Thermodynamic potential of interacting Bose-Einstein gas confined in harmonic potential

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We investigate the interaction effect between atoms and the finite size effect of a Bose-Einstein gas at finite temperature. Using a mean field approach, we derive the thermodynamic potential on finite systems and obtain the condensate fraction, the chemical potential and the internal energy with the interaction and the finite size effects taken into account. In this approach, we can treat thermodynamic quantities as those of the ideal Bose gas. It is found that the interaction effect shifts the transition temperature by a few percent toward the lower temperature. Above the transition temperature, these quantities agree with the noninteracting Bose gas.

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I. INTRODUCTION

Bose-Einstein condensation (BEC) was first observed in dilute ultracold alkali atoms of rubidium [1], lithium [2] and sodium [3]. Furthermore, Mewes et al. and Ensher et al. measured the condensate fraction and the energy of rubidium atoms [4,5]. It revealed that the transition temperature \( T_0 \) is shifted not only by the interaction effect but also by the finite size effect by a few percent, where \( T_0 \) denotes the transition temperature of the noninteracting Bose gas within the external field in the thermodynamic limit. This means that both the interaction and the finite size effects play an important role in the real Bose gases. In fact, the number of trapped atoms is typically \( N = 10^3 \sim 10^6 \), and this may not be sufficiently large to take the thermodynamic limit. For the noninteracting Bose gas, the condensate fraction confined in a spherical potential can be analytically given as [4,5],

\[
\frac{N_0}{N} = 1 - \left( \frac{T}{T_0} \right)^3 - 3 \frac{\zeta(2)}{2 \zeta(3)^{2/3}} \frac{1}{N^{1/3}} \left( \frac{T}{T_0} \right)^2, \tag{1.1}
\]

where the first two terms in the right hand side correspond to the condensate fraction in the thermodynamic limit and the third term is the finite size correction.

On the other hand, these experimental findings have stimulated much interest in the theory of the interacting Bose gas. Since BEC occurs when atoms are dilute and cold, we can treat the interaction of atoms as the two-body interacting Bose gas. In this case, the s-wave scattering length characterizes the strength of the two-body interaction. Under these conditions, the Gross-Pitaevskii (GP) equation can well describe the behavior of the interacting Bose gas at zero temperature [6,7,11]. This is a mean field approach for the order parameter associated with the condensate. Using the GP equation, several authors [12] studied the ground state and the excitation properties of the condensate.

To study BEC at finite temperature, the Bogoliubov approximation at zero temperature was extended by Griffin [13]. It is called the Hartree-Fock-Bogoliubov (HFB) theory. In particular, Popov approximation to the HFB theory has been employed to explain the experimental results [2]. This approximation neglect the anomalous average of the fluctuating field operator in the HFB theory. With the Popov approximation, thermodynamic quantities, such as the condensate fraction and the internal energy, agree with the experimental results at low temperature. However, recent experimental data of the excitation frequencies of the condensates indicate a discrepancy with these approximate results near the transition temperature \( T_0 \) \( (T/T_0 > 0.6) \) [13].

In this paper, we derive the thermodynamic potential for the interacting Bose gas within a mean field approximation which is different from Bogholubov approximation. With this thermodynamic potential, we obtain the thermodynamic quantities; the condensate fraction, the entropy and the internal energy. These quantities have the same form as that of the ideal Bose gas, but the energy \( E_i \) contains the interaction effect and varies as a function of the temperature \( T \) and the total number \( N \). Therefore, we must determine not only the chemical potential \( \mu \) but also the energy \( E_i \) as a function of \( T \) and \( N \) in a self-consistent fashion. In particular, the chemical potential determines the transition temperature on the condition that the chemical potential \( \mu \) is equal to the ground state energy \( E_0 \) at \( T = T_0 \). Here, we choose the repulsive interaction where the scattering length \( a \) is positive, and numerically solve the chemical potential and the energy \( E_i \). By determining the chemical potential near \( T \sim T_0 \), we find that the interaction effect shifts \( T_0 \) by a few percent toward the lower temperature which should be compared with the previous estimations of the semiclassical approximation [14].

This paper is organized in the following way. In the next section, we derive the thermodynamic potential for the interacting Bose gas at finite temperature. Then, we obtain thermodynamic quantities in a self-consistent way. In section 3, we carry out the numerical evaluation of the chemical potential, the condensate fraction and the internal energy, in particular near \( T_0 \). Section 4 summarizes
what we have clarified in this paper.

