

Canonical statistics of trapped ideal and interacting Bose gases

Hongwei Xiong,^{1,2} Shujuan Liu,¹ Guoxiang Huang,³ and Zaixin Xu³

¹*Department of Applied Physics, Zhejiang University of Technology, Hangzhou 310032, China*

²*Zhijiang College, Zhejiang University of Technology, Hangzhou 310012, China*

³*Department of Physics, East China Normal University, Shanghai 200062, China*

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The mean ground-state occupation number and condensate fluctuations of interacting and noninteracting Bose gases confined in a harmonic trap are considered by using a canonical ensemble approach. To obtain the mean ground-state occupation number and the condensate fluctuations, an analytical description for the probability distribution function of the condensate is provided directly starting from the analysis of the partition function of the system. For the ideal Bose gas, the probability distribution function is found to be a Gaussian one for the case of the harmonic trap. For the interacting Bose gas, using a unified approach the condensate fluctuations are calculated based on the lowest-order perturbation method and on Bogoliubov theory. It is found that the condensate fluctuations based on the lowest-order perturbation theory follow the law $\langle \delta^2 N_0 \rangle \sim N$, while the fluctuations based on Bogoliubov theory behave as $N^{4/3}$.

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I. INTRODUCTION

The experimental achievement of Bose-Einstein condensation (BEC) in dilute alkali-metal atoms [1], spin-polarized hydrogen [2], and recently in metastable helium [3] has greatly stimulated theoretical research [4–6] on ultracold bosons. Among the several intriguing questions on the statistical properties of trapped interacting Bose gases, the problem of condensate fluctuations $\langle \delta^2 N_0 \rangle$ of the mean ground-state occupation number $\langle N_0 \rangle$ is of central importance. Apart from the intrinsic theoretical interest, it is foreseeable that such fluctuations will become experimentally testable in the near future [7]. On the other hand, the calculations of $\langle \delta^2 N_0 \rangle$ are crucial to investigate the phase collapse time of the condensate [8,9].

It is well known that within a grand-canonical ensemble the fluctuations of the condensate are given by $\langle \delta^2 N_0 \rangle = N_0(N_0 + 1)$, implying that δN_0 becomes of order N when the temperature approaches zero. To avoid this sort of unphysically large condensate fluctuations, a canonical (or a microcanonical) ensemble has to be used to investigate the fluctuations of the condensate. On the other hand, because in the experiment the trapped atoms are cooled continuously from the surrounding, the system can be taken as being in contact with a heat bath but the total number of particles in the system is conserved. Thus it is necessary to use the canonical ensemble to investigate the statistical properties of the trapped weakly interacting Bose gas.

Within the canonical as well as the microcanonical ensembles, the condensate fluctuations have been studied systematically in the case of an ideal Bose gas in a box [10–14] and in the presence of a harmonic trap [14–21]. Recently, the question of how interatomic interactions affect the condensate fluctuations has been the subject of several theoretical investigations [22–27]. Idziaszek *et al.* [23] investigated the condensate fluctuations of interacting Bose gases using the lowest-order perturbation theory and a two-gas model,

while Giorgini *et al.* [22] addressed this problem within a traditional particle-number–nonconserving Bogoliubov approach. Recently, Kocharovskiy *et al.* [26] supported and extended the results of the work of Giorgini *et al.* [22] using a particle-number–conserving operator formalism.

Although the condensate fluctuations are thoroughly investigated in Refs. [22–26], to the best of our knowledge up to now an analytical description of the probability distribution function for the interacting Bose gas directly from the microscopic statistics of the system has not been given. Note that as soon as the probability distribution function of the system is obtained, it is straightforward to get the mean ground-state occupation number and the condensate fluctuations. The purpose of the present work is to attempt to provide such an analytical description of the probability distribution function of interacting and noninteracting Bose gases based on the analysis of the partition function of the system.

We shall investigate in this paper the condensate fluctuations of interacting and noninteracting Bose gases confined in a harmonic trap. The analytical probability distribution function of the condensate will be given directly from the partition function of the system using a canonical ensemble approach. For an ideal Bose gas, we find that the probability distribution of the condensate is a Gaussian function. In particular, our method can be easily extended to discuss the probability distribution function for a weakly interacting Bose gas. A unified way is given to calculate the condensate fluctuations from the lowest-order perturbation theory and from Bogoliubov theory. We find that different methods of approximation for the interacting Bose gas give quite different predictions concerning the condensate fluctuations. We show that the fluctuations based on the lowest-order perturbation theory follow the law $\langle \delta^2 N_0 \rangle \sim N$, while the fluctuations based on the Bogoliubov theory behave as $N^{4/3}$.

The paper is organized as follows. Section II is devoted to outlining the canonical ensemble, which is developed to discuss the probability distribution function of Bose gases. In Sec. III, we investigate the condensate fluctuations of the ideal Bose gas confined in a harmonic trap. In Sec. IV, the

condensate fluctuations of the weakly interacting Bose gas are calculated based on the lowest-order perturbation theory. In Sec. V, the condensate fluctuations due to collective excitations are obtained based on Bogoliubov theory. Finally, Sec. VI contains a discussion and summary of our results.

II. FLUCTUATIONS AND MEAN GROUND-STATE OCCUPATION NUMBER OF THE CONDENSATE IN THE CANONICAL ENSEMBLE

According to the canonical ensemble, the partition function of the system with N trapped interacting bosons is given by

$$Z[N] = \sum_{\sum_{\mathbf{n}} N_{\mathbf{n}} = N} \exp[-\beta(\sum_{\mathbf{n}} N_{\mathbf{n}} \varepsilon_{\mathbf{n}} + E_{\text{int}})], \quad (1)$$

where $N_{\mathbf{n}}$ and $\varepsilon_{\mathbf{n}}$ are the occupation number and energy level of the state $\mathbf{n} = \{n_x, n_y, n_z\}$, respectively. $\beta = 1/k_B T$ and $\{n_x, n_y, n_z\}$ are non-negative integers. E_{int} is the interaction energy of the system. For convenience, by separating out the ground-state $\mathbf{n} = \mathbf{0}$ from the state $\mathbf{n} \neq \mathbf{0}$, we have

$$Z[N] = \sum_{N_0=0}^N \{\exp[-\beta(E_0 + E_{\text{int}})] Z_0(N, N_0)\}, \quad (2)$$

where $Z_0(N, N_0)$ stands for the partition function of a fictitious system comprising $N - N_0$ trapped ideal noncondensed bosons:

$$Z_0(N, N_0) = \sum_{\sum_{\mathbf{n} \neq \mathbf{0}} N_{\mathbf{n}} = N - N_0} \exp\left[-\beta \sum_{\mathbf{n} \neq \mathbf{0}} N_{\mathbf{n}} \varepsilon_{\mathbf{n}}\right]. \quad (3)$$

