Critical temperature and condensate fraction of the trapped interacting Bose gas with finite-size effects

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Abstract

The critical temperature and condensate fraction of a trapped interacting Bose gas are investigated when both atom-atom interaction and finite-size effects are taken into account. Canonical ensemble is used to obtain the equations on the condensate fraction for the trapped interacting Bose gas near and below the critical temperature. In our approaches corrections due to atom-atom interaction and finite-size effects are obtained simultaneously for the critical temperature and condensate fraction of the system. Analytical high-order correction to the condensate fraction is given in this work. 

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I. INTRODUCTION

The experimental realization of Bose-Einstein condensation (BEC) in the dilute alkali-metal atoms [1] and more recently in the atomic hydrogen [2] has stimulated a new interest in the theoretical study of the inhomogeneous Bose gas. Thermodynamic properties such as critical temperature, condensate fraction have been investigated by several authors for the trapped Bose gas recently [3].

In the presence of an anisotropic harmonic potential of the form
\[ V_{\text{ext}}(\mathbf{r}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \]
the noninteracting model gives the critical temperature
\[ T_0^c = \frac{k_B \hbar \omega_{ho}}{N \zeta(3)} \]
where \( \omega_{ho} = (\omega_x \omega_y \omega_z)^{1/3} \) is the geometrical average of the oscillator frequencies. \( \zeta(n) \) is Riemann \( \zeta \) function. In the large-\( N \) limit, the condensate fraction is
\[ \xi = \frac{N_0}{N} = 1 - \frac{\zeta(3)}{N} \left( \frac{k_B T}{\hbar \omega_{ho}} \right)^3 \]
Finite-size effects [4] and interatomic interaction will give corrections to the thermodynamic properties of the system. The correction to the critical temperature due to finite-size effects has shown to be
\[ \delta T_0^c / T_0^c \simeq -0.73 \frac{\bar{\omega}}{\omega_{ho}} N^{-1/3} \]
where \( \bar{\omega} = (\omega_x + \omega_y + \omega_z)/3 \) is the mean frequency.

Although the atom clouds realized in the present experiments are very dilute, the effects due to interatomic interaction are important at low temperature. Researches show that atom-atom interaction will give leading corrections when \( N \) is larger than \( 10^5 \) for the alkalis. In fact the question of how two-body forces affect the thermodynamic properties of these systems have been the object of several theoretical investigations [3]. Using a local density approximation Giorgini, Pitaevskii, and Stringari [3] obtained the shift of the critical temperature due to interatomic interaction:
\[ \delta T_0^c / T_0^c \simeq -1.33 a N^{1/6} / a_{ho} \]
where \( a_{ho} = \sqrt{\hbar/m \omega_{ho}} \) is the harmonic oscillator length. Recently Monte Carlo simulation [7] is also used to investigate the thermodynamic properties of the trapped interacting Bose gases.

In this work, we investigate the critical temperature and the condensate fraction of the system when both atom-atom interaction and finite-size effects are taken into account. Canonical ensemble is used to obtain the analytical high-order correction due to interatomic interaction. Especially, finite-size effects are obtained simultaneously. To obtain the shift of
the critical temperature, we give the analytic description of the condensation fraction near the critical temperature.

The paper is planned as follows. In Sec.II we outline the canonical ensemble. In Sec.III we give the condensate fraction of the system near the critical temperature. The shift of the critical temperature agrees with the usual results [3,4,6]. In Sec.IV we obtain the analytical high-order correction to the condensate fraction due to atom-atom interaction. The lowest-order correction agrees with the well-established results [3,6,8]. In Sec.V the correction to the condensate fraction beyond mean field theory is given.

II. PARTITION FUNCTION OF THE TRAPPED INTERACTING BOSE GASES

Canonical ensemble and saddle-point method have been used to investigate the thermodynamic properties of the interacting uniform Bose gases [9]. In this work canonical ensemble is used to discuss the trapped interacting Bose gases. The partition function of $N$ trapped interacting bosons is given by

$$\begin{align*}
Q(N) = \Sigma_n \exp (-\beta E_n) = \Sigma_{\{n_x,n_y,n_z\}} \exp \left[ -\beta \left( \Sigma_{n_x,n_y,n_z} N_{n_x,n_y,n_z} \varepsilon_{n_x,n_y,n_z} + E_{int} \right) \right],
\end{align*}$$

(1)

where $N_{n_x,n_y,n_z}$ and $\varepsilon_{n_x,n_y,n_z}$ are the occupation numbers and energy level of the state $\{n_x,n_y,n_z\}$ respectively. $E_{int}$ is the interaction energy of the system.