II. THERMODYNAMICS FOR INTERACTING BOSE GAS

We derive the thermodynamic potential for the interacting Bose gas within a mean field approach. To begin with, we construct the effective Hamiltonian in this system. The Hamiltonian for the interacting Bose gas confined in an external potential $V_{\text{ext}}$ can be written as

$$H = \int dr \hat{\Psi}^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) \right] \hat{\Psi}(r) + \frac{1}{2} \int dr dr' \hat{\Psi}^\dagger(r) V(r-r') \hat{\Psi}(r') \hat{\Psi}(r),$$

(2.1)

where $\hat{\Psi}(r)$ is the boson field operator and $V(r-r')$ is the two-body atomic potential. Here, we choose the spherical harmonic potential for the $V_{\text{ext}}$ for simplicity. Thus, the $V_{\text{ext}}$ is given as

$$V_{\text{ext}}(r) = \frac{1}{2} m \omega^2 r^2.$$  

(2.2)

Since we are interested in the dilute and cold Bose gas, we replace $V(r-r')$ by an effective interaction of the $\delta$-function type,

$$V(r-r') = g \delta^{(3)}(r-r'),$$

(2.3)

where the coupling constant $g$ is related to the $s$-wave scattering length $a$ through

$$g = \frac{4 \pi \hbar^2 a}{m}.$$  

(2.4)

The scattering length is an important length scale in this system. A typical value of the scattering length $a$ is of the order of $nm$. The boson field operator for the ideal system can be written as

$$\hat{\Psi}(r) = \frac{1}{\sqrt{V}} \sum_k a_k e^{i k \cdot r}.$$  

(2.5)

But for the general case, the corresponding field operator is a sum over all normal modes \[13\]

$$\hat{\Psi}(r) = \sum_n a_n \chi_n(r),$$

(2.6)

when $\chi_n(r)$’s define any complete set of normalized single-particle wave function $a_n$ is a bosonic annihilation operator for the single-particle state $n$. In our case, $\chi_n(r)$ is given as

$$\chi_n(r) \equiv u_{n_x n_y n_z}(x, y, z) = N_{n_x} N_{n_y} N_{n_z} e^{-\frac{1}{2}(x/a_{ho})^2} H_{n_x}(x/a_{ho}) H_{n_y}(y/a_{ho}) H_{n_z}(z/a_{ho}),$$

(2.7)

where $H_n(\xi)$ is the Hermite polynomial, and $N_n$ is the normalization constant which can be written as

$$N_n = \sqrt{\frac{a_{ho}^{-1}}{\pi^{1/2} 2^n n!}},$$

(2.8)

where $a_{ho}$ denotes the harmonic oscillator length

$$a_{ho} = \sqrt{\frac{\hbar}{m \omega}}.$$  

(2.9)

This is also an important length scale in this system. It is typically of the order of $\mu m$. From Eqs. (2.1) and (2.4), the Hamiltonian can be written as

$$H = \sum_n \varepsilon_n a_n^\dagger a_n + \frac{2 \pi \hbar^2 a}{m} \sum_{(m)} \langle n_1 n_2 | n_3 n_4 \rangle a_n^\dagger a_{n_2} a_{n_3} a_{n_4},$$

(2.10)

with

$$\varepsilon_n = \hbar \omega \left( n_x + n_y + n_z + \frac{3}{2} \right);$$

(2.11)

$$\langle n_1 n_2 | n_3 n_4 \rangle = \int dr \chi_{n_1}^\dagger(r) \chi_{n_2}(r) \chi_{n_3}(r) \chi_{n_4}(r).$$

(2.12)

Now we consider the first order perturbation theory for the thermodynamic potential \[14\]. The first order correction is given by the diagonal part of the interacting Hamiltonian in Eq. (2.10). This corresponds to ignoring the anomalous average. Therefore, the effective Hamiltonian can be written as

$$\hat{H}_{\text{eff}} = \sum_i \varepsilon_i n_i + \hbar \omega \frac{4 \pi a}{a_{ho}} \sum_{i,j} U_{ij} n_i n_j,$$