Assuming $A_0(N, N_0)$ is the free energy of the fictitious system, we have

$$A_0(N, N_0) = -k_B T \ln Z_0(N, N_0). \quad (4)$$

The calculation of the free energy $A_0(N, N_0)$ is nontrivial because there is a requirement that the number of noncondensed bosons is $N - N_0$ in the summation of the partition function $Z_0(N, N_0)$. Using the saddle-point method developed by Darwin and Fowler [28], it is straightforward to obtain a useful relation between the free energy $A_0(N, N_0)$ and the fugacity z_0 of the fictitious $N - N_0$ noninteracting bosons

$$-\beta \frac{\partial}{\partial N_0} A_0(N, N_0) = \ln z_0, \quad (5)$$

where the fugacity z_0 is determined by

$$N_0 = N - \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp[\beta \varepsilon_{\mathbf{n}}] z_0^{-1} - 1}. \quad (6)$$

We have given a simple derivation of Eqs. (5) and (6) in the Appendix.

Using the free energy $A_0(N, N_0)$, the partition function of the system becomes

$$Z[N] = \sum_{N_0=0}^N \exp[q(N, N_0)], \quad (7)$$

where

$$q(N, N_0) = -\beta(E_0 + E_{\text{int}}) - \beta A_0(N, N_0). \quad (8)$$

It is obvious that $(1/Z[N]) \exp[q(N, N_0)]$ represents the probability finding N_0 atoms in the condensate.

To obtain the probability distribution function of the system, let us first investigate the largest term in the sum of the partition function $Z[N]$. Assume the number of the condensed atoms is N_0^p in the largest term of the partition function. The largest term $\exp[q(N, N_0^p)]$ is determined by requiring that $(\partial/\partial N_0)q(N, N_0)|_{N_0=N_0^p} = 0$, i.e.,

$$-\beta \frac{\partial}{\partial N_0^p} (E_0 + E_{\text{int}}) - \beta \frac{\partial}{\partial N_0^p} A_0(N, N_0^p) = 0. \quad (9)$$

Using Eq. (5), we obtain

$$\ln z_0^p = \beta \frac{\partial}{\partial N_0^p} (E_0 + E_{\text{int}}). \quad (10)$$

In addition, from Eq. (6), the most probable value N_0^p is determined by

$$N_0^p = N - \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp[\beta \varepsilon_{\mathbf{n}}] (z_0^p)^{-1} - 1}. \quad (11)$$

In the case of an ideal Bose gas, from Eq. (10) one obtains $\ln z_0^p = \beta \varepsilon_0$. Thus N_0^p is the same as the mean ground-state occupation number obtained by using a grand-canonical ensemble approach. For sufficiently large N , the sum $\sum_{N_0=0}^N$ in Eq. (7) may be replaced by the largest term, since the error omitted in doing so is statistically negligible. In this situation, Eq. (11) shows the equivalence between the canonical ensemble and the grand-canonical ensemble for large N .

The other terms in the partition function (7) will contribute to the fluctuations of the condensate, and lead to the deviation of $\langle N_0 \rangle$ from the most probable value N_0^p . If $N_0 \neq N_0^p$, we have $(\partial/\partial N_0)q(N, N_0) \neq 0$. Assuming

$$\frac{\partial}{\partial N_0} q(N, N_0) = \alpha(N, N_0), \quad (12)$$

from Eqs. (5) and (8) we obtain

$$\ln z_0 = \beta \frac{\partial}{\partial N_0} (E_0 + E_{\text{int}}) + \alpha(N, N_0). \quad (13)$$

By Eqs. (6) and (13), we have

$$N_0 = N - \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp[\beta \varepsilon_{\mathbf{n}}] \exp\left(-\beta \frac{\partial}{\partial N_0}(E_0 + E_{\text{int}}) - \alpha(N, N_0)\right) - 1}. \quad (14)$$

Combining Eqs. (11) and (14), we get the following equation for determining $\alpha(N, N_0)$:

$$N_0 - N_0^p = \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp[\beta \varepsilon_{\mathbf{n}}] \exp\left(-\beta \frac{\partial}{\partial N_0^p}(E_0 + E_{\text{int}})\right) - 1} - \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp[\beta \varepsilon_{\mathbf{n}}] \exp\left(-\beta \frac{\partial}{\partial N_0}(E_0 + E_{\text{int}}) - \alpha(N, N_0)\right) - 1}. \quad (15)$$

Once we know E_0 and E_{int} of the system, it is straightforward to obtain $\alpha(N, N_0)$ from Eq. (15). Using $\alpha(N, N_0)$, one can obtain the probability distribution function of the system.

From Eq. (12), we obtain the following result for $q(N, N_0)$:

$$q(N, N_0) = \int_{N_0^p}^{N_0} \alpha(N, N_0) dN_0 + q(N, N_0^p). \quad (16)$$

Thus the partition function of the system becomes

$$Z[N] = \sum_{N_0=0}^N \{\exp[q(N, N_0^p)] G(N, N_0)\}, \quad (17)$$

where

$$G(N, N_0) = \exp\left[\int_{N_0^p}^{N_0} \alpha(N, N_0) dN_0\right]. \quad (18)$$

Assuming $P(N_0|N)$ is the probability to find N_0 atoms in the condensate, $G(N, N_0)$ represents the ratio $[P(N_0|N)]/[P(N_0^p|N)]$, i.e., the relative probability to find N_0 atoms in the condensate. From Eq. (18), the normalized probability distribution function is given by

$$G_n(N, N_0) = A \exp\left[\int_{N_0^p}^{N_0} \alpha(N, N_0) dN_0\right], \quad (19)$$

where A is a normalization constant and is given by the condition $A \int G(N, N_0) dN_0 = 1$.

As soon as we know $G(N, N_0)$, the statistical properties of the system can be clearly described. From Eqs. (17) and (18), one obtains the mean ground-state occupation number $\langle N_0 \rangle$ and fluctuations $\langle \delta^2 N_0 \rangle$ in the canonical ensemble:

$$\langle N_0 \rangle = \frac{\sum_{N_0=0}^N N_0 \exp[q(N, N_0)]}{\sum_{N_0=0}^N \exp[q(N, N_0)]} = \frac{\sum_{N_0=0}^N N_0 G(N, N_0)}{\sum_{N_0=0}^N G(N, N_0)}, \quad (20)$$

$$\langle \delta^2 N_0 \rangle = \langle N_0^2 \rangle - \langle N_0 \rangle^2 = \frac{\sum_{N_0=0}^N N_0^2 G(N, N_0)}{\sum_{N_0=0}^N G(N, N_0)} - \left[\frac{\sum_{N_0=0}^N N_0 G(N, N_0)}{\sum_{N_0=0}^N G(N, N_0)} \right]^2. \quad (21)$$

Starting from Eqs. (20) and (21), one can calculate the mean ground-state occupation number and fluctuations for ideal and interacting Bose gases.