From (1)

$$\begin{align*}
Q(N) &= \Sigma_{N_0=0}^N \left\{ \exp \left[ -\beta \left( E_0 + E_{int} \right) \right] \right\} Q_0 (N - N_0) ,
\end{align*}$$

(2)

where $Q_0 (N - N_0) = \Sigma_{\{n_x,n_y,n_z\}} \exp \left[ -\beta \left( \Sigma_{n_x,n_y,n_z} N_{n_x,n_y,n_z} \varepsilon_{n_x,n_y,n_z} \right) \right]$ stands for the partition function of a fictitious system of $N - N_0$ trapped noninteracting atoms. $E_0$ is the energy of the condensate. For convenience, we have separated out the ground state $n_x = n_y = n_z = 0$ from the states $\{n_x,n_y,n_z\} \neq 0$, so that we first carry out the primed summation over all $\{n_x,n_y,n_z\} (\{n_x,n_y,n_z\} \neq 0)$ with a fixed value $(N - N_0)$ of the partial sum $\Sigma_{\{n_x,n_y,n_z\}}$ and then carry out a summation over all possible values of $N_0$, i.e. $N_0 = 0$ to $N_0 = N$. Assume
\( A_0 (N - N_0) \) is the free energy of the fictitious system. \( A_0 (N - N_0) = -\frac{1}{\beta} \ln Q_0 (N - N_0) \). From (2)

\[
Q(N) = \sum_{N_0=0}^{N} \exp \left[ -\beta (E_0 + E_{int}) - \beta A_0 (N - N_0) \right].
\] (3)

The sum \( \sum_{N_0=0}^{N} \) in (3) maybe replaced by the largest term in the sum, for the error omitted in doing so will be statistically negligible. With this approximation we do not investigate the fluctuations of the system. However, this approximation is reasonable because we can give the occupation number of the energy level \( \varepsilon_{x,y,z} \), which agrees with the widely used mean occupation number in the frame of grand-canonical ensemble. Neglecting all terms but the largest in (3), the number of bosons in the condensate can be obtained as:

\[
-\beta \frac{\partial}{\partial N_0} (E_0 + E_{int}) - \beta \frac{\partial}{\partial N_0} A_0 (N - N_0) = 0.
\] (4)

The calculations of the free energy \( A_0 (N - N_0) \) of the fictitious noninteracting Bose gas is nontrivial because there is a requirement that the number of the particles is \( N - N_0 \) in the summation of the partition function. Using the saddle-point method of integration developed by Darwin and Fowler [10] it is straightforward to find that

\[
-\beta \frac{\partial}{\partial N_0} A_0 (N - N_0) = \ln z_0 \text{ in which } z_0 \text{ is the fugacity of the fictitious Bose gas.}
\]

In addition, the fugacity \( z_0 \) is determined by

\[
N - N_0 = \sum_{n_x,n_y,n_z}^\prime \frac{1}{\exp \left[ \beta \varepsilon_{n_x,n_y,n_z} \right] z_0^{-1} - 1}.
\] (5)

We can easily understand (5) in terms of Bose-Einstein distribution of the trapped noninteracting Bose gas. Using the relation \(-\beta \frac{\partial}{\partial N_0} A_0 (N - N_0) = \ln z_0\), (4) becomes

\[
-\beta \frac{\partial}{\partial N_0} (E_0 + E_{int}) + \ln z_0 = 0.
\] (6)

Equations (5) and (6) will be used to discuss the corrections due to atom-atom interaction and finite-size effects. Once we know the interaction energy of the system, it is easy to obtain the correction due to atom-atom interaction. In addition, finite-size effects are separated off in (5). Omitting interactions between atoms, we can obtain \( \ln z = \beta \varepsilon_{000} \) from (6). From (5) the number of the thermal atoms \( N_T \) is given by
\[ N_T = N - N_0 = \sum_{n_x,n_y,n_z}^{\prime} \frac{1}{\exp \left[ \beta (\varepsilon_{n_x,n_y,n_z} - \varepsilon_{000}) \right] - 1}. \] (7)

