left(1 + A_k \right) \gamma_k (b_k + b_{-k}^\dagger)_{\gamma_k}. \quad (8)
\end{align*}
$$

$A_k$ is chosen to make the off-diagonal term vanish. That is,

$$
2(\epsilon_k^0 + n g) A_k + n g (1 + A_k^2) = 0,
$$

and we obtain $A_k (= A_{-k})$ as

$$
A_k = \frac{E_k - (\epsilon_k^0 + n g)}{n g}, \quad (10)
$$

where

$$
E_k = \sqrt{(\epsilon_k^0 + n g)^2 - (n g)^2}. \quad (11)
$$

The positive sign was selected in Eq. \((10)\) to give positive excited energy values. Note that $(1 + A_k)/(1 - A_k) = \epsilon_k^0/E_k$.

Substituting $A_k$ into the Hamiltonian in Eq. \((8)\), we obtain the following compact form of the Hamiltonian

$$
\begin{align*}
\hat{H} &= \frac{1}{2} n^2 V g + \sum_{k \neq 0} \frac{1}{1 - A_k^2} [(\epsilon_k^0 + n g) A_k^2 + n g A_k] \\
&+ \sum_{k \neq 0} E_k b_k^\dagger b_k + \sum_{k \neq 0} G_k (b_k + b_{-k}^\dagger), \quad (12)
\end{align*}
$$

where

$$
G_k = \frac{n g}{\sqrt{N}} \frac{(1 + A_k) \gamma_k}{\sqrt{1 - A_k^2}}. \quad (13)
$$

We can regard the system as a collection of quantum mechanical harmonic oscillators exposed to additional forces given by linear terms. The linear terms $b_k$ and $b_k^\dagger$ can be made to eliminate by a linear transformation of the form

$$
\begin{align*}
b_k &= c_k + \alpha_k, \\
b_k^\dagger &= c_k^\dagger + \alpha_{-k}, \quad (14)
\end{align*}
$$

where the new operators $c_k$ and $c_k^\dagger$ satisfy the bosonic commutator relations. Note that $\alpha_{k}^\dagger = \alpha_{-k}$ and commutes with $c_k$. 
Substituting the new operators in Eq. (14) into Eq. (12), we can rewrite the Hamiltonian in Eq. (12) as

\[ \hat{H} = \frac{1}{2} n^2 V g + \sum_{k \neq 0} \frac{1}{1 - A_k^2} \left[ (\epsilon_k^0 + ng) A_k^2 + ng A_k \right] \]

\[ \quad + \sum_{k \neq 0} \left( E_k c_k^\dagger c_k + E_k \alpha_k c_k + 2 G_k \alpha_k \right) \]

\[ \quad + \sum_{k \neq 0} (E_k \alpha_{-k} + G_k) c_k + \sum_{k \neq 0} (E_k \alpha_k + G_{-k}) c_k^\dagger. \]  

(15)

Here, we choose \( \alpha_k = -G_{-k}/E_k \) to make the linear terms vanish. Then, the Hamiltonian in Eq. (15) is now diagonalized in terms of new operators as follows

\[ \hat{H} = \frac{1}{2} n^2 V g + \sum_{k \neq 0} \frac{1}{1 - A_k^2} \left[ (\epsilon_k^0 + ng) A_k^2 + ng A_k \right] \]

\[ \quad - \sum_{k \neq 0} \frac{G_k G_{-k}}{E_k} + \sum_{k \neq 0} E_k c_k^\dagger c_k \]

\[ = \hat{H}_g + \sum_{k \neq 0} E_k n_k. \]  

(16)

Using Eqs. (10), (11), (13), and the chosen \( \alpha_k \), the above Hamiltonian \( \hat{H}_g \) produces the general form of the ground state energy as

\[ E_g = \frac{1}{2} n^2 V g + \sum_{k \neq 0} \left[ E_k - (\epsilon_k^0 + ng) \right] + \frac{n^2 g^2}{N} \sum_{k \neq 0} \frac{\epsilon_k^0}{E_k^2} \langle 0 | \gamma_k \gamma_{-k} | 0 \rangle \]

\[ \equiv E_0 + E_1 + E_2. \]  

(17)

From the relation of the interaction strength, \( g^2 \)

\[ \frac{4 \pi \hbar^2 a}{m} = g - \frac{g^2}{2V} \sum_{k \neq 0} \frac{1}{\epsilon_k^0} + ... , \]  

(18)

we obtain the ground state energy density of the first two terms as

\[ \frac{1}{V} (E_0 + E_1) = \frac{2 \pi \hbar^2 a n^2}{m} \left[ 1 + \frac{128}{15 \sqrt{\pi}} (na^3)^{1/2} \right]. \]  

(19)

Note that \( \sum_k \) is replaced with \( V \int d^3 k / (2 \pi)^3 \) during the calculation. The first two terms, \( E_0 \) and \( E_1 \) in the ground state energy are exactly same as those obtained through conventional methods in the literature \[1,2,3\].