III. IDEAL BOSE GASES

We now study the condensate fluctuations of the system with N noninteracting bosons trapped in an external potential. The potential is a harmonic one with the form

$$V_{\text{ext}}(\mathbf{r}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad (22)$$

where m is the mass of atoms, and ω_x, ω_y , and ω_z are frequencies of the trap along three coordinate-axis directions. The single-particle energy level has the form

$$\varepsilon_{\mathbf{n}} = \left(n_x + \frac{1}{2}\right) \hbar \omega_x + \left(n_y + \frac{1}{2}\right) \hbar \omega_y + \left(n_z + \frac{1}{2}\right) \hbar \omega_z. \quad (23)$$

From Eq. (11), one can get easily the most probable value N_0^p , which reads

$$N_0^p = N - N \left(\frac{T}{T_c^0}\right)^3 - \frac{3\bar{\omega}\zeta(2)}{2\omega_{\text{ho}}[\zeta(3)]^{2/3}} \left(\frac{T}{T_c^0}\right)^2 N^{2/3}, \quad (24)$$

where $T_c^0 = (\hbar \omega_{\text{ho}}/k_B)[N/\zeta(3)]^{1/3}$ is the critical temperature of the ideal Bose gas in the thermodynamic limit. $\bar{\omega} = (\omega_x + \omega_y + \omega_z)/3$ and $\omega_{\text{ho}} = (\omega_x \omega_y \omega_z)^{1/3}$ are arithmetic and geometric averages of the oscillator frequencies, respectively. When obtaining Eq. (24), we have used the following expression of the density of states [30]:

$$\rho(E) = \frac{1}{2} \frac{E^2}{(\hbar \omega_{\text{ho}})^3} + \frac{3 \bar{\omega} E}{2 \omega_{\text{ho}} (\hbar \omega_{\text{ho}})^2}. \quad (25)$$

On the basis of the same density of states, a detailed study of the critical temperature and the ground-state occupation number was given recently in [31].

In a thermodynamic equilibrium, the deviation from the most probable value N_0^p is small, therefore we can use the approximation $\exp[-\alpha(N, N_0)] \approx 1 - \alpha(N, N_0)$. From Eq. (15) and the single-particle energy level (23), we find the result for $\alpha(N, N_0)$,

$$\alpha(N, N_0) = - \frac{\zeta(3)(N_0 - N_0^p)}{\zeta(2)N(T/T_c^0)^3}. \quad (26)$$

When obtaining $\alpha(N, N_0)$, we have used the expansion $g_3(1 + \delta) \approx \zeta(3) + \zeta(2)\delta$ [32], where $g_3(z)$ belongs to the class of functions $g_\alpha(z) = \sum_{n=1}^{\infty} z^n/n^\alpha$ and $\zeta(n)$ is the Riemann ζ function. From Eqs. (18) and (26), we obtain the normalized probability distribution function of the harmonically trapped ideal Bose gas

$$G_{\text{ideal}}(N, N_0) = A_{\text{ideal}} \exp \left[- \frac{\zeta(3)(N_0 - N_0^p)^2}{2\zeta(2)N(T/T_c^0)^3} \right], \quad (27)$$

where A_{ideal} is a normalization constant. It is interesting to note that the expression (27) is a Gaussian distribution function. From the formulas (20), (21), (24), and (27) we can obtain $\langle N_0 \rangle$ and $\langle \delta^2 N_0 \rangle$ for the ideal Bose gas.

In Fig. 1(a) and Fig. 1(b), we plot $\langle N_0 \rangle/N$ as a function of temperature for $N=200$ and $N=10^3$ ideal bosons confined in an isotropic harmonic trap. The dashed line displays $\langle N_0 \rangle/N$ in the thermodynamic limit, while the solid line displays $\langle N_0 \rangle/N$ within the grand-canonical ensemble (or N_0^p within the canonical ensemble). The dotted line displays $\langle N_0 \rangle/N$ within the canonical ensemble. When $N > 10^3$, $\langle N_0 \rangle/N$ from the canonical ensemble agrees well with that from the grand-canonical ensemble. Obviously, in the case of $N \rightarrow \infty$, $\langle N_0 \rangle/N$ obtained from the canonical ensemble coincides with that from the grand-canonical ensemble.

From the formulas (20) and (21) and the results (24) and (27), we can obtain the condensate fluctuations of the ideal Bose gas. In Fig. 2, we plot the numerical result of $\delta N_0 = \sqrt{\langle \delta^2 N_0 \rangle}$ (solid line) for $N=10^3$ ideal bosons confined in an isotropic harmonic potential. The dashed line displays the result of Holthaus *et al.* [21], where the saddle-point method is developed to avoid the failure of the standard saddle-point approximation below the onset of BEC.

In Fig. 2, the dotted line displays the result given in Refs. [15,22]. Our results coincide with those of Refs. [15,22] when T/T_c^0 is smaller than T_m/T_c^0 , which corresponds to the maximum fluctuations $\langle \delta^2 N_0 \rangle_{\text{max}}$. In fact, when $T/T_c^0 < T_m/T_c^0$, from Eqs. (20), (21), and (27), we obtain the analytical result for the condensate fluctuations:

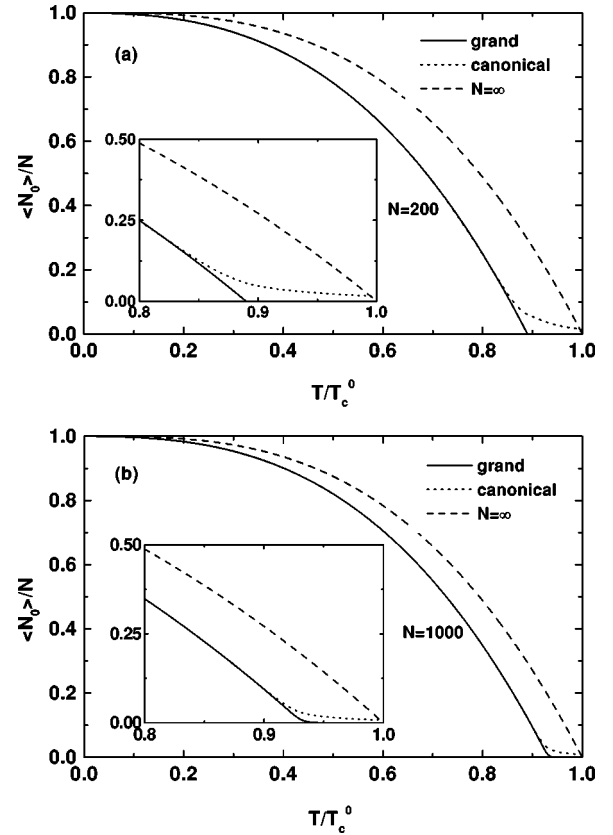


FIG. 1. Relative mean ground-state occupation number $\langle N_0 \rangle/N$ vs T/T_c^0 for $N=200, 10^3$ noninteracting bosons confined in an isotropic harmonic trap. The dashed line shows $\langle N_0 \rangle/N$ in the thermodynamic limit, the solid line shows $\langle N_0 \rangle/N$ within the grand-canonical ensemble, while the dotted line displays $\langle N_0 \rangle/N$ within the canonical ensemble. When $N \rightarrow \infty$, the mean ground-state occupation number of the canonical ensemble coincides with that of the grand-canonical ensemble.

$$\langle \delta^2 N_0 \rangle = \frac{\pi^2}{6\zeta(3)} N \left(\frac{T}{T_c^0} \right)^3, \quad (28)$$

which recovers the result given in Refs. [15,22]. This shows the validity of the probability distribution function (27) for studying the statistical properties of the system. At the critical temperature, however, our results give

$$\langle \delta^2 N_0 \rangle|_{T=T_c} = \left(1 - \frac{2}{\pi} \right) \frac{\pi^2 N}{6\zeta(3)}, \quad (29)$$

which is much smaller than the result of Ref. [22]. This difference is apprehensible because the analysis of Giorgini *et al.* [22] holds in the canonical ensemble except near and above T_c^0 , while our result holds also for the temperature near T_c^0 . Near the critical temperature, our result (solid line) agrees with that of Holthaus *et al.* [21]. The results given by Eqs. (28) and (29) show a normal behavior of the condensate fluctuations for the harmonically trapped ideal Bose gas.

The fluctuations of the condensate can also be evaluated at $T=0$. In the case of $T \rightarrow 0$, from Eq. (27) we get

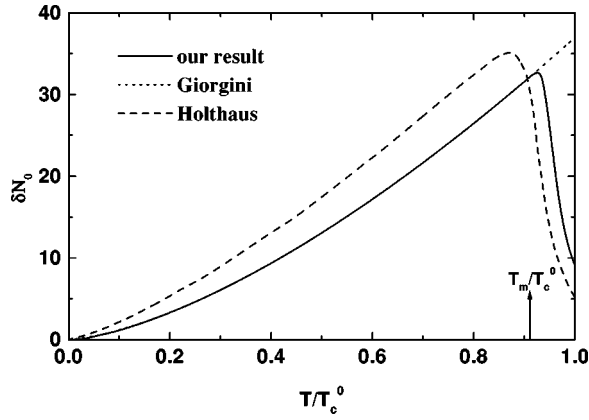


FIG. 2. Root-mean-square fluctuations δN_0 for $N=10^3$ noninteracting bosons confined in an isotropic harmonic traps. The solid line displays δN_0 obtained from the probability distribution function Eq. (27), while the dashed line shows the result of Holthaus *et al.* [21]. The dotted line displays the result of Giorgini *et al.* [22] [Eq. (28)]. The arrow marks the temperature corresponding to the maximum condensate fluctuations. Below T_m , the solid line coincides with the result of Giorgini *et al.* [22]. Near T_c , our result agrees with that of Holthaus *et al.* [21].

$G(N, N_0) = A_{\text{ideal}}$ if $N_0 = N$, while $G(N, N_0) \rightarrow 0$ when $N_0 \neq N$. Therefore, we obtain $\langle N_0 \rangle \rightarrow N$ and $\langle \delta^2 N_0 \rangle \rightarrow 0$ when $T \rightarrow 0$.

Note that our results are reliable although the disputable saddle-point method is used to investigate the fluctuations of the condensate. It is well known that the applicability of the saddle-point approximation for the condensed Bose gas has been the subject of a long debate [12,29]. Recently, the analysis given in Ref. [17] showed that the fluctuations are overestimated and do not appear to vanish properly with temperature using the conventional saddle-point method. Our discussions on the condensate fluctuations are reasonable due to two reasons. (i) As proven in Ref. [21], the most probable value Eq. (11) for the noninteracting Bose gas is still correct, even when carefully dealing with the failure of the standard saddle-point method below the critical temperature. (ii) In the usual statistical method, $\langle N_0 \rangle$ and $\langle \delta^2 N_0 \rangle$ are obtained through the first and second partial derivatives of the partition function, respectively. When the saddle-point approximation is used to calculate the partition function of the system, the error will be overestimated in the second partial derivative of the partition function. Thus one cannot obtain correct condensate fluctuations using the usual method. However, in our approach here what we used is the reliable result given by Eqs. (11) and (14). The probability distribution function of the ground state occupation number can be obtained directly from Eqs. (11) and (14), without resorting to the second partial derivative of the partition function. $\langle N_0 \rangle$ and $\langle \delta^2 N_0 \rangle$ are obtained from the probability distribution function in our approach. The correct description of δN_0 near zero temperature and critical temperature also shows the validity of our method. Thus our approach has provided in some sense a simple method recovering the applicability of

the saddle-point method through the calculations of the probability distribution function of the system.

IV. INTERACTING BOSE GASES BASED ON THE LOWEST-ORDER PERTURBATION THEORY

Below the critical temperature, Bose-Einstein condensation results in a sharp enhancement of the density in the central region of the trap. This makes the interacting effect between atoms much more important than above T_c . The correction to the condensate fraction and critical temperature due to the interatomic interaction has been discussed within the grand-canonical ensemble [33–36] and the canonical ensemble [37,31]. In this section, we investigate the role of interaction on the condensate fluctuations of a weakly interacting Bose gas.

Using the lowest-order perturbation theory, the interaction energy of the system takes the form

$$E_{\text{int}} = 2g \int n_0(\mathbf{r}) n_T(\mathbf{r}) d^3 \mathbf{r} + g \int n_T^2(\mathbf{r}) d^3 \mathbf{r}, \quad (30)$$

where $g = 4\pi\hbar^2 a/m$ is the coupling constant fixed by the s -wave scattering length a . $n_0(\mathbf{r})$ and $n_T(\mathbf{r})$ are the density distributions of the condensate and normal gas, respectively.