This is the exact conclusion in the frame of grand-canonical ensemble for the trapped noninteracting Bose gas. This shows the equivalence between the grand-canonical ensemble and canonical ensemble in the calculations of the condensate fraction. In addition, it shows that neglecting all terms but the largest in (3) is reasonable. In the absence of interaction, from (7), the condensate fraction is given by

\[ \xi = 1 - \left( \frac{T}{T_c} \right)^3 - \frac{3\omega_\zeta (2)}{2\omega_\zeta (3)^{2/3}} \left( \frac{T}{T_0} \right)^2 N^{-1/3}. \] (8)

The third term in (8) is the finite-size correction to the ideal Bose gas in the thermodynamic limit. In short, (3) and (8) account for both interatomic interaction and finite-size effects. We will use (3) and (8) to calculate the critical temperature and condensate fraction of the system.

III. CRITICAL TEMPERATURE AND CONDENSATE FRACTION NEAR \( T_C \)

A. Interaction energy of the system near the critical temperature

The parameter expressing the importance of the interatomic interaction compared to the kinetic energy is \( \frac{E_{\text{int}}}{E_{\text{kin}}} \propto \frac{N_0|a|}{\bar{a} \hbar} \), where \( a \) is the scattering length between bosons. Near the critical temperature \( \frac{N_0|a|}{\bar{a} \hbar} \ll 1 \). This means that \( E_{\text{kin}} >> E_{\text{int}} \). In this case we can use the method of pseudopotentials developed by Huang and Yang \([11]\) to calculate the interaction energy of the system.

In the method of pseudopotentials, the actual Hamiltonian of the system is replaced by an effective Hamiltonian, such that the ground state and the low-lying energy levels of the system are given equally well by the new Hamiltonian. With hard-sphere approximation, the boundary conditions between atoms are replaced by the pseudopotential operator \( g \delta^{(3)}(\vec{r}) \frac{\partial}{\partial r} r \) in the effective Hamiltonian, where \( g = \frac{4\pi a \hbar^2}{m} \). The effective Hamiltonian of the system may be taken to be
\[ \hat{H} = -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \cdots + \nabla_N^2 \right) + \Sigma_{i=1}^N V_{\text{ext}}(\vec{r}_i) + \Sigma_{i<j} \omega_{ij}, \]

where \( \omega_{ij} = g \Sigma_{i<j} \delta^{(3)}(\vec{r}_i - \vec{r}_j) \frac{\partial}{\partial r_{ij}} r_{ij}. \) For a trapped dilute Bose gas near the critical temperature the pseudopotentials can be regarded as perturbation terms. The energy levels to the first order in \( a \) may be obtained through the usual perturbation theory.

In the general case of a system containing an arbitrary number \( N \) of bosons, the unperturbed normalized wave function of the system is given by

\[ \Psi_N = \left( \frac{N_{\alpha_1}! N_{\alpha_2}! \cdots}{N!} \right)^{1/2} \Sigma_P [\phi_{\alpha_1} \phi_{\alpha_2} \cdots \phi_{\alpha_N}], \]

where the sum is taken over all permutations of the different suffixes \( \alpha_1, \alpha_2, \cdots, \alpha_N \) and the numbers \( N_{\alpha_i} \) show how many of these suffixes have the same value \( \alpha_i \) (with \( \Sigma N_{\alpha_i} = N \)). From the first-order perturbation theory the interaction energy \( E_{\text{int}} \) of the system is given by

\[ E_{\text{int}} = \langle \Psi_N | \Sigma_{i<j} \omega_{ij} | \Psi_N \rangle. \]

Thus, the operators \( (\partial/\partial r_{ij}) r_{ij} \) will be operating on a set of functions which are well behaved for all values of \( r_{ij} \); accordingly, these operators may be replaced by the unit operators. Basing on the investigation of the various permutations [1] of the single particle states the interaction energy takes the form,

\[ E_{\text{int}} = g \frac{(N_0^2 - N_0)}{2} \int \phi_0^4(\vec{r}) d^3\vec{r} + 2g N_0 \int \phi_0^2(\vec{r}) n_T(\vec{r}) d^3\vec{r} + g \int n_T^2(\vec{r}) d^3\vec{r}. \]

