Condensate fluctuations of interacting Bose gases within a microcanonical ensemble

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Condensate fluctuations of interacting Bose gases within a microcanonical ensemble

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Abstract

Based on counting statistics and Bogoliubov theory, we present a recurse relation for the microcanonical partition function for a weakly interacting Bose gas with a finite number of particles in a cubic box. According to this microcanonical partition function, we calculate numerically the distribution function, condensate fraction and condensate fluctuations for a finite and isolated Bose-Einstein condensate. For the ideal and weakly interacting Bose gases, we compare the condensate fluctuations with those in the canonical ensemble. The present approach yields an accurate account of the condensate fluctuations for temperatures close to the critical region. We emphasize that the interactions between excited atoms turn out to be important for moderate temperatures.

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I. INTRODUCTION

The enormous experimental progress in the manipulation of Bose-Einstein condensates (BECs) [1] has stimulated a great interest in the physics of the ultracold gases and also brought up some problems which still await final solutions. Among others, the issue of statistical properties of the finite systems has been a subject of intensive theoretical studies [2–4] since in the experiment the total number of the particles is roughly fixed and finite. However, the standard textbook approach based on the grandcanonical ensemble, where the energy and the particle number are fixed on average, may not be able to approximate well the experimental situations. Particularly, the grand canonical ensemble predicts the unphysically large condensate fluctuations. Hence, one must resort to the microcanonical and canonical ensembles which are free of these flaws.

Statistical properties [5–10] and, in particular, condensate fluctuations have been investigated for ideal and weakly interacting Bose gases (WIBGs), both within the canonical [11–21] and microcanonical [11, 18, 19, 21–24] ensembles, where the differences between ideal Bose gases (IBGs) in the canonical and microcanonical ensembles have also been explored [11, 24]. Specific experimental conditions determine which statistics should be used to study a particular system. Magnetic or optical confinement in the BEC experiments [25, 26] suggests that the system is thermally isolated and thus the microcanonical ensemble description of the trapped condensate is needed [15]. For a WIBG in a microcanonical ensemble, several useful papers have been published dealing with some limiting cases [18, 19, 21], but to our best knowledge, so far there has been no microcanonical approach based on the recursive scheme to treat this problem valid for temperatures close to the critical region. In particular, the problem of fluctuations in the interacting gas is more complex and less clear than in the case of the IBG. Under such a circumstance, the issue of the fluctuations as well as the thermodynamics for the WIBGs requires a more refined approach.

In the present paper, we develop a recursive scheme by using counting statistics and Bogoliubov approximation. This recurrence algorithm, as an enhanced version of the earlier ones applied to the IBG [24] in the microcanonical ensemble and the WIBG in the canonical ensemble [27], gives an accurate description of fluctuations and thermodynamics in the WIBGs at finite temperatures. Based on Hartree-Fock approximation, we include the interactions between out of condensate atoms to study the fluctuations for temperatures close to the critical region, since the Bogoliubov approximation is valid only for temperatures out of the critical region. Using this recurrence relation, we calculate numerically the partition function, the condensate fraction, and the condensate fluctuations, and compare the microcanonical fluctuations with the canonical ones. We show that the particle-number constraint and the interactions between out of condensate atoms are of importance for moderate temperatures.

The paper is organized as follows. In the framework of counting statistics and Bogoliubov theory, in Sec. II we derive the recurrence relation for the microcanonical partition function in the WIBGs, where interactions between excited atoms and particle-number constraint are considered. In Sec. III we present the numerical analysis of the distribution function, the condensation fraction, and the condensate fluctuations. Conclusions are made in Sec. IV.

II. MICROCANONICAL PARTITION FUNCTION AND PHYSICAL QUANTITIES

In the statistical physics the partition function entirely specifies the statistical properties, so our first priority is to determine the partition function in the microcanonical ensemble. A system can be divided into two parts: N_e particles occupying excited levels with the energy E_e, and $N_0 = N - N_e$ particles in the ground state. In the microcanonical ensemble, the partition function of N bosons with total energy E is given by

$$\Omega(N,E) = \sum_{N_e=0}^{N} \Omega_e(N_e,E_e)\Omega_0(N_0,E_0), \tag{1}$$

where the total energy $E = E_0 + E_e$ and total particle number $N = N_0 + N_e$. Here the partition function Ω_e depends on the condensed number of particles N_0 because of $N = N_0 + N_e$. For a WIBG in a cubic box with periodic boundary conditions, the energy of the condensate subsystem $E_0 = N_0\epsilon_0 = 0$ since $\epsilon_0 = 0$. In addition, the partition function $\Omega_0(N - N_e, 0) = 1$. Consequently, the formula (1) becomes

$$\Omega(N,E) = \sum_{N_e=0}^{N} \Omega_e(N_e,E_e). \tag{2}$$

According to Bogoliubov approximation [28], the boson operator $\hat{a}_{\mathbf{k}}$ can be written in terms of the quasiparticle creation $\hat{b}^+_{\mathbf{k}}$ and annihilation $\hat{b}_{\mathbf{k}}$ operators as $\hat{a}_{\mathbf{k}} = u_{\mathbf{k}}\hat{b}_{\mathbf{k}} + v_{\mathbf{k}}\hat{b}^+_{-\mathbf{k}}$.