Below the critical temperature, by the Thomas-Fermi (TF) approximation the density distribution of the condensate reads

$$n_0(\mathbf{r}) = \frac{\mu - V_{\text{ext}}(\mathbf{r})}{g}, \quad (31)$$

where μ is the chemical potential of the system. The temperature dependence of the chemical potential is then fixed by the number of atoms in the condensate,

$$\mu(N_0, T) = \frac{\hbar \omega_{\text{ho}}}{2} \left(\frac{15N_0 a}{a_{\text{ho}}} \right)^{2/5}, \quad (32)$$

where $a_{\text{ho}} = (\hbar/m\omega_{\text{ho}})^{1/2}$ is the harmonic oscillator length. Moreover, since $\mu = \partial E_0 / \partial N_0$, the energy per particle in the condensate turns out to be

$$\varepsilon_0^{\text{TF}} = E_0 / N_0 = \frac{5}{7} \mu(N_0, T). \quad (33)$$

As a first-order approximation, omitting the interaction between condensed and noncondensed atoms, the partition function of the system is given by

$$Z_{\text{int}}[N] = \sum_{N_0=0}^N \{ \exp[-\beta N_0 \varepsilon_0^{\text{TF}}] Z_0(N, N_0) \}. \quad (34)$$

From Eq. (11), the most probable value reads

$$N_0^p = N - \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp\{\beta[\varepsilon_{\mathbf{n}} - \mu(N_0^p, T)]\} - 1}. \quad (35)$$

Using the density of states, i.e., Eq. (25), one obtains the result for the most probable value N_0^p ,

$$N_0^p = N(1 - t^3) - \frac{\zeta(2)}{\zeta(3)} \frac{\mu(N_0^p, T)t^3 N}{k_B T} - \frac{3\bar{\omega}\zeta(2)}{2\omega_{\text{ho}}[\zeta(3)]^{2/3}} t^2 N^{2/3}, \quad (36)$$

where $t = T/T_c^0$ is the reduced temperature. Introducing the scaling parameter η [4],

$$\eta = \frac{\mu(T=0)}{k_B T_c^0} = 1.57 \left(\frac{N^{1/6} a}{a_{\text{ho}}} \right)^{2/5}, \quad (37)$$

Eq. (36) becomes

$$N_0^p = N(1 - t^3) - \frac{\zeta(2)}{\zeta(3)} \eta N t^2 \left(\frac{N_0^p}{N} \right)^{2/5} - \frac{3\bar{\omega}\zeta(2)}{2\omega_{\text{ho}}[\zeta(3)]^{2/3}} t^2 N^{2/3}. \quad (38)$$

Note that the corrections due to the interatomic interaction and finite number of particle of the system can be obtained simultaneously when Eq. (38) is used to calculate $\langle N_0 \rangle$ and $\langle \delta^2 N_0 \rangle$ of the system. The second term on the right-hand side of Eq. (38) accounts for the correction of the interaction effect. The correction due to the interatomic interaction coincides with the lowest-order thermal depletion obtained in the grand-canonical ensemble approach [4].

For other N_0 , assuming $(\partial/\partial N_0)q(N, N_0) = \alpha(N, N_0)$, we get

$$N_0 = N - \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp\{\beta[\varepsilon_{\mathbf{n}} - \mu(N_0, T)]\} \exp[-\alpha(N, N_0)] - 1}. \quad (39)$$

Combining Eqs. (35) and (39), one obtains the result for $\alpha(N, N_0)$,

$$\alpha(N, N_0) = - \frac{\zeta(3)(N_0 - N_0^p)}{\zeta(2)Nt^3} + \frac{\mu(N_0^p, T) - \mu(N_0, T)}{k_B T}. \quad (40)$$

The probability distribution function of the interacting Bose gas is then

$$\begin{aligned} G_{\text{int}}(N, N_0) &= A_{\text{int}} \exp \left[\int_{N_0^p}^{N_0} \alpha(N, N_0) dN_0 \right] \\ &= \frac{A_{\text{int}}}{A_{\text{ideal}}} G_{\text{ideal}}(N, N_0) R_{\text{int}}(N, N_0), \end{aligned} \quad (41)$$

where A_{int} is a normalization constant. $G_{\text{ideal}}(N, N_0)$ is the probability distribution function given by the formula (27)

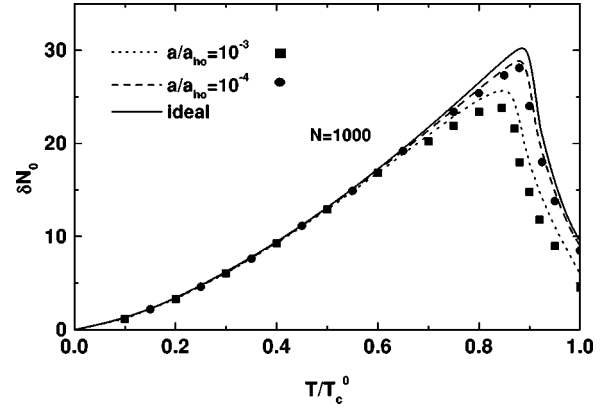


FIG. 3. The numerical result of δN_0 for $N=1000$ interacting bosons confined in an isotropic harmonic trap with $a/a_{\text{ho}}=10^{-4}$ and $a/a_{\text{ho}}=10^{-3}$, respectively. The dotted and dashed lines show condensate fluctuations when interactions between condensed and noncondensed atoms are omitted. The condensate fluctuations are displayed with circles and squares when interactions between condensed and noncondensed atoms are considered. The crossover from the interacting to noninteracting Bose gases is clearly shown in the figure.

for the ideal harmonically trapped Bose gas. The correction $R_{\text{int}}(N, N_0)$ originating from the interatomic interaction takes the form

$$\begin{aligned} R_{\text{int}}(N, N_0) &= \exp \left\{ \frac{\hbar \omega_{\text{ho}}}{2k_B T} \left(\frac{15a}{a_{\text{ho}}} \right)^{2/5} \left[(N_0^p)^{2/5} (N_0 - N_0^p) \right. \right. \\ &\quad \left. \left. - \frac{5}{7} [N_0^{7/5} - (N_0^p)^{7/5}] \right] \right\}. \end{aligned} \quad (42)$$

Note that $G_{\text{int}}(N, N_0)$ is not a Gaussian distribution function because of the existence of the non-Gaussian factor $R_{\text{int}}(N, N_0)$.

From Eqs. (21) and (41) we can obtain the numerical result of $\langle \delta^2 N_0 \rangle_{\text{int}}$. In Fig. 3, we have provided the numerical result of δN_0 for $N=1000$ interacting bosons confined in an isotropic harmonic trap with $a/a_{\text{ho}}=10^{-4}$ and $a/a_{\text{ho}}=10^{-3}$, respectively. The crossover from the interacting to the noninteracting Bose gases is clearly shown. From Fig. 3, we find that the repulsive interaction between atoms results in a decrease of the condensate fluctuations. For an attractive interaction, we anticipate that the corrections between atoms result in an increase in the condensate fluctuations.