(2.13)

where $n_i = a_i^\dagger a_i$ and

$$U_{ij} = F_{i,j,1} F_{j,1,i} F_{i,1,j},$$

$$F_{i,j} = \frac{1}{\pi^2 a^2 \omega} \int d\xi e^{-2 \xi^2} H_i^2(\xi) H_j^2(\xi).$$

(2.14)

Now we rewrite Eq. (2.13) in the following way

$$\hat{H}_{\text{eff}} = \hat{H}_0 + \hat{H'},$$

(2.15)

with

$$\hat{H}_0 = \sum_i E_i n_i - \hbar \omega \frac{4 \pi a}{a_{ho}} \sum_{i,j} U_{ij} \nu_i \nu_j,$$

(2.16)

$$\hat{H'} = \hbar \omega \frac{4 \pi a}{a_{ho}} \sum_{i,j} U_{ij} (n_i - \nu_i) (n_j - \nu_j),$$

(2.17)

$$E_i = \varepsilon_i + \hbar \omega \frac{8 \pi a}{a_{ho}} \sum_j U_{ij} \nu_j.$$  

(2.18)
Here, we minimize $\hat{H}'$ by taking $\nu_i$ the mean occupation numbers

$$\nu_i = \langle n_i \rangle = \frac{\text{Tr} \ n_i \ e^{-\left(\hat{H}_0 - \mu \hat{N}\right)/k_B T}}{\text{Tr} \ e^{-\left(\hat{H}_0 - \mu \hat{N}\right)/k_B T}} = \frac{1}{e^{(E_i - \mu)/k_B T} - 1}.$$ 

Then, the thermodynamic potential $\Omega = -pV$ can be given as

$$\Omega = -k_B T \ln \text{Tr} \ e^{-\left(\hat{H}_0 - \mu \hat{N}\right)/k_B T},$$
$$\approx -\hbar \omega \sum_{ij} U_{ij} \langle n_i \rangle \langle n_j \rangle + k_B T \sum_i \ln \left(1 - e^{-(E_i - \mu)/k_B T}\right),$$

where the first term in the right hand side is the first order correction. We note that Eq. (2.19) can be also determined by the condition

$$0 = \left( \frac{\partial \Omega}{\partial (\langle n_i \rangle)} \right)_{T,\mu,V,(n_i)\neq\langle n_i \rangle}$$
$$= - \sum_j U_{ij} \langle n_j \rangle + \sum_j \frac{1}{e^{(E_j - \mu)/k_B T} - 1}.$$ 

This condition means that the thermodynamic potential $\Omega$ is a minimum with respect to any change of state at constant $T$, $V$ and $\mu$ in a state of thermal equilibrium.

Now we derive the thermodynamic quantities from Eqs. (2.20) and (2.21). First, we obtain the total number $N$ from Eq. (2.20) with the condition of Eq. (2.21)

$$N = - \left( \frac{\partial \Omega}{\partial \mu} \right)_{T,V}$$
$$= - \left( \frac{\partial \Omega}{\partial \mu} \right)_{T,V,(n_i)} - \sum_i \left( \frac{\partial \Omega}{\partial \langle n_i \rangle} \right) \left( \frac{\partial \langle n_i \rangle}{\partial \mu} \right)$$
$$= \sum_i \frac{1}{e^{(E_i - \mu)/k_B T} - 1}.$$ 

We can determine the chemical potential $\mu$ and the energy $E_i$ from Eqs. (2.18) and (2.22) which should be solved self-consistently. Then, we obtain the thermodynamic quantities through Eq. (2.20) with Eq. (2.21). For example, the entropy $S$ can be given by

$$S = - \left( \frac{\partial \Omega}{\partial T} \right)_{V,\mu}$$
$$= - \left( \frac{\partial \Omega}{\partial T} \right)_{V,\mu,(n_i)} - \sum_i \left( \frac{\partial \Omega}{\partial \langle n_i \rangle} \right) \left( \frac{\partial \langle n_i \rangle}{\partial T} \right)$$
$$= k_B \sum_i \left[ (1 + \langle n_i \rangle) \ln(1 + \langle n_i \rangle) - \langle n_i \rangle \ln \langle n_i \rangle \right],$$

where we also use the condition Eq. (2.21). Finally, the internal energy $E$ can be given as