The Hamiltonian can thus be approximated by [17]

$$\hat{H} = \hat{H}_B + E_{ex}(N, N_0) = \sum_{\mathbf{k}\neq 0} \epsilon_{\mathbf{k}} \hat{b}^{+}_{\mathbf{k}} \hat{b}_{\mathbf{k}} + E_{ex}(N, N_0), \tag{3}$$

where $\epsilon_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} + gn_0)^2 - (gn_0)^2} = \varepsilon_{\mathbf{k}}\sqrt{1 + 2gn_0/\varepsilon_{\mathbf{k}}}$ is the celebrated Bogoliubov energy spectrum. $E_{ex}(N, N_0)$ is the interaction energy between the excited atoms, which can be determined by the Hartree-Fock approximation: $E_{ex} = \frac{g}{2V} N_e^2$ [17, 29] with $V = L^3$ being the volume and $g = 4\pi\hbar^2 a/m$ being the coupling constant fixed by the s-wave scattering length a. Here $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$, m is the atomic mass. $n_0 = N_0/L^3$ and $n = N/L^3$ denote the ground-state and total particle densities, respectively. Bogoliubov amplitudes satisfy the relations: $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = (\varepsilon_{\mathbf{k}} + gn_0)/\epsilon_{\mathbf{k}}$ and $u_{\mathbf{k}} v_{\mathbf{k}} = gn_0/2\epsilon_{\mathbf{k}}$, i.e., the normalization condition $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$. Note that Bogoliubov amplitudes $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are functions of the condensed particle number N_0, respectively. In the case of a three-dimensional box with periodic boundary conditions, we note that $\mathbf{k} = 2\pi\mathbf{j}/L$ with $\mathbf{j} = \{j_x, j_y, j_z\}$ being integers, and the energy spectrum

$$\epsilon_{\mathbf{j}} = \epsilon_1 \sqrt{[\mathbf{j}^2 + 2N_0 a n^{1/3}/(LN^{1/3}\pi)]^2 - [2N_0 a N^{1/3}/(LN^{1/3}\pi)]}, \tag{4}$$

or

$$\epsilon_{\mathbf{j}} = \epsilon_1 |\mathbf{j}| \sqrt{\mathbf{j}^2 + 4N_0 a n^{1/3}/(N^{1/3}\pi)}, \tag{5}$$

where $\epsilon_1 = \frac{2\pi^2\hbar^2}{mL^2}$ is the energy gap between the ground state and the first excited state in the box. It is clear that the energy spectrum of the weakly interacting gas depends on the actual number of condensed atoms N_0 and the gas parameter $an^{1/3}$: $\epsilon_{\mathbf{j}} = \epsilon_{\mathbf{j}}(N_0, an^{1/3})$. For repulsive interaction, as discussed throughout this work, the scattering length $a > 0$, and thus the criterion for weak interaction reads $an^{1/3} \ll 1$.

The total number of the excited particles given by the expectation value of the operator $\hat{N}_e = \sum_{\mathbf{k}>\mathbf{0}} \hat{a}^{+}_{\mathbf{k}} \hat{a}_{\mathbf{k}}$ takes the form

$$\langle N_e \rangle = \sum_{\mathbf{j}>\mathbf{0}} [n_{\mathbf{j}}(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2) + v_{\mathbf{j}}^2], \tag{6}$$

where $n_{\mathbf{j}} = \langle \hat{b}^{+}_{\mathbf{j}} \hat{b}_{\mathbf{j}} \rangle$ is the number of elementary excitations in the state $\mathbf{j}$. Here the actual number N_e of the excited particles differs from the total number of excitations due to the Bogoliubov transformation. And the energy of a given configuration of excitations in various $\{n_{\mathbf{j}}\}$ is given by

$$E_e(N_e) = \sum_{\mathbf{j}\neq 0} n_{\mathbf{j}} \epsilon_{\mathbf{j}} + E_{ex}(N_e), \tag{7}$$

where the energy spectrum $\epsilon_{\mathbf{j}}$, given by Eq. (5), depends on the number of the condensed atoms N_0 (or the number of the excited atoms N_e): $\epsilon_{\mathbf{j}} = \epsilon_{\mathbf{j}}(N_0)$ [or $\epsilon_{\mathbf{j}} = \epsilon_{\mathbf{j}}(N_e)$]. So the total energy E_e of the excited subsystem depends on the actual number N_e of the exited atoms: $E_e = E_e(N_e)$. In order to enforce the constraint on the total particle number rigorously, in Eq. (3) we write the energy spectrum as a function of the actual number of condensed particles. That is, when including the interaction between out of the excited atoms, we use the energy spectrum in which $\epsilon_{\mathbf{j}} = \epsilon_{\mathbf{j}}(N_0)$ [17].