To obtain (12) we used the fact that \( n_T(\vec{r}) = \Sigma_{l \neq 0} N_l \phi_l^2(\vec{r}) \) is the density distribution of the thermal atoms. Near the critical temperature, the density distribution of the condensate is \( n_0(\vec{r}) = N_0 \phi_0^2(\vec{r}) = N_0 \left( \frac{m \omega_0}{\pi \hbar} \right)^{3/2} \exp\left[ -\frac{m}{\hbar} (\omega_x x^2 + \omega_y y^2 + \omega_z z^2) \right]. \) The density distribution of the thermal atoms can be obtained using Bose-Einstein distribution and the semiclassical approximation of the energy level of a single particle. Near the critical temperature \( \frac{k_B T}{\hbar \omega_{ho}} \propto N^{1/3} \). In the available traps \( N \) ranges from a few thousand to several millions, thus \( \hbar \omega_{ho} \ll k_B T_c, \) i.e. the energy level of the thermal atoms can be approximated as continuous. In addition, this means that the semiclassical approximation for the normal gas
is expected to work well on a wide range of temperatures \[3\]. In terms of Bose-Einstein distribution

\[ n_T(\vec{r}) = \int d^3\vec{p} (2\pi\hbar)^{-3} |\exp (\beta\varepsilon(\vec{p}, \vec{r})) - 1|^{-1} \]

where \( \varepsilon(\vec{p}, \vec{r}) = \frac{p^2}{2m} + V_{\text{ext}}(\vec{r}) \) is the semiclassical energy in phase space and \( \beta = 1/k_B T \). Density distribution of the thermal atoms in the coordinate space would be

\[ n_T(\vec{r}) = \lambda_T^{-3} \frac{g_{3/2}}{2} (\exp[-V_{\text{ext}}(\vec{r})/(k_B T)]) \]

where \( \lambda_T = \left[2\pi\hbar^2/(mk_BT)^{1/2} \right] \) is the thermal wavelength. \( g_{3/2}(z) \) belongs to the class of functions \( g_{\alpha}(z) = \sum_{n=1}^{\infty} z^n/n^\alpha \). By integrating the semiclassical approximation \( n_T(\vec{r}) \) over space one obtain the condensate fraction \( \xi = 1 - \left(\frac{r}{\lambda_T}\right)^3 \), which does not account for finite-size effects. However, in this paper the semiclassical approximation \( n_T(\vec{r}) \) is used to calculate the interaction energy of the system, i.e. used to calculate the high-order correction due to interatomic interaction. Thus the adoption of the semiclassical approximation will omit only higher-order modification, which is of the order of the multiplication of the corrections due to the interatomic interaction and finite-size effects. Because the finite-size effects have been separated off in (3), we can give finite-size effects although semiclassical approximation is used to calculate the correction due to interatomic interaction.

Using the geometrical average of the oscillator frequencies \( \omega_{ho} \), \( n_T(r) = \lambda_T^{-3} g_{3/2} (\exp[-m\omega_{ho}^2 r^2/2k_B T]) \). Introducing the width of the normal gas \( R_T = \sqrt{2k_B T/m\omega_{ho}^2} \) and defining the rescaled variable through \( r = R_T \tau \), we can obtain \( n_T(\tau) = \lambda_T^{-3} g_{3/2} (\exp[-\tau^2]) \). Near the critical temperature \( k_B T >> \hbar \omega_{ho} \), the classical Boltzmann distribution \( n_{cl}(\tau) \propto \lambda_T^{-3} \exp[-\tau^2] \) gives a zero-order approximation for the density distribution of the thermal cloud. Thus we take the trial function of the form

\[ n_T^G(\tau) = \eta_1 \lambda_T^{-3} \exp[-\eta_2 \tau^2] \]  \hspace{1cm} (13)

where \( \eta_1 \) and \( \eta_2 \) are two dimensionless variational parameters. Another reason for the adoption of the Gaussian trial function lies in the fact that there is a factor \( \exp[-\tau^2] \) in \( n_T(\tau) \). \( \eta_1 \) and \( \eta_2 \) are determined by the requirement that \( \int |n_T^G(\tau) - n_T(\tau)| d^3\tau \) obtain the minimum. Results of numerical calculations show that \( \eta_1 = 2.587, \eta_2 = 1.146 \) and \( \int |n_T^G(\tau) - n_T(\tau)| d^3\tau / \int n_T(\tau) d^3\tau = 0.0017 \). So the Gaussian distribution \( n_T^G(\tau) \) agrees very well with \( n_T(\tau) \). We should note that the Gaussian distribution \( n_T^G(\tau) \) is different from the
classical Boltzmann distribution because of the variational parameters $\eta_1$ and $\eta_2$.