$$E = \sum_i \frac{E_i}{e^{(E_i - \mu)/k_B T} - 1}. $$

We obtain the thermodynamic quantities from Eq. (2.20) by solving $E_i$ and $\mu$ from Eqs. (2.18) and (2.20) self-consistently. This is a mean field approach within the first order perturbation theory. The chemical potential cannot exceed the energy $E_i$ at any temperature. At the transition temperature, the chemical potential is equal to the ground state energy. Therefore, the transition temperature has to be determined by the chemical potential. We note that the second term of Eq. (2.18) shifts the transition temperature. If we choose $U_{ij}$ as a constant i.e. $U_i$, then it only causes the constant shift for all $E_i$, but the transition temperature does not change. Therefore, the second term of Eq. (2.18) plays an important role to understand the interacting Bose gas. We also note that, when we put $g = 0$, Eq. (2.22) reproduces the total number of the noninteracting Bose gas confined in the spherical harmonic potential, because there are no constraints in between the chemical potential $\mu$ and the energy $E_i$. Therefore, when we consider the interaction effect, we can also investigate the finite size effect at the same time.

### III. NUMERICAL RESULTS

We present the numerical results of thermodynamic quantities which appear in Eqs. (2.22) and (2.24). First, we numerically solve the chemical potential $\mu$ and the energy $E_i$ by using Eqs. (2.18) and (2.22) with the iteration method. Then, we obtain $\mu$ and $E_i$ as a function of $T$ and $N$. If the temperature of this system is lowered at fixed $N$, the chemical potential $\mu$ given by Eq. (2.22) increases. It finally reaches the ground state energy $E_0$, since the chemical potential cannot exceed the ground state energy. Therefore, we can define the transition temperature $T_c$ as $\mu = E_0$ at $T = T_c$. We note that the transition temperature $T_c$ for the noninteracting Bose gas confined in the spherical harmonic potential can be given as

$$T_c = T_0 \left( 1 - \frac{\zeta(2)}{2 \zeta(3)^{2/3}} \frac{1}{N^{1/3}} \right),$$

where the second term is the finite size effect, and $T_0$ denote the transition temperature in the thermodynamic limit which can be written as

$$T_0 = \frac{\hbar \omega}{k_B} \left( \frac{N}{\zeta(3)} \right)^{1/3}.$$

Because the interaction effect also shifts the transition temperature $T_c$, we have to redefine the transition temperature.
For $T > T_0$, we solve Eqs. (2.18) and (2.22) with fixed $N$ and given $T$. Here, the total number $N$ and the strength of the interaction with the repulsive force are chosen to be $N = 1000$ and $a / a_{ho} = 7 \times 10^{-3}$, respectively. In Fig. 3, we show the calculated values of the chemical potential $\mu / k_B T_0$ as a function of $T / T_0$. As can be seen, when $T / T_0 \sim 0.91$, $\mu / k_B T_0$ approaches to a finite value. This means that the chemical potential $\mu$ reaches the ground state energy $E_0$. Therefore, the transition temperature becomes $T / T_0 \sim 0.91$ (see, Fig. 3). Comparing this result with the transition temperature $T_c / T_0 \sim 0.93$ given by Eq. (5.1), the interaction effect further shifts the transition temperature about 2 percent toward the lower temperature.

For $T < T_0$, the chemical potential $\mu$ is equal to the ground state energy $E_0$. In this case, since the ground state occupation numbers $N_0$ diverges, we have to rewrite Eq. (2.18) as follows

$$E_i = \varepsilon_i + \hbar \omega \frac{8 \pi a}{a_{ho}} U_{i,0} N + \hbar \omega \frac{8 \pi a}{a_{ho}} \sum_{j \neq 0} \langle n_j \rangle (U_{i,j} - U_{i,0}),$$  

(3.3)

where we use the relation $N = N_0 + \sum_{j \neq 0} \langle n_j \rangle$. Under this condition, we solve Eq. (3.3) with $\mu / k_B T_0 = 0.178$. We note that $\mu / k_B T_0$ is 0.159 for the noninteracting model at the transition temperature, since $\mu$ is $3/2 \hbar \omega$ in our approach.