In the microcanonical ensemble the system is assumed to be found with equal probability $1/\Omega$ in any microstate. The microstates are nothing but the configurations of occupation numbers, $\{n\} = \{n_0, n_1, \cdots\}$. The microcanonical partition function reads:

$$\Omega_e(N_e, E_e) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \sum_{n_\infty=0}^{\infty} \delta_{\langle \hat{H} \rangle, E_e} \delta_{N_e, \langle N_e \rangle}, \tag{8}$$

which cannot be explicitly evaluated because of the restrictions $\delta_{\langle \hat{H} \rangle, E_e}$ and $\delta_{\langle N_e \rangle, N_e}$. The actual number of condensate atoms, N_0, affects the partition function Ω_e since $N_e = N - N_0$ within the canonical ensemble. To proceed, we shall use the counting statistics to establish a recursive scheme, that allows to determine the microcanonical partition function numerically.

Analogously to the case of an IBG [24], in the excited subsystem of a WBG we now turn to the quasiparticle counting statistics. Let $P_{\mathbf{j}}[n|N_e, E_e(N_e)]$ be the probability to find n quasiparticles out of a total of N_e excited particles occupying the $\mathbf{j}$'th ($\mathbf{j} > \mathbf{0}$) state. This quantity can be represented by $P_{\mathbf{j}}[n|N_e, E_e(N_e)] = P_{\mathbf{j}}^{\geq}[n|N_e, E_e(N_e)] - P_{\mathbf{j}}^{\geq}[n+1|N, E_e(N_e)]$, where $P_{\mathbf{j}}^{\geq}[n|N_e, E_e(N_e)]$ is the probability to find at least n quasiparticles in the state $\mathbf{j}$. The computation of $P_{\mathbf{j}}^{\geq}[n|N_e, E_e(N_e)]$ involves summations given in Eq. (8), but the sum over $n_{\mathbf{j}}$ starts at $n_{\mathbf{j}} = n$ rather than at $n_{\mathbf{j}} = 0$. This leads to

$$\begin{aligned} P_{\mathbf{j}}^{\geq}[n|N_e, E_e(N_e)] &= \frac{1}{\Omega_e[N_e, E_e(N_e)]} \sum_{n_1=0}^{\infty} \cdots \sum_{n_{\mathbf{j}}=n}^{\infty} \cdots \sum_{n_\infty=0}^{\infty} \delta_{\langle \hat{H} \rangle, E_e(N_e)} \delta_{\langle N_e \rangle, N_e} \\ &= \frac{1}{\Omega_e[N_e, E_e(N_e)]} \sum_{n_1=0}^{\infty} \cdots \sum_{n'_{\mathbf{j}}=0}^{\infty} \cdots \sum_{n_\infty=0}^{\infty} \delta_{\langle \hat{H} \rangle, E'_e(N'_e)} \delta_{\langle N'_e \rangle, N'_e}. \end{aligned} \tag{9}$$

where $N'_e = N_e - n(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2)$ and $E_e(N'_e) = \sum_{\mathbf{j} \neq 0} n_{\mathbf{j}} \epsilon_{\mathbf{j}} - n\epsilon_{\mathbf{j}} + g[N_e - n(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2)]^2/2V$. It is noted that the right hand side of Eq. (9) stands for the microcanonical partition function for system of N'_e excited atoms which share the total energy $E_e(N'_e)$. That is, the probability function $P^{\geq}_{\mathbf{j}}[n|N_e, E_e(N_e)]$ has the form

$$P^{\geq}_{\mathbf{j}}[n|N_e, E_e(N_e)] = \frac{1}{\Omega_e[N_e, E_e(N_e)]}\Omega_e[N_e - n(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2), E_e(N'_e)]. \tag{10}$$

Thus, we find

$$P_{\mathbf{j}}[n|N_e, E_e(N_e)] = \frac{\Omega_e[N_e - n(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2), E_e(N'_e)]}{\Omega_e[N_e, E_e(N_e)]} - \frac{\Omega_e[N_e - (n+1)(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2), [N_e, E_e(N''_e)]}{\Omega_e[N_e, E_e(N_e)]}, \tag{11}$$

where N'_e and $E_e(N'_e)$ were defined in Eq. (9), $N''_e = N_e - (n+1)(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2)$, and $E_e(N''_e) = \sum_{\mathbf{j}\neq 0} n_{\mathbf{j}}\epsilon_{\mathbf{j}} - (n+1)\epsilon_{\mathbf{j}} + g[N_e - (n+1)(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2)]^2/2V$. The mean occupation of quasiparticle excitations in mode $\mathbf{j}$ when the system is composed of N_e excited atoms and N_0 condensed atoms can be expressed as:

$$\langle n_{\mathbf{j}}\rangle_{N_0}^{N_e} = \sum_{n=0}^{N_e} n P_{\mathbf{j}}[n|N_e, E_e(N_e)]. \tag{12}$$

Substituting Eq. (11) into Eq. (12), we can readily obtain

$$\langle n_{\mathbf{j}}\rangle_{N_0}^{N_e} = \frac{1}{\Omega_e[N_e, E_e(N_e)]}\sum_{n=1}^{N_e}\Omega_e[N_e - n(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2), E_e(N'_e)]. \tag{13}$$

This is just the number of elementary excitation $n_{\mathbf{j}}$ in Eq. (6). Combining Eqs. (13) and (6), we get the recurrence relation for the microcanonical partition function:

$$\Omega_e[N_e, E_e(N_e)] = \frac{1}{N_e - \sum_{\mathbf{j}\neq\mathbf{0}} v_{\mathbf{j}}^2}\sum_{\mathbf{j}\neq\mathbf{0}}\sum_{n=1}^{N_e}(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2)\Omega_e[N_e - n(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2), E_e(N'_e)], \tag{14}$$

where we have taken $N_e = \langle N_e\rangle$. This recurrence algorithm is one of main results in this work. In principle, substituting Eq. (14) into Eq. (2), we can analyze numerically the thermodynamic properties of the WIBGs at finite temperatures.