Combining (12) and (13) we have

$$E_{\text{int}} = \frac{g}{2} \left( \sqrt{2\pi a_{ho}} \right)^3 \eta_1^2 + \left( 2 - \frac{1}{2^{3/2}} \right) \eta_1 g \lambda_T^{-3} N_0 + \frac{\eta_1 g \lambda_T^{-3}}{2^{3/2}} \eta_2 N,$$

where we have used the fact that $a_{ho} >> \lambda_T$ and $k_B T >> \hbar \bar{\omega}$ near the critical temperature.

**B. shift of the critical temperature and condensate fraction near $T_c$**

We introduce a scaling parameter which accounts for the role of the two-body repulsive interaction. This parameter $\theta$ is fixed by the ratio between $gn_T (\vec{r} = 0, T^0_c)$ and the critical temperature $k_B T^0_c$. $\theta = \frac{gn_T (\vec{r} = 0, T^0_c)}{k_B T^0_c} = \frac{\eta_1 \sqrt{2/\pi} a_{ho}}{\zeta(3)^{1/3}} \frac{N_{1/6}}{a_{ho}}$. The scaling parameter $\theta$ can also be written in the form $\theta = 0.65 \eta_1^{5/2}$, where $\eta = \mu (T = 0) / k_B T^0_c = \left( \frac{\zeta(3)^{1/3} 15^{2/3}}{2} \right)^{1/5} \left( N_{1/6} \frac{a}{a_{ho}} \right)^{2/5}$ is also an important scaling parameter accounting for the role of interatomic interaction [3,12]. Obviously $\theta$ stands for high-order correction due to interatomic interaction, compared to the parameter $\eta$. From (3), (4), and (14) we can obtain the equation on the condensate fraction.

$$1 - \xi = \frac{t^3}{\zeta(3)} g_3 (z_0) + \frac{3 \zeta(2)}{2 \zeta(3) 2^{3/2}} \frac{\bar{\omega}}{\omega_{ho}} t^2 N^{-1/3},$$

$$- \frac{\zeta(3)^{1/2} \theta N^{1/2}}{\eta t} \xi - \left( 2 - \frac{1}{2^{3/2}} \right) \theta t^{1/2} + \ln z_0 = 0,$$

where we have used the reduced temperature $t = T/T^0_c$. From (13) and (14) the condensate fraction is given by

$$\xi = \frac{1 - t^3 - 4.51 \frac{a}{a_{ho}} N^{1/6} t^{7/2} - \frac{3 \zeta(2)}{2 \zeta(3) 2^{3/2}} \frac{\bar{\omega}}{\omega_{ho}} t^2 N^{-1/3}}{1 + 1.16 \frac{a}{a_{ho}} N^{2/3} t^2}. $$

The third term in the numerator of (17) represents the correction due to the interaction between atoms, while the last term in the numerator accounts for the correction due to the finite-size effects. By setting $\xi = 0$ in (17) one can obtain the shift of the critical temperature,

$$\frac{\delta T^0}{T^0_c} = \frac{\delta T_{\text{int}}}{T^0_c} + \frac{\delta T_{\text{finite}}}{T^0_c} = -1.50 \frac{a}{a_{ho}} N^{1/6} - \frac{\zeta(2)}{2 \zeta(3) 2^{3/2} \omega_{ho}} \bar{\omega} N^{-1/3}.$$

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The first term in (18) is the shift due to interatomic interaction. It agrees with the results based on the local density approximation [3,6]. Because of the denominator in (17), close to $T_0$ the condensate fraction will increase slowly with decreasing the temperature. Especially, it shows that there is only high-order correction of the scaling parameter $\eta$ due to interatomic interaction. We should note that (17) holds only when $\frac{N_0a}{\hbar\omega} << 1$. The second contribution in (18) gives exactly the usual results due to the finite-size effects.