IV. THE PARTICLE DEPLETION

Accurate determination of the fractional depletion of the zero momentum state for an interacting gas is increasingly needed with the advance of the experimental technique on the BEC states. The particle distribution of the dilute system is obtained from Eq. (7) and (14) as

\[ n_k = \langle 0 | a_k^\dagger a_k | 0 \rangle \]

\[ = \frac{A_k^2}{1 - A_k^2} + \frac{(1 + A_k)^2}{1 - A_k^2} \langle 0 | \alpha_{-k} \alpha_k | 0 \rangle \]

\[ = \frac{1}{2} \left( \epsilon_k^0 + ng \right) + \frac{n^2 g^2}{N} \frac{\epsilon_k^0}{E_k} \langle 0 | \gamma_k \gamma_{-k} | 0 \rangle. \]  

(20)

The dominant part of the unknown quantity \( \langle \gamma_k \gamma_{-k} \rangle \) is obtained by iteration method. Applying the definition of \( \gamma_k \) in Eq. (6), it is written as

\[ \langle 0 | \gamma_k \gamma_{-k} | 0 \rangle = \langle 0 | \sum_{q, q' \neq 0} a_{k+q}^\dagger a_{-k+q}^\dagger a_{q'} a_{-q'} | 0 \rangle. \]  

(21)
It is known that the dominant contribution arises when a particle interacts with itself and it belongs to the term where \( \mathbf{q}' = \mathbf{k} + \mathbf{q} \). Then, we separate the dominant contribution into two parts \( \mathbf{q} = \mathbf{q}' \) and \( \mathbf{q} \neq \mathbf{q}' \) again.

\[
\langle 0 | \gamma_{k-k} | 0 \rangle = (0) \sum_{q'=k+q} a^\dagger_{k+q} a^{}_{q'=k-q} a^{}_{q'} | 0 \rangle + (0) \sum_{q'=k+q} a^\dagger_{k+q} a^{}_{q} a^\dagger_{-k-q} a^{}_{q'} | 0 \rangle
\]

\[
= (0) \sum_{q=q' \neq 0} a^\dagger_{q} a^{}_{q} a^\dagger_{q} a^{}_{q} | 0 \rangle + (0) \sum_{q\neq q' \neq 0} a^\dagger_{q} a^{}_{q} a^\dagger_{q} a^{}_{q} | 0 \rangle
\]

\[+(k \text{ dependent minor terms}).\]  

(22)

The term for \( \mathbf{q} \neq \mathbf{q}' \) vanishes using the argument of random phase approximation. Within this approximation we obtain the dominant part of \( \langle \gamma_k \gamma_{-k} \rangle \) as

\[
\langle 0 | \gamma_{k} | 0 \rangle = \sum_{q \neq 0} n_q^2 + \ldots
\]

\[
= \sum_{q \neq 0} \left\{ \frac{1}{2} \left( \frac{c_q^0 + n g}{E_q} - 1 \right) \right\}^2 + \ldots
\]

\[
= N \left( \pi - \frac{8}{3} \right) p + \ldots. \tag{23}
\]

The new variable \( p = \sqrt{n a^2}/\pi \) \((0 < p \ll 1)\) accounts for the diluteness of the system and will be used for the expansion.

When we back \( \langle \gamma_k \gamma_{-k} \rangle \) in Eq. (23) into Eq. (20) by iteration method, we obtain a new \( n_k \) as

\[
n_k = \frac{1}{2} \left( \frac{c_k^0 + n g}{E_k} - 1 \right) + \frac{n^2 g^2 c_k^0 c_k^0}{E_k^4} \left( \pi - \frac{8}{3} \right) p + \ldots. \tag{24}
\]

Putting the new \( n_k \) into Eq. (23), we obtain \( \langle \gamma_k \gamma_{-k} \rangle \) as

\[
\langle 0 | \gamma_{k} | 0 \rangle \approx \sum_{q \neq 0} \left\{ \frac{c_q^0 + n g}{E_q} - 1 \right\} + \frac{n^2 g^2 c_k^0 c_k^0}{E_k^4} \left( \pi - \frac{8}{3} \right) p^2 + \ldots
\]

\[
= N \left[ \left( \pi - \frac{8}{3} \right) p + 2 \left( \pi - \frac{8}{3} \right) \left( \frac{10}{3} - \pi \right) p^2 + 2 \pi \left( \pi - \frac{8}{3} \right)^2 p^3 \right]. \tag{25}
\]

We see the dominant part of \( \langle \gamma_k \gamma_{-k} \rangle \) is \( k \)-independent. Therefore, \( E_2 \) in Eq. (17) can be written as

\[
E_2 = \frac{n^2 g^2}{N} \langle 0 | \gamma_{k} | 0 \rangle \sum_{q \neq 0} \frac{1}{c_q^0 + 2 n g}. \tag{26}
\]