From the mathematical point of view, similar to the case of the canonical ensemble [17, 27], the calculations must be performed within the approximation that $\Omega_e[N_e, E_e(N_e)] = \frac{1}{N_e - \sum_{\mathbf{j}\neq\mathbf{0}} v_{\mathbf{j}}^2}\sum_{n=1}^{N_e}\sum_{\mathbf{j}\neq\mathbf{0}}(u_{\mathbf{j}}^2 + v_{\mathbf{j}}^2)\Omega_e[N_e - n, E_e(N'_e)]$, where $E_e(N'_e)$ was defined in Eq. (9). Physically, the actual numbers of excited atoms become integers in the partition functions $\Omega_e[N_e - n, E_e(N'_e)]$ given by the simple formula. Like in the recurrence alogrithm of the IBG [24], here the initial conditions $\Omega_e(N_e \geq 0, 0) = 1$ and $\Omega_e(0, E_e > 0) = 0$ have to be used so as to the iterative procedure can proceed. For finite energy E_e the sum over $\mathbf{j}$ is finite since $\Omega_e(N_e, E_e < 0) \equiv 0$.

The recurrence algorithm is an enhanced version of the earlier one applied to the IBG case where $u_{\mathbf{j}} = 1$ and $v_{\mathbf{j}} = 0$. Unlike in the WIBG case where $E_e = E_e(N_e)$, the energy E_e of the subsystem and the particle number N_e are two independent control parameters for an IBG. In this special case, Eq. (14) simplifies to $\Omega_e(N_e, E_e) = \frac{1}{N_e}\sum_{n=1}^{N}\sum_{\mathbf{j}>\mathbf{0}}\Omega_e(N_e - n, E_e - n\epsilon_{\mathbf{j}})$ with $\Omega_e(0,0) = 1$. We obtain finally the partition function (2), which is equal exactly to the recurrence relation $\Omega(N, E) = \frac{1}{N}\sum_{n=1}^{N}\sum_{\mathbf{j}=\mathbf{0}}\Omega(N - n, E - n\epsilon_{\mathbf{j}})$ derived directly from the IBG case. Similarly to the case of the WIBGs within a canonical statistics [27, 30], here we have to separate the ground sate from the excited state since $N_e \neq \sum_{\mathbf{j}\neq 0} n_{\mathbf{j}}$ in the WIBG case.

Eqs. (2) and (14) yield the expression for the condensate distribution function

$$P_0(N_0) = \frac{\Omega_e[N - N_0, E_e(N_e)]}{\Omega(N, E)}. \tag{15}$$

This is just the probability to find N_0 condensate atoms for the system of N atoms. The mean number of the atoms in the ground state is given by

$$\langle N_0 \rangle = \sum_{N_0=0}^{N} N_0 P_0(N_0). \tag{16}$$

To express our result in terms of temperature, we determine the microcanonical temperature T according to the thermodynamical relation

$$\frac{1}{T} = \frac{\partial S(N, E)}{\partial E}, \tag{17}$$

where the entropy $S(N, E) = k_B \ln \Omega(N, E)$ with k_B being Boltzmann constant.

In the microcanonical ensemble, since the total number of the particles is conserved, $\langle N \rangle = N = N_e + N_0$, the fluctuations of condensed and excited atoms are equal, $\langle \delta^2 N_0 \rangle = \langle \delta^2 N_e \rangle$. The fluctuations are divided into two parts [21]: $\langle \delta^2 N_e \rangle = \langle \delta^2 N_e \rangle_T + \langle \delta^2 N_e \rangle_Q$. The thermal fluctuations are given by

$$\begin{aligned}\langle \delta^2 N_e \rangle_T &= \sum_{\mathbf{k},\mathbf{q}\neq 0} [(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)(u_{\mathbf{q}}^2 + v_{\mathbf{q}}^2)(\langle \hat{n}_{\mathbf{k}} \hat{n}_{\mathbf{q}} \rangle - \langle \hat{n}_{\mathbf{k}} \rangle \langle \hat{n}_{\mathbf{q}} \rangle) \\ &= \sum_{N_0=0}^{N} {N_0}^2 P_0(N_0) - \langle N_0 \rangle^2. \end{aligned} \tag{18}$$