In Fig. 4, we show the condensation fraction as a function of $T / T_0$. The dotted line refers to the condensation fraction of the noninteracting Bose gas in the thermodynamic limit, and the solid line represents the condensation fraction including the finite size effect (see, Eq. (1.1)). Finally, the condensation fraction with the interaction and the finite size effects is shown as solid circles. These correspond to each other at $T > T_0$. This means that we can ignore the atom-atom interaction because the number density is low at $T > T_0$. On the other hand, at near the transition temperature, atoms must occupy the ground state energy $E_0$. Since the number density becomes high at this temperature, the atom-atom interaction becomes strong, and shifts the transition temperature. Although the finite size effect can also shift the transition temperature, it disappears at large $N$ limit. Therefore, the interaction effect is more important than the finite size effect.

In Fig. 4, we show the results for the internal energy $E / N k_B T_0$ as a function of $T / T_0$. It reveals that the internal energy curve changes slope near the transition temperature. We note that the specific heat can be calculated by differentiating the internal energy with respect to the temperature $T$. Therefore, this result means that the specific heat is discontinuous at the transition temperature. As can be seen from the result of Ensher et al. [5], the derivative of the internal energy is discontinuous at the transition temperature. This behavior of our calculated internal energy is in a good agreement with the experimental result.

Finally, we compare our results with the semiclassical results. In the semiclassical approximation, the dimensionless parameter $E_{int} / E_{kin} = N a / a_{ho}$ is important to discuss the two-body atomic interaction energy $E_{int}$ compared to the kinetic energy $E_{kin}$. For the Thomas-Fermi (TF) limit ($N a / a_{ho} \gg 1$), the chemical potential $\mu_0$ can be written in terms of this parameter [17] as

$$\mu_0 = \frac{\hbar \omega}{2} \left( 15 N a / a_{ho} \right)^{2/5}.$$  

(3.4)

In our case, $\mu_0 / k_B T_0 = 0.342$. This is about twice as large as the $\mu / k_B T_0 = 0.178$. Since we take the parameter $N a / a_{ho} \sim 1$, it does not achieve the TF limit. Therefore, the kinetic term plays an important role in this value. Further, the interaction term $U_{ij}$ in Eq. (2.18) suppresses the total number $N$ of $N a / a_{ho}$. The shift of the transition temperature $\delta T_0 / T_0$ in the semiclassical approximation for the large $N$ limit can be given as [14]

$$\frac{\delta T_0}{T_0} = -1.3 \frac{a}{a_{ho}} N^{1/6}.$$  

(3.5)

In our case, the shift of the transition temperature $\delta T_0 / T_0$ is about 3 percent. Because of the interaction term $U_{ij}$, the transition temperature is also suppressed by its term in our model.

### IV. CONCLUSIONS

We have presented the thermodynamic potential of the interacting Bose gas confined in the spherical harmonic potential within a mean field approach. In this approach, we minimize the interacting Hamiltonian $H'$ under the condition that the mean occupation numbers $\nu_i$ should be the Bose distribution function. Then, we can derive the thermodynamic potential in a self-consistent fashion. With this thermodynamic potential, we obtain the thermodynamic quantities which have the same form as that of the ideal Bose gas. Further, we carry out the numerical calculations of the chemical potential, the condensate fraction and the internal energy. In particular, because the energy $E_i$ also varies as a function of $T$ and $N$ in our approach, we have to solve $E_i$ and $\mu$ with the conditions that $\mu$ cannot exceed $E_i$ at any temperature. Further, since we take the parameter $N a / a_{ho} \sim 1$ which corresponds neither to the TF limit nor to the noninteracting limit for the semiclassical point of view, we cannot expect $\mu$ from the semiclassical approximation. Then, we find that the interaction effect shifts the transition temperature $T_0$ given by $\mu = E_0$ at $T = T_c$ about 2 percent toward the lower temperature compared with the noninteracting model including the finite size effect.
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FIGURE CAPTIONS

FIG. 1. Chemical potential $\mu/k_B T_0$ as a function of $T/T_0$. The solid line refers to the noninteracting model. Solid circles show the calculated values of the interacting case.

FIG. 2. Condensate fraction $N/N_0$ as a function of $T/T_0$. The solid line is drawn with Eq. (1.1) and the dotted line is the thermodynamic limit. Solid circles are the same as in Fig. 1.

FIG. 3. The same as Fig. 2 just below the transition temperature. Open circles are numerical results of the noninteracting case.

FIG. 4. Internal energy $E/Nk_B T_0$ as a function of $T/T_0$. The solid line is the noninteracting case. Solid circles are the same as in Fig. 3.
FIG. 1
FIG. 2
FIG. 4