The interaction between condensed and noncondensed atoms gives high-order correction to the thermodynamic properties of the system. Near the critical temperature, i.e., when $N_0 a/a_{\text{ho}} \ll 1$ [4], we have $n_0(\mathbf{r}) = N_0 (m\omega_{\text{ho}}^2/\pi\hbar)^{3/2} e^{-m(\omega_x x^2 + \omega_y y^2 + \omega_z z^2)/\hbar}$. In addition, we can adopt the semiclassical approximation for the normal gas [4], i.e., $n_T(\mathbf{r}) = \lambda_T^{-3} g_{3/2}(e^{-\beta V_{\text{ext}}(\mathbf{r})})$ with $\lambda_T = [2\pi\hbar^2/(mk_B T)]^{1/2}$ being the thermal wavelength. From Eqs. (11) and (30), it is straightforward to obtain the most probable value N_0^p near the critical temperature:

$$\frac{N_0^p}{N} = \frac{1-t^3 - \frac{\zeta(2)}{\zeta(3)} \left[2 - \frac{S}{\zeta(3/2)} \right] \theta t^{7/2} - \frac{3\zeta(2)}{2[\zeta(3)]^{2/3}} \frac{\bar{\omega}}{\omega_{\text{ho}}} t^2 N^{-1/3}}{1 + \frac{\zeta(2)\theta N^{1/2} t^2}{[\zeta(3)]^{1/2} \zeta(3/2)}}, \quad (43)$$

where $S = \sum_{i,j=1}^{\infty} 1/\zeta(3)[ij(i+j)]^{3/2}$. When obtaining Eq. (43), we have introduced a scaling parameter $\theta = gn_T(\mathbf{r} = \mathbf{0}, T_c^0)/k_B T_c^0 = 2.02(a/a_{\text{ho}})N^{1/6}$. θ can also be written in the form of $\theta = 0.65\eta^{5/2}$. By setting $N_0^p = 0$, from Eq. (43) we obtain the shift of the critical temperature:

$$\frac{\delta T_c^0}{T_c^0} = -1.65 \frac{a}{a_{\text{ho}}} N^{1/6} - \frac{\zeta(2)}{2[\zeta(3)]^{2/3}} \frac{\bar{\omega}}{\omega_{\text{ho}}} N^{-1/3}. \quad (44)$$

The first term on the right-hand side of Eq. (44) is the shift due to the interatomic interaction. It agrees with the results based on the local-density approximation [33] obtained by using the grand-canonical ensemble approach. The second term in Eq. (44) gives exactly the usual results due to effects of the finite number of particles [4]. Thus in our approach, within the canonical ensemble the corrections due to the effects of the finite particle number and the interatomic interactions can be obtained simultaneously.

Below the critical temperature, the most probable value is given by

$$\frac{N_0^p}{N} = 1 - t^3 - \frac{\zeta(2)}{\zeta(3)} t^3 \left[\frac{\eta \xi^{2/5}}{t} + 1.49 \frac{\eta t^2}{\xi^{2/5}} F(w) + 0.14 \eta^{5/2} t^{1/2} \right] - \frac{3\bar{\omega}\zeta(2)}{2\omega_{\text{ho}}[\zeta(3)]^{2/3}} t^2 N^{-1/3}, \quad (45)$$

where $w = (\eta \xi^{2/5}/t)^{1/2}$. $F(w)$ is defined by

$$F(w) = 0.53(1 - 0.5e^{-0.23w^3} - 0.5e^{-1.51w^3}). \quad (46)$$

Omitting the high-order terms of the parameter η , the expression (45) gives exactly the lowest-order correction of Eq. (38).

From Eq. (30), we can obtain the probability distribution function of the condensate when the interaction between condensed and noncondensed atoms is considered. Combining with the most probable value, one obtains $\langle N_0 \rangle$ and δN_0 of the interacting Bose gases. In Fig. 4, the experimental parameter by Ensher *et al.* [38] is used to plot $\langle N_0 \rangle/N$ within the canonical ensemble. Our results (solid line) agree well with the conclusion of Ref. [33] (circles) where the semiclassical approximation is used in the frame of the grand-canonical ensemble. We can also obtain the numerical results for δN_0 in the presence of the interaction between condensed and noncondensed atoms. The numerical result of δN_0 is displayed in Fig. 3 with $a/a_{\text{ho}} = 10^{-4}$ (circles) and $a/a_{\text{ho}} = 10^{-3}$ (squares), respectively. Our calculations show that

the repulsive interaction between the condensed and noncondensed atoms lowers the condensate fluctuations further.

V. INTERACTING BOSE GASES BASED ON BOGOLIUBOV THEORY

Condensate fluctuations due to collective excitations have been recently investigated by Giorgini *et al.* [22] within the traditional particle-number-nonconserving Bogoliubov approach. In Ref. [22], the fluctuations from collective excitations are shown to follow the law $\langle \delta^2 N_0 \rangle \sim N^{4/3}$. In this section, the Bogoliubov theory will be developed based on our canonical statistics to discuss the condensate fluctuations originating from collective excitations. According to the Bogoliubov theory [39,40], the total number of particles out of the condensate is given by

$$N_T = \sum_{nl \neq 0} N_{nl} = \sum_{nl \neq 0} (u_{nl}^2 + v_{nl}^2) f_{nl}. \quad (47)$$

The real quantities u_{nl} and v_{nl} satisfy the relations

$$u_{nl}^2 + v_{nl}^2 = \frac{[(\varepsilon_{nl}^B)^2 + g^2 n_0^2]^{1/2}}{2\varepsilon_{nl}^B}, \quad (48)$$

$$u_{nl}v_{nl} = -\frac{gn_0}{2\varepsilon_{nl}^B}, \quad (49)$$

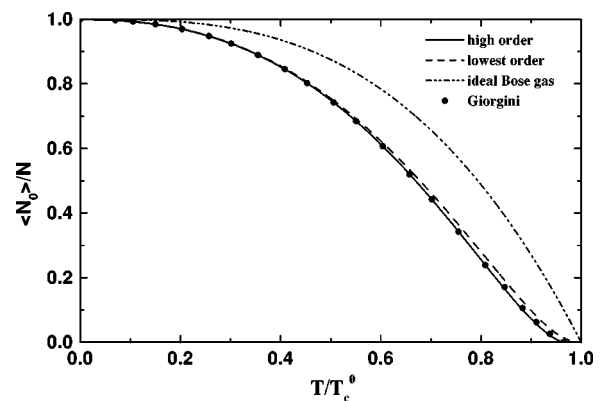


FIG. 4. Displayed is $\langle N_0 \rangle/N$ of the trapped interacting Bose gases with the experimental parameters of Ensher *et al.* [38]. The dashed-dotted line shows $\langle N_0 \rangle/N$ of the ideal Bose gas, while the circles show the result of Giorgini *et al.* [33]. The numerical results of the lowest order and high order $\langle N_0 \rangle/N$ within the canonical ensemble are displayed with dashed and solid lines, respectively.