The quantum fluctuations are written as

$$\langle \delta^2 N_e \rangle_Q = 4 \sum_{\mathbf{k}\neq 0} u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 (\langle \hat{n}_{\mathbf{k}} \hat{n}_{-\mathbf{k}} \rangle + \langle \hat{n}_{\mathbf{k}} \rangle + \frac{1}{2}), \tag{19}$$

which would not vanish even at $T = 0$ in the WIBGs. The average of an arbitrary operator $\hat{f}$ in Eqs. (18) and (19) can be given by $\langle \hat{f} \rangle = \sum_{N_0=0}^{N} \langle \hat{f} \rangle_{N_0}^{N_e} P_0(N_0)$, in which the mean occupation $\langle \hat{n}_{\mathbf{k}} \rangle$ is given by Eq. (13), and the correlation with the opposite momenta is $(\langle \hat{n}_{\mathbf{k}} \hat{n}_{-\mathbf{k}} \rangle)_{N_0}^{N_e} = \frac{1}{\Omega_e(N_e,\ E_e)} \sum_{n_{\mathbf{l}}, n_{\mathbf{j}} \neq 0} \Omega_e\{N_e - (n_{\mathbf{l}} + n_{\mathbf{j}})(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2),\ E_e[N_e - (n_{\mathbf{l}} + n_{\mathbf{j}})(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)]\}$, with $E_e[N_e - (n_{\mathbf{l}} + n_{\mathbf{j}})(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)] = \sum_{\mathbf{k} \neq 0} n_{\mathbf{k}} \epsilon_{\mathbf{k}} - (n_{\mathbf{l}} + n_{\mathbf{j}}) \epsilon_{\mathbf{k}} + g[N_e - (n_{\mathbf{l}} + n_{\mathbf{j}})(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)]^2/2V$. Eqs. (14) and (15) together with (18) and (19) provide the complete statistical information for the WIBG at finite temperatures.

III. NUMERICAL ANALYSIS

In principle, with the knowledge of the microcanonical partition function we can study all statistical properties of the system in a standard way. The recursive scheme derived above can be applied to calculation of the statistical properties for the weakly interacting systems at finite temperatures. The physical quantities, such as the mean condensate population and the condensate fluctuations, should be dependent on the interaction strength since the explicit form of the recurrence relation for the partition function depends on the gas parameter $an^{1/3}$.

When neglecting the interactions between out of condensate atoms, we can use the rigorous spectrum (Bogoliubov energy spectrum) approximation: $\epsilon_{\mathbf{k}}(N_0)$, where N_0 is the actual condensed particle number and is current. Although in this approximation the total particle number is conserved, configurations of the excitation correspond to different number of excited atoms and thus may lead to different excitation spectrum. Moreover, the Bogoliubov approximation with the rigorous energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ as a mean field theory is valid only for the well-formed condensate when fluctuations are much less than the order parameter, i.e., $\langle \delta N_0 \rangle \ll \langle N_0 \rangle$. In other words, it holds only for low temperatures, compared to the transition temperature. Therefore, instead of the rigorous energy spectrum $\epsilon_{\mathbf{k}}(N_0)$, we take the common average approximation (Bogoliubov-Popov energy spectrum): $\epsilon_{\mathbf{k}}(N_0) = \epsilon_{\mathbf{k}}(\langle N_0 \rangle)$, with $\langle N_0 \rangle$ being determined from self-consistency equation $\langle N_0 \rangle = \sum_{N_0=0}^{N} N_0 P_0(N_0)$ [13, 14, 17]. In the grand canonical ensemble where the total particle number and the total energy are fluctuate, the Popov-approximation is well established for the analysis of the finite-temperature properties of the WIBGs and is not valid only in a very small interval near T_c, given by $T_c - T < an^{1/3} T_c \ll T_c$ [13, 31]. The method using

Bogoliubov-Popov spectrum $\epsilon_{\mathbf{k}}(\langle N_0 \rangle)$ holds in the microcanonical ensemble except too near and, of course, above the transition point [13]. In such a case we obtain the formulas for the partition function $\Omega(N,E) = \sum_{N_0=0}^{N} \Omega_e[N-N_0, E_e(\langle N_0 \rangle)]$ and the distribution function $P_0(N_0) = \frac{\Omega_e[N-N_0, E_e(\langle N_0 \rangle)]}{\Omega(N,E)}$. In order to apply the recurrence relation to calculation of the weakly interacting Bose gas close to the critical region, we take into account of the interactions between out of condensed atoms . In such a approach, to ensure the conservation of the number of atoms, we keep only the Hartree-Fock contribution to interactions between quasi-particles and use the energy spectrum dependent on the actual number of the condensed atoms [17].

In what follows, we will adopt the three energy spectrum approximations as follows [17]: (i) rigorous energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ without E_{ex} term; (ii) energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ with inclusion of E_{ex} term; (iii) average spectrum $\epsilon_{\mathbf{k}}(\langle N_0 \rangle)$ without E_{ex} term. We first calculate the distribution function $NP_0(N_0)$, then plot the condensate fraction $\langle N_0 \rangle / N$, and at the end of this section study the root-mean-square condensate fluctuations $\langle \delta N_0 \rangle$.