Finally substituting Eq. (25) into Eq. (20), we obtain the particle depletion from the zero momentum condensate as

\[
\frac{N - N_0}{N} = \frac{1}{N} \sum_{q \neq 0} n_q
\]

\[
= \frac{1}{2N} \sum_{q \neq 0} \left( \frac{c_q^0 + n g}{E_q} - 1 \right)
\]

\[
+ \frac{n^2 g^2}{N} \sum_{q \neq 0} \frac{c_q^0 c_q^0}{E_q^3} \left[ \left( \pi - \frac{8}{3} \right) p + 2 \left( \pi - \frac{8}{3} \right) \left( \frac{10}{3} - \pi \right) p^2 + \ldots \right]
\]

\[
= \frac{8}{3} \sqrt{\frac{n a^3}{\pi}} + 2 \left( \pi - \frac{8}{3} \right) n a^3 + \ldots. \tag{27}
\]

We obtained the next order correction term of the particle depletion beyond the textbook result as \( 2(\pi-8/3)n a^3 \frac{1}{12} \). If we repeat the above procedure, we can obtain the higher order terms too within the given approximation scheme. In the following section, we discuss the next order correction to the ground state energy density which originates from the fluctuation contribution of the condensate.
V. THE HIGHER ORDER CORRECTION TO THE GROUND STATE ENERGY DENSITY

This approximation of $\langle \gamma_k \gamma_{-k} \rangle$ also gives us a simple result for the condensation fluctuation correction $E_2$ in Eq. (20) to the ground state energy density, but the integral carries an ultraviolet divergence. The same divergence in $E_1$ was handled through the expression of the scattering length $a$ to order of $g^2$ as given in Eq. (13). However, for the calculation of $E_2$ such a simple cancellation scheme is not possible, because it is now necessary to expand $a$ up to $g^3$. Therefore, we resort to an alternative cutoff procedure called minimal subtraction renormalization scheme. The justification for this scheme to the current problem is given in detail in Ref. [5].

In this scheme the ultraviolet divergence in Eq. (20) can be regularized by imposing a cutoff procedure in the $k$ space. With the cutoff $|k| < \Lambda$ where $\Lambda$ is an arbitrary separation between short distance effects, the divergence can be handled by introducing a counter term in the Hamiltonian. That is, linear, quadratic, and other power ultraviolet divergences are removed as part of the regularization scheme by subtracting the appropriate power of $k$ from the momentum space integrated. In this case $1/k^2$ is subtracted from the integral. The justification for this procedure is that the terms that are subtracted are dominated by short distances and can be canceled by counter terms in the Hamiltonian. Also, we note that the result is independent of the potential used, since the fluctuation contribution from the condensate considered here is a generic feature for any potential.

Following this prescription, we obtain $E_2$ in a dimensionless form

$$E_2 = -\frac{2g}{N\sqrt{V}} \langle 0|\gamma_k \gamma_{-k} |0 \rangle \sum_{q \neq 0} \left( \frac{1}{c_q^0 + 2ng} - \frac{1}{c_q^0} \right),$$

(28)

where $E_c = n^2 gV/2 = 2\pi \hbar^2 an^2 V/m$. The summation part in Eq. (28) is obtained by integration independently as

$$\sum_{q \neq 0} \left( \frac{1}{c_q^0 + 2ng} - \frac{1}{c_q^0} \right) = -\frac{4m^2 ng}{\pi^2 \hbar^2} \int_0^\infty dq \frac{dq}{q^2 + \frac{4mng}{\hbar^2}}$$

$$= -\frac{2mV}{\hbar^2} p$$

(29)

Substituting Eqs. (18), (24) and (29) into Eq. (28), this approximation gives the result for the condensation fluctuation correction, $E_2$,

$$\frac{E_2}{E_c} = 16\pi \left( \pi - \frac{8}{3} \right) p^2 + 32\pi \left( \pi - \frac{8}{3} \right) \left( \frac{10}{3} - \pi \right) p^3 + O(p^4).$$

(30)

Thus, the present calculation gives $C_{20} = 16(\pi - 8/3)$, and $C_{30} = (32/\sqrt{\pi})(\pi - 8/3)(10/3 - \pi)$. The $C_{20}$ is exactly the same as one from our previous functional Schrödinger picture method. The higher order contribution to the ground state energy in Eq. (30) comes from the interactions of particles out of and into the condensate. This term represents the fluctuation contribution from the excited states and disappears if the number of condensate particles is conserved strictly.

VI. SUMMARY AND DISCUSSIONS

In this paper we revived the ground state energy density calculating of an interacting dilute Bose gas. Hugenholtz and Pines have given a general form of the series expansion in terms of $\sqrt{na^3}$. Till now only the first few coefficients are known. In view of the fundamental interest of homogeneous dilute interacting Bose gas, it is desirable to know about the coefficients of higher order expansion.

There are at least two possible sources to give contributions for the unknown coefficients of $na^3$ terms. One is the fluctuation from condensation and produces a universal result. The other is from the three-body interaction and not universal because it depends on the radial potential. Here we used the standard canonical transformation method of two-body interaction. We obtained the next order terms in the particle depletion and the ground state energy density coming from the condensate fluctuation. They are $2(\pi - 8/3)$ and $16(\pi - 8/3)$ respectively. Furthermore, the coefficient of $(na^3)^{3/2}$ term is $(32/\sqrt{\pi})(\pi - 8/3)(10/3 - \pi)$ in this approximation.

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