IV. CONDENSATE FRACTION OF THE SYSTEM BELOW $T_C$

A. lowest-order correction due to interatomic interaction and finite-size effects

Below the critical temperature $\frac{N_0a}{\hbar\omega} >> 1$, i.e. $E_{int} >> E_{kin}$. In this case we can use the well-known Thomas-Fermi approximation. With the Thomas-Fermi approximation the density profile of the condensate is $n_0(\vec{r}) = \frac{\mu - V_{ext}(\vec{r})}{g} \theta (\mu - V_{ext}(\vec{r}))$. The normalization condition on $n_0(\vec{r})$ provides the relation between chemical potential and number of particles in the condensate: $\mu = \frac{1}{2} \left( \frac{15 N_0 a}{\hbar \omega} \right)^{2/5}$. From Gross-Pitaevskii (GP) equation [13] and the well-known Virial theorem the energy of the condensate turns out to be $E_0 = (5/7) \mu N_0 [3]$. Omitting atom-atom interactions in the normal gas and the interaction between the condensate and normal gas, from (5) and (6)

$$N_0 = N - N_T = N - \sum_{n_x,n_y,n_z}^\prime \frac{1}{\exp [\beta (\varepsilon_{n_x n_y n_z} - \mu)] - 1}, \quad (19)$$

From (13) it is easy to obtain the following result

$$\xi = 1 - t^3 - \frac{\zeta(2)}{\zeta(3)} \frac{\mu}{k_B T} - \frac{3\omega \zeta(2)}{2\omega \zeta(3)^{2/3}} t^2 N^{-1/3}, \quad (20)$$

where the last term in (20) is the correction due to finite-size effects [4]. Using the relation $\mu/k_B T = \eta \xi^{2/5}/t$, the third term in (20) gives exactly the usual lowest-order modification due to atom-atom interactions [3,6,8].

$$\xi = 1 - t^3 - \frac{\zeta(2)}{\zeta(3)} \eta \xi^{2/5} t^2 - \frac{3\omega \zeta(2)}{2\omega \zeta(3)^{2/3}} t^2 N^{-1/3}. \quad (21)$$
This proves the equivalence between canonical ensemble and grand-canonical ensemble, even in the presence of interatomic interactions. We will give high-order modification in the following.

### B. high-order modification due to interatomic interactions

Equation (21) is obtained by omitting the interaction between thermal atoms and interaction between thermal atoms and the condensate. When these two sorts of interactions are considered

\[
E_0 + E_{\text{int}} = \frac{5}{7} \mu N_0 + 2 g \int n_0(\vec{r}) n_T(\vec{r}) d^3\vec{r} + g \int n_T^2(\vec{r}) d^3\vec{r}. \tag{22}
\]

The calculations of (22) are straightforward. The results is given by

\[
E_0 + E_{\text{int}} = \frac{5}{7} \mu N_0 + \frac{16 \pi \eta_1 \mu R^3_\mu}{15 \lambda_T^3} - \frac{16 \pi \eta_1 \eta_2}{35 \lambda_T^3} \mu^2 + \frac{\eta_1 g \lambda_T^{-3}}{2^{3/2}} (N - N_0), \tag{23}
\]

where \( R_\mu = \sqrt{2 \mu / m \omega_{\text{ho}}^2} \) is the radius of the condensate. \( R^3_\mu / \lambda_T^3 = \alpha_{R\lambda} N^{1/2} t^{3/2} N_0^{3/5} \), where \( \alpha_{R\lambda} = 0.294 (a/a_{\text{ho}})^{3/5} \). From (23)

\[
- \beta \frac{\partial}{\partial N_0} (E_0 + E_{\text{int}}) = - \left( 1 - 0.89 \eta^{5/2} t^{1/2} \right) \frac{\mu}{k_B T} - 1.01 \eta^{5/2} t^{1/2}. \tag{24}
\]

From (3), (3), and (24) we can obtain the condensate fraction below the critical temperature,

\[
\xi = 1 - t^3 - \frac{\zeta(2)}{\zeta(3)} t^3 \left[ \left( 1 - 0.89 \eta^{5/2} t^{1/2} \right) \eta^{2/5} t + 1.01 \eta^{5/2} t^{1/2} \right] - \frac{3}{2 \omega_{\text{ho}}} \frac{\zeta(2)}{\zeta(3)} t^{2/3} N^{-1/3}. \tag{25}
\]