A. Distribution function $P_0(N_0)$

Now we use our method to calculate the distribution functions for a WIBG in a box with periodic boundary conditions. In Fig. 1 we plot the distribution function $P_0(N_0)$ multiplied by N as a function of N_0 for the total particle number of $N = 100$ at the temperature $T/T_c^0 = 0.85$ in the three energy spectrum approximations. $T_c^0 = 2\pi\hbar^2 n^{2/3}/k_B m[\zeta(3/2)]^{2/3}$ is the ideal-gas thermodynamic critical temperature in a box for fixed particle density n. The distribution functions $P_0(N_0)$, which determine the thermal fluctuations and mean condensate fraction, calculated with the rigorous spectrum without E_{ex} term merge with those obtained by average spectrum without E_{ex} term. However, the distribution functions $P_0(N_0)$ obtained in the model with rigorous and average spectrum without E_{ex} term differ substantially from the results obtained in the model assuming Bogoliubov Hamiltonian H_B with inclusion of interactions between excited atoms. Comparison between the ideal and weakly interacting gases in Fig. 1 reveals that the interactions between atoms increase the distribution function significantly and essentially sharpen the peak at the intermediate temperatures, and that the interactions lead to an increase in the value of N_0 corresponding to the maximum of the distribution function $P_0(N_0)$. This suggests that the condensation

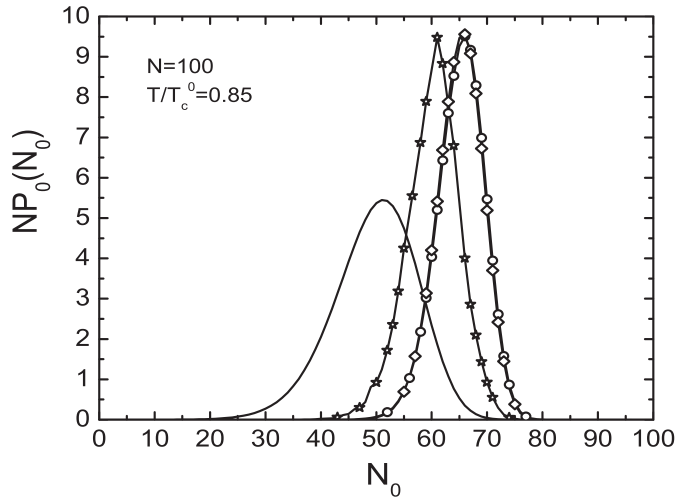

FIG. 1: Distribution function multiplied by N, $NP_0(N_0)$, versus condensate particle number N_0 for a WIBG with $N = 100$ and $an^{1/3} = 0.1$, described by the rigorous (circles) $\epsilon_{\mathbf{k}}(N_0)$ and average Bogoliubov-Popov $\epsilon_{\mathbf{k}}(\langle N_0 \rangle)$ spectrum without E_{ex} term (diamonds). Solid line represents the distribution function of an IBG, while starts correspond to the results for the model assuming the energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ with E_{ex} term.

of the particles at intermediate temperatures should occur more easily in the WIBGs than in the IBGs. This suggestion will be verified in the next subsection where the condensation fraction is discussed.

B. Condensate fraction $\langle N_0 \rangle / N$

Figure 2 depicts the condensate fraction $\langle N_0 \rangle / N$ for an ideal ($an^{1/3} = 0$, solid line) and weakly interacting ($an^{1/3} = 0.05$, solid lines with symbols) Bose gas of $N = 200$ particles in a box with periodic boundary conditions. When the interactions between out of condensate atoms are neglected, the mean condensate population $\langle N_0 \rangle$ obtained from the rigorous spectrum is in agreement with that obtained from the average energy spectrum. Fig. 2 shows that the interactions between out of condensate atoms turn out to be of significance in the regime near the critical region. We can see from Fig. 2 that the repulsive inter-particle interaction stimulates BEC, and yields an increase in the mean condensate occupation $\langle N_0 \rangle$ at intermediate temperatures, as compared to the ideal gas. This result, which has been obtained by different ways [13, 14, 27] within the canonical ensemble, occurs for the attraction

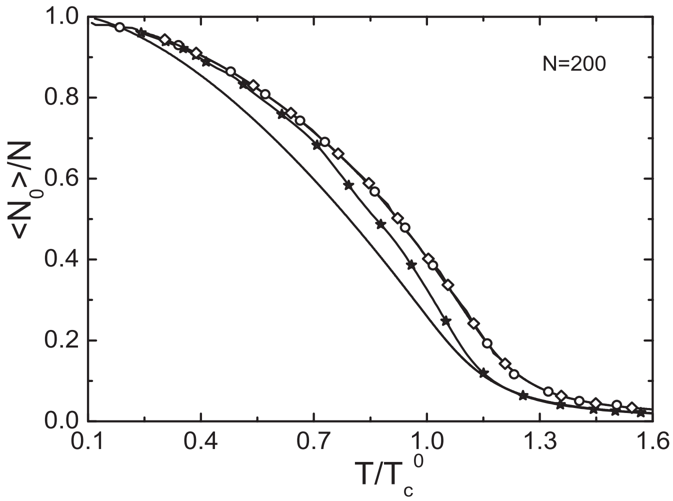

FIG. 2: Condensate fraction $\langle N_0 \rangle / N$ versus normalized temperature T/T_c^0 for a WIBG with $N = 200$ and $an^{1/3} = 0.05$, described by the rigorous (circles) $\epsilon_{\mathbf{k}}(N_0)$ and average $\epsilon_{\mathbf{k}}(\langle N_0 \rangle)$ Bogoliubov-Popov spectrum (diamonds). Solid line represents the condensate fraction of an IBG, while starts correspond to the results for the model assuming the energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ with E_{ex} term. $T_c^0 = 2\pi\hbar^2 n^{2/3}/k_B m[\zeta(3/2)]^{2/3}$ is the ideal-gas thermodynamic critical temperature in a box.

in momentum space and energetic reasons [32].