where f_{nl} is the number of the collective excitations excited in the system at the thermal equilibrium

$$f_{nl} = \frac{1}{\exp[\beta \varepsilon_{nl}^B] - 1}. \quad (50)$$

In addition, the energy of the collective excitations entering Eqs. (48) and (49) is given by the dispersion law [41]

$$\varepsilon_{nl}^B = \hbar \omega_{ho} (2n^2 + 2nl + 3n + l)^{1/2}. \quad (51)$$

These phononlike collective excitations are in excellent agreement with the measurement of experiments. The dispersion law (51) is valid if the conditions $N_0 a / a_{ho} \gg 1$ and $\varepsilon_{nl} \ll \mu$ are satisfied. The contribution to the condensate fluctuations due to these discrete low-energy modes is important because $f_{nl}, u_{nl}^2 + v_{nl}^2, u_{nl}v_{nl} \propto 1/\sqrt{2n^2 + 2nl + 3n + l}$ at low excitation energies.

In Eq. (47), N_{nl} can be regarded as the effective occupation number of noncondensed atoms, while

$$N_{nl}^B = \frac{N_{nl}}{u_{nl}^2 + v_{nl}^2} = f_{nl} \quad (52)$$

is the occupation number of the collective excitations. From the form of f_{nl} , one can construct the partition function of the collective excitations in the frame of the canonical ensemble,

$$Z_B = \sum_{\{N_{nl}\}} \exp\left[-\beta \sum_{nl} N_{nl}^B \varepsilon_{nl}^B\right]. \quad (53)$$

From Eq. (52), Z_B becomes

$$Z_B = \sum_{\{\sum N_{nl} = N\}} \exp\left[-\beta \sum_{nl} N_{nl} \varepsilon_{nl}^{\text{eff}}\right], \quad (54)$$

where $\varepsilon_{nl}^{\text{eff}} = \varepsilon_{nl}^B / (u_{nl}^2 + v_{nl}^2)$ can be taken as an effective energy level of the thermal atoms. In this case, Z_B is the partition function of a fictitious boson system, which is composed of N noninteracting bosons whose energy level is determined by $\varepsilon_{nl}^{\text{eff}}$. From Eq. (54), the most probable value N_0^p is given by

$$N_0^p = N - \sum_{nl \neq 0} \frac{1}{\exp[\beta(\varepsilon_{nl}^{\text{eff}} - \varepsilon_{nl=0}^{\text{eff}})] - 1}. \quad (55)$$

It is obvious that the occupation number of low n, l in Eq. (55) coincides with that of Eq. (47). The other N_0 is determined by

$$N_0 = N - \sum_{nl \neq 0} \frac{1}{\exp[\beta(\varepsilon_{nl}^{\text{eff}} - \varepsilon_{nl=0}^{\text{eff}})] \exp[-\alpha(N, N_0)] - 1}. \quad (56)$$

From Eqs. (55) and (56), we obtain

$$\alpha(N, N_0) \approx - \frac{N_0 - N_0^p}{\sum_{nl \neq 0} (u_{nl}^2 + v_{nl}^2)^2 f_{nl}^2}. \quad (57)$$

When getting Eq. (57), we have used the approximation $f_{nl} \approx k_B T / \varepsilon_{nl}^B$ for low-energy collective excitations. Thus the probability distribution function of the condensate is given by

$$G_B(N, N_0) = A_B \exp\left[-\frac{(N_0 - N_0^p)^2}{2 \sum_{nl \neq 0} (u_{nl}^2 + v_{nl}^2)^2 f_{nl}^2}\right], \quad (58)$$

where A_B is a normalization constant. Therefore, the condensate fluctuations due to the collective excitations read

$$\begin{aligned} \langle \delta^2 N_0 \rangle_{\text{collective}} &= \frac{\sum_{N_0=0}^N N_0^2 G_B(N, N_0)}{\sum_{N_0=0}^N G_B(N, N_0)} \\ &= \left[\frac{\sum_{N_0=0}^N N_0 G_B(N, N_0)}{\sum_{N_0=0}^N G_B(N, N_0)} \right]^2. \end{aligned} \quad (59)$$

Equations (58) and (59) provide the formulas for calculating the condensate fluctuations originating from the collective excitations.

Below the temperature T_m which corresponds to the maximum fluctuations, we obtain the analytical result for the condensate fluctuations,

$$\begin{aligned} \langle \delta^2 N_0 \rangle_{\text{collective}} &= \frac{\pi^2}{12 \zeta(2)} B \left(\frac{m a^2 k_B T_c}{\hbar^2} \right)^{2/5} N^{4/3} \\ &= \frac{1}{2} B \left(\frac{m a^2 k_B T_c}{\hbar^2} \right)^{2/5} N^{4/3}, \end{aligned} \quad (60)$$

where B is a dimensionless parameter, which is the same as that obtained in Ref. [22]. Note that compared with the result obtained by Ref. [22], the coefficient in Eq. (60) differs by a factor $\frac{1}{2}$. The expression (60) shows clearly that the condensate fluctuations due to the collective excitations are anomalous, i.e., proportional to $N^{4/3}$. Note that $G_B(N, N_0)$ is a Gaussian distribution function. The anomalous behavior of the condensate fluctuations comes from the factor $2 \sum_{nl \neq 0} (u_{nl}^2 + v_{nl}^2)^2 f_{nl}^2$, which is proportional to $N^{4/3}$.

At the critical temperature $G_B(T = T_c) = \exp[-N_0^2 / \gamma]$, where $\gamma = 2 \sum_{nl} (u_{nl}^2 + v_{nl}^2)^2 f_{nl}^2$. In this case, we obtain the analytical result of the condensate fluctuations,

$$\langle \delta^2 N_0 \rangle_{T=T_c} = 0.18 \gamma = 0.18 B \left(\frac{m a^2 k_B T_c}{\hbar^2} \right)^{2/5} N^{4/3}. \quad (61)$$

From Eqs. (60) and (61), we find that the behavior of the condensate fluctuations based on the Bogoliubov theory is rather different from that of the lowest-order perturbation theory.