In (25) the terms comprises \( \eta^{5/2} \) represents high-order correction to the condensate fraction due to interatomic interaction. Omitting the terms comprises \( \eta^{5/2} \), we can obtain the lowest-order correction (21). Essentially, (21) and (25) are transcendental equations on the condensate fraction. We can easily give the numerical solution of the condensate fraction. In Fig.1 and Fig.2 we used the experimental parameter by Ensher et al. [14], where the cloud consists of \( 4 \times 10^4 \) atoms at the transition and \( a/a_{\text{ho}} = 5.4 \times 10^{-3} \). According to Fig.2 the high-order correction (25) agrees well with the condensate fraction (17) in the
region $\frac{N_0 a}{\hbar^2} \ll 1$. From (17) and (23), close to $T_0$ the condensate fraction increase quite slowly with decreasing the temperature. However, the lowest-order correction (21) is rather different from the dashed line near the critical temperature. The difference between (17) and (21) lies in the fact that there is only high-order correction due to interatomic interaction near the critical temperature, while there is only lowest-order correction in (21). Fig.2 demonstrates the validity of (24) over the whole range of temperature below $T_c$.

In the preceding calculations we neglects the role of the interaction between the condensate and the thermal atoms on the density distributions of the condensate and the thermal atoms. In the frame of Hartree-Fork model [3,8], the densities of the condensate and the thermal component are given as follows.

$$n_0(\vec{r}) = \frac{\mu - V_{ext}(\vec{r}) - 2gn_T(\vec{r})}{g} \theta (\mu - V_{ext}(\vec{r}) - 2gn_T(\vec{r})),$$  \hspace{1cm} (26)

$$n_T(\vec{r}) = \frac{\lambda}{\bar{v}^{3/2}} \left[ e^{-(v_{ext}(\vec{r})+2g(n_0(\vec{r})+n_T(\vec{r})-\mu)/k_BT} \right].$$ \hspace{1cm} (27)

Using (3), (5), (22) and (26), (27) and the usual iterative procedure we can obtain the numerical conclusion of the condensate fraction. The numerical conclusion is illustrated in Fig.3.

V. CONDENSATE FRACTION BEYOND MEAN-FIELD THEORY

In the preceding calculations of the condensate fraction, GP equation is used to obtain the energy $E_0$ of the condensate. GP equation is expected to be valid if the system is dilute, i.e. $n|a|^3 \ll 1$. Obviously, correction to GP equation would modify the condensate fraction of the system. The first correction to the mean-field approximation have been investigated by Timmermans, Tommasini, and Huang [15] and by Braaten and Nieto [16]. For large $N_0$, using the local density approximation, the density distribution of the condensate is given by

$$n_0(\vec{r}) = \frac{\mu - V_{ext}(\vec{r})}{g} - \frac{4n^{3/2}}{3\pi^2\hbar^2} [\mu - V_{ext}(\vec{r})]^{3/2},$$ \hspace{1cm} (28)

with $\mu$ given by
\[
\mu = \frac{\hbar \omega_{ho}}{2} \left( \frac{15N_0 a}{a_{ho}} \right)^{2/5} \left( 1 + \sqrt{\pi a^3 n(0)} \right). \tag{29}
\]

The parameter \(a^3 n(0)\) can be directly expressed in terms of the relevant parameters of the system. \(a^3 n(0) = \frac{15^{2/5}}{8\pi} \left( N_0^{1/6} \frac{a}{a_{ho}} \right)^{12/5} = 0.0078\eta^6 \xi^{2/5}.\) Using the relation \(E_0 = 5N_0\mu/7\) and (3), (3) we can obtain the correction to the condensate fraction below \(T_c\)

\[
\xi = 1 - t^3 - \frac{\zeta(2)}{\zeta(3)} t^3 \left[ (1 - 0.89\eta^{5/2} t^{1/2} + 0.16\eta^3 \xi^{1/5}) \frac{\eta \xi^{2/5}}{t} + 1.01\eta^{5/2} t^{1/2} \right] - \frac{3\omega \zeta(2)}{2\omega_{ho} \zeta(3)^{2/3}} t^2 N^{-1/3}. \tag{30}
\]

The term \(0.16\eta^3 \xi^{1/5}\) is the correction due to the modification of the GP equation. It gives higher-order correction of the scaling parameter \(\eta\), compared to the high-order correction due to interatomic interactions.