We would like to point out that in Fig. 2 (as well as in the following figures) the numerical results determined from the microcanonical ensemble are missing at very low temperatures, which arises from the large uncertainty in the determination of the microcanonical temperature at low energies of the system. Unlike in the IBG case where all particles occupy the ground state at $T = 0$, as follows from Eq. (6), the mean number $\langle N_e \rangle$ of the excited atoms would not vanish even at $T = 0$.

C. Root-mean-square condensate fluctuations $\langle \delta N_0 \rangle$

We are now in a position to calculate the condensate fluctuations in the microcanonical ensemble. In Fig. 3 we plot the average condensate fluctuations as a function of temperature for (a) $N = 100$ and (b) $N = 200$ with $an^{1/3} = 0, 0.1$. Noteworthy, the effect of the weak interaction between atoms on the condensate fluctuations is of great significance for the system with small N. The condensate fluctuations plotted in Fig. 3 shows the following novel features:

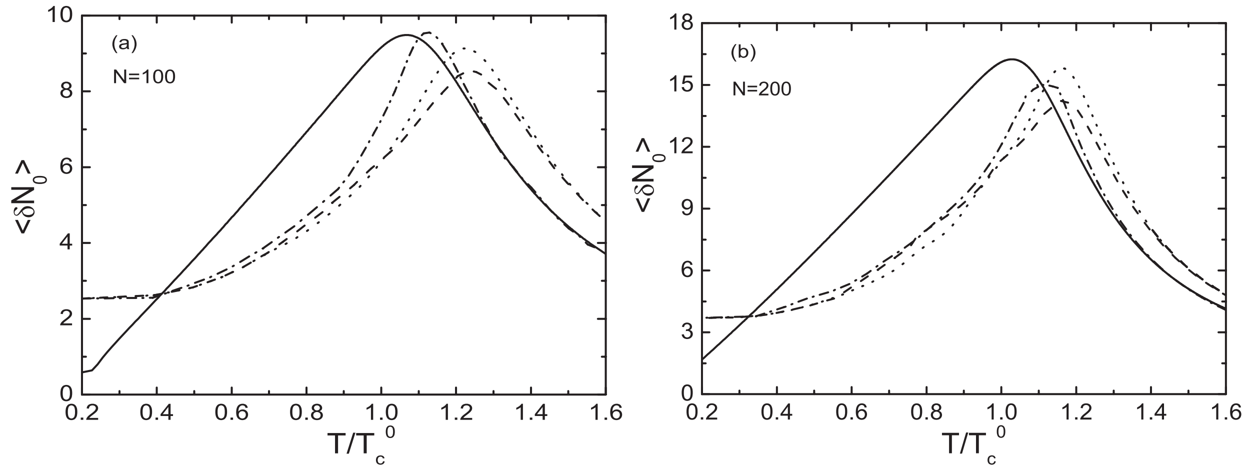

FIG. 3: Root-mean-square condensate fluctuations $\langle \delta N_0 \rangle$ versus normalized temperatures T/T_c^0 for a WIBG of (a) $N = 100$ and (b) $N = 200$ with $an^{1/3} = 0.1$, obtained from Bogoliubov spectrum $\epsilon_{\mathbf{k}}(N_0)$ with (dot-dashed line) and without (dotted line) energy E_{ex} of interactions between excited atoms. Solid lines represent the calculations of an IBG, while dashed lines correspond to the results based on the average spectrum approximation $\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}}(\langle N_0 \rangle)$ without inclusion of E_{ex}.

(i). For interacting particles, the above energy approximations yield slight different condensate fluctuations for temperatures much lower than the critical region. However, below the transition temperature the dependence of $\langle \delta N_0 \rangle$ on T/T_c^0 is even qualitatively different from the non-interacting limit. This agrees well with the results obtained in different approaches [14, 15, 17, 21].

(ii). Both Figs. 2 and 3 show that for the low enough temperatures ($T < 0.8T_c$), all curves nearly merge to the same curve. As expected, the difference among the three approaches is very slight at low temperatures. For the small particle number $N = 100$, at temperatures near the critical region, the result obtained by the Bogoliubov Hamiltonian H_B with energy of interactions between thermal atoms differs substantially from the corresponding that obtained in the model with average spectrum. However, when the particle number N is up to 200, the differences between the energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ with energy of interactions E_{ex} and the average spectrum $\epsilon_{\mathbf{k}}(\langle N_0 \rangle)$ is small even at temperatures near the critical point, which is similar to result obtained in the canonical ensemble [17].