VI. DISCUSSION AND CONCLUSION

In this paper, a canonical ensemble approach has been developed to investigate the mean ground-state occupation number and condensate fluctuations for interacting and non-interacting Bose gases. Different from the conventional methods, the analytical probability distribution function of the condensate has been obtained directly from the partition function of the system. Based on the probability distribution function, we have calculated the thermodynamic properties of the Bose gas, such as the condensate fraction and the fluctuations. Through the calculations of the probability distribution function, we have provided a simple method to recover the applicability of the saddle-point method for studying the condensate fluctuations. In fact, the theory of the improved saddle-point method developed in this work can be applied straightforwardly to consider the condensate fluctuations in other physical systems, such as the interacting Bose gas confined in a box [42], the interacting Bose gas in low dimensions, etc. The probability distribution function can also be used to discuss other interesting problems, such as the phase diffusion of the condensate.

For the harmonically trapped interacting Bose gas, we found that different approximations for weakly interacting Bose gases give quite different theoretical predictions concerning the condensate fluctuations. In our opinion, the lowest-order perturbation theory gives in some sense the condensate fluctuations due to normal thermal atoms, while the Bogoliubov theory gives the condensate fluctuations originating from the collective excitations. The contributions to the condensate fluctuations due to the collective excitations mainly come from the low-energy modes, and it is obvious that the condensate fluctuations based on the lowest-order perturbation theory miss the contributions coming from the collective excitations. Considering the fact that the contributions due to low-energy thermal atoms in the lowest-order perturbation theory are relatively small, the overall condensate fluctuations may be written as

$$\langle \delta^2 N_0 \rangle_{\text{all}} = \langle \delta^2 N_0 \rangle_{\text{int}} + \langle \delta^2 N_0 \rangle_{\text{collective}}, \quad (62)$$

where $\langle \delta^2 N_0 \rangle_{\text{int}}$ and $\langle \delta^2 N_0 \rangle_{\text{collective}}$ are condensate fluctuations due to the normal thermal atoms and the collective excitations, respectively.

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APPENDIX

In this appendix, the method of saddle-point integration described by Darwin and Fowler [28] is used to investigate the partition function of the fictitious $N - N_0$ noninteracting bosons. The partition function of the fictitious system is given by

$$Z_0(N_T) = \sum_{\substack{N_{\mathbf{n}}=N_T \\ \mathbf{n} \neq \mathbf{0}}} \exp \left[-\beta \sum_{\mathbf{n} \neq \mathbf{0}} N_{\mathbf{n}} \varepsilon_{\mathbf{n}} \right], \quad (A1)$$

where $N_T = N - N_0$ is the number of particles out of the condensate.

Because of the restriction $\sum_{\mathbf{n} \neq \mathbf{0}} N_{\mathbf{n}} = N_T$ in the summation of Eq. (A1), $Z_0(N_T)$ cannot be explicitly evaluated. To proceed, we define a generating function for $Z_0(N_T)$ in the following manner. For any complex number z , we take

$$G_0(T, z) = \sum_{N_T=0}^{\infty} z^{N_T} Z_0(N_T). \quad (A2)$$

The generating function can be evaluated easily. The result of $G_0(T, z)$ is given by

$$G_0(T, z) = \prod_{\mathbf{n} \neq \mathbf{0}} \frac{1}{1 - z \exp[-\beta \varepsilon_{\mathbf{n}}]}. \quad (A3)$$

To obtain $Z_0(N_T)$, we note that by definition $Z_0(N_T)$ is the coefficient of z^{N_T} in the expansion of $G_0(T, z)$ in powers of z . Therefore, we have

$$Z_0(N_T) = \frac{1}{2\pi i} \oint dz \frac{G_0(T, z)}{z^{N_T+1}}, \quad (A4)$$

where the contour of integration is a closed path in the complex z plane about $z=0$. Let $g(z)$ be defined by

$$\exp[g(z)] = \frac{G_0(T, z)}{z^{N_T+1}}; \quad (A5)$$

then $Z_0(N_T)$ becomes

$$Z_0(N_T) = \frac{1}{2\pi i} \oint dz \exp[g(z)]. \quad (A6)$$

The saddle point z_0 is determined by

$$\frac{\partial g(z_0)}{\partial z_0} = 0. \quad (A7)$$

From Eq. (A5) we obtain

$$N_T = z_0 \frac{\partial}{\partial z_0} \ln G_0(T, z_0) - 1. \quad (A8)$$

By Eq. (A3), one gets

$$N_T = \sum_{\mathbf{n} \neq \mathbf{0}} \frac{1}{\exp[\beta \varepsilon_{\mathbf{n}}] z_0^{-1} - 1}. \quad (\text{A9})$$

Noting that Eq. (A9) is exactly the equation to determine the number of condensed atoms within the grand-canonical ensemble, the saddle point z_0 can also be regarded as the fugacity of the fictitious $N - N_0$ noninteracting bosons.

Expanding the integrand of Eq. (A6) about $z = z_0$, we have

$$Z_0(N_T) = \frac{1}{2\pi i} \oint dz \exp \left[g(z_0) + \frac{1}{2} (z - z_0)^2 \frac{\partial^2}{\partial z_0^2} g(z_0) + \dots \right], \quad (\text{A10})$$

where

$$\frac{\partial^2}{\partial z_0^2} g(z_0) = \frac{G_0''(T, z_0)}{G_0(T, z_0)} - \frac{N_T^2 - N_T}{z_0^2}. \quad (\text{A11})$$

By setting $z - z_0 = iy$, we obtain

$$Z_0(N_T) \approx \frac{\exp[g(z_0)]}{2\pi} \int_{-\infty}^{\infty} \exp \left[-\frac{1}{2} \frac{\partial^2}{\partial z_0^2} g(z_0) y^2 \right] dy. \quad (\text{A12})$$

Thus we have

$$Z_0(N_T) = \frac{G_0(T, z_0)}{z_0^{N_T+1} [2\pi g''(z_0)]^{1/2}}. \quad (\text{A13})$$

With these results, the free energy $A_0(N, N_0)$ of the fictitious system is then given by

$$A_0(N, N_0) = -k_B T \left\{ \ln G_0(T, z_0) - N_T \ln z_0 - \ln z_0 - \frac{1}{2} \ln [2\pi g''(z_0)] \right\}. \quad (\text{A14})$$

In the case of $N_T \gg 1$, the last two terms in Eq. (A14) can be omitted. Therefore,

$$A_0(N, N_0) = -k_B T [\ln G_0(T, z_0) - N_T \ln z_0]. \quad (\text{A15})$$

From Eq. (A3), we obtain the relation between $A_0(N, N_0)$ and z_0 of the fictitious system:

$$-\beta \frac{\partial}{\partial N_0} A_0(N, N_0) = \ln z_0. \quad (\text{A16})$$

Equations (A9) and (A16) are useful relations used in the text.

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