Another correction to the condensate fraction beyond mean-field approximation is given by the quantum depletion of the condensate. There are atoms which do not occupy the condensate at zero temperature because of quantum depletion effects. We can use local density approximation to write the density of atoms out of the condensate. Timmermans, Tommasini, and Huang [13] gives \(n_{out}(\vec{r}) = (8/3) [n(\vec{r}) a^3 / \pi]^{1/2}\). Integration of \(n_{out}(\vec{r})\) yields the result

\[
\xi_{out} = \int n_{out}(\vec{r}) d^3\vec{r} = \frac{5\sqrt{\pi}}{8} \sqrt{a^3 n(0)}. \tag{31}
\]

Combining (30) and (31)

\[
\xi = 1 - t^3 - \frac{\zeta(2)}{\zeta(3)} t^3 \left[ (1 - 0.89\eta^{5/2} t^{1/2} + 0.16\eta^3 \xi^{1/5}) \frac{\eta \xi^{2/5}}{t} + 1.01\eta^{5/2} t^{1/2} \right] - 0.11\eta^3 \xi^{1/5} - \frac{3\omega \zeta(2)}{2\omega_{ho} \zeta(3)^{2/3}} t^2 N^{-1/3}. \tag{32}
\]

The term \(-0.11\eta^3 \xi^{1/5}\) is the correction due to quantum depletion.

Compared to the finite-size effects, the corrections to the mean-field approximation have a different dependence on the parameter \(N\) and \(a/a_{ho}\). The corrections beyond mean field
theory become larger than finite-size effects when $N$ is larger than about $10^6$. In Fig.4 we give numerical conclusion of (32). The corrections beyond mean field theory become important when the temperature is much lower than the critical temperature.

VI. CONCLUSION

To conclude, the canonical ensemble is used to obtain the equations on the condensate fraction (3) and (4), which account for interaction effects. Finite-size effects can be obtained simultaneously because these effects are comprised in (3). (3) and (4) are used to investigate the condensate fraction near and below the critical temperature. From the condensate fraction near the critical temperature, we obtain the shift of the critical temperature due to atom-atom interaction and finite-size effects simultaneously. In addition, the analytical high-order correction due to interatomic interaction is obtained in this work.

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FIGURES

FIG. 1. Theoretical prediction for the condensate fraction vs $T/T_c^0$ for $N = 4 \times 10^4$ rubidium atoms in a trap with $a/a_{ho} = 5.4 \times 10^{-3}$. The dashed line shows the noninteracting model in the thermodynamical limit. The dotted line is obtained from the numerical solution of (21), which accounts for the lowest-order correction due to interatomic interaction. The solid line is obtained from (25) which accounts for high-order correction.

FIG. 2. The upper solid line shows the lowest-order correction (21) due to interatomic interaction. The lower solid line represents the high-order correction (25). The dashed line shows the condensate fraction near $T_c$, which is obtained from (17). Equation (17) holds when $N_{a0}a/a_{ho} << 1$. In the region $N_{a0}a/a_{ho} << 1$, the lower solid line agrees well with the dashed line. This demonstrates the validity of (25) over the whole range of temperature $T < T_c$, even close to $T_c^0$.

FIG. 3. The solid line is obtained from (25). The dashed line is a self-consistent numerical solution of (5), (6), (22), and (26), (27) using iterative method.

FIG. 4. The solid line is obtained from (25) which accounts for high-order correction due to interatomic interaction. The dotted line is obtained from (32), in which the corrections beyond mean field theory are comprised. The corrections beyond mean-field theory become important when the temperature is much lower than the critical temperature (shown in the inset).
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Fig. 1

$N_0/N$ vs. $T/T_c^0$

- Ideal Bose gas
- Lowest-order correction
- High-order correction
Fig. 2

- Condensate fraction near $T_c$
- Lowest-order correction
- High-order correction

$N_0/N$ vs. $T/T_c^0$
Fig. 3

- Dashed line: iterative method
- Solid line: high-order correction
Fig. 4

- high-order correction
- beyond mean-field

$N_0 / N$

$T / T_c^0$

Fig. 4