(iii). The microcanonical fluctuations are smaller in the WIBG than in the IBG at moderate temperatures. This happens because the fluctuations are suppressed by the pairs of strongly coupled modes in the WIBG [13, 15].

(iv). Near the critical regions, the condensate fluctuations are smaller in the energy spectrum approximation with E_{ex} term than in the average energy approximation. For the dilute Bose gas, the Bogoliubov approximation with rigorous energy spectrum and the Bogoliubov-Popov approximation with average energy spectrum are invalid in the critical region, but the critical point lacks a unique definition for the smooth phase transition. This implies that the improved calculations are reasonable in this temperature region, if one takes into account the conservations of the particle number and total energy and includes the interactions between out of condensate atoms.

(v). The interactions essentially enhance the condensate fluctuations at very low temperatures. Physically, this behavior follows from the fact that the excited atoms are forced by the interactions to occupy the excited levels at very low temperatures (even at $T = 0$), so that $N_0(T = 0) < N$, as pointed out in Sec.III B.

(vi). The peak position and the width of the distribution function $P_0(N_0)$ determine the values of $\langle N_0 \rangle$ and $\langle \delta N_0 \rangle$, respectively [17]. Fig. 2 shows that, in the approach based on the energy spectrum $\epsilon_{\mathbf{k}}(N_0)$ with E_{ex} term, the temperature corresponding to the peak of $P_0(N_0)$ is shifted toward lower values (compared to the other two approaches), although it increases because of weak interaction between atoms (compared to the ideal Bose gas case). Therefore, this approach predicts an increase in the mean number of condensed atoms at moderate temperatures, but does not indicate the increase of the transition temperature on the level of the mean number of condensed atoms (See Fig. 2). However, in this approach the transition temperature on the level of condensate fluctuations, which is determined by the width of $P_0(N_0)$ and quantum fluctuations given by Eq. (19), is predicted to increase because of interaction between atoms (See Figs. 3 and 4).

It is interning to study whether or not the differences between the canonical and microcanonical fluctuations will hold in the WIBGs. Fig. 4 shows the root-mean-square fluctuations in the canonical and microcanonical ensembles, respectively, as functions of the temperature for an ideal ($an^{1/3} = 0$) and weakly interacting ($an^{1/3} = 0.1$) gas. It can been seen from Fig. 4 that the microcanonical fluctuations are smaller than the canonical ones [14] both in IBGs and WIBGs, as expected. Again, Fig. 4 show that, both within microcanonical and canonical ensembles the transition temperature $T_c(N)$ which can be defined by the position of the peak of the fluctuations [17] increases because of the effects of interactions between atoms. We would like to point out that, for Bogoliubov-Popov approximation with

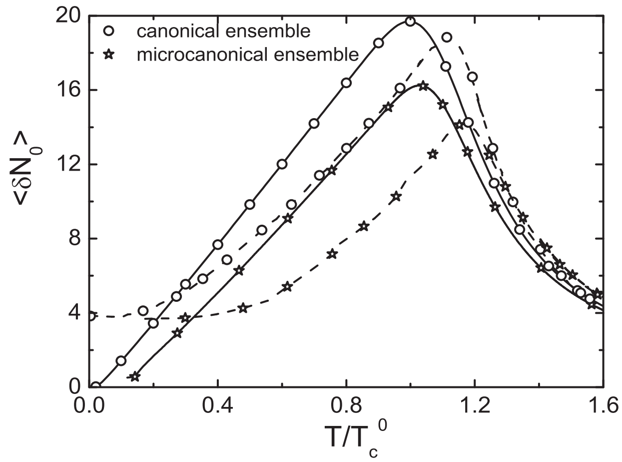

FIG. 4: Root-mean-square condensate fluctuations $\langle \delta N_0 \rangle$ versus normalized temperatures T/T_c^0 for an ideal ($an^{1/3} = 0$, solid lines) and weakly interacting ($an^{1/3} = 0.1$, dashed lines) Bose gas of $N = 200$ particles in a cubic box. The circles and starts represent the canonical and microcanonical fluctuations [14], respectively.

average energy spectrum, we are not sure of the physical significance near the critical region shown in Figs. 2, 3 and 4, since the Bogoliubov-Popov energy spectrum is questionable when temperatures are so close to the critical value. However, the ultimate verification can be done in experiments. Noteworthy, although the fluctuations at very low temperatures cannot be determined because of large numerical errors, for the IBGs the microcanonical fluctuations would vanish for zero temperature since all N particles occupy the ground state. However, in the weakly interacting gas there exist positive quantum fluctuations given by Eq. (19) at zero temperature.

IV. CONCLUSIONS

In the present work we have presented a recursive scheme which, for the first time, yields an accurate account of the distribution function, condensate fraction and fluctuations for a finite WIBG within the microcanonical ensemble. This recursion algorithm is an enhanced version of the earlier ones both for an IBG in the canonical and microcanonical ensembles and for a WIBG in the canonical ensemble.

In a WIBG, we have used three approaches for calculations of the condensate statistics: (i) with the energy spectrum dependent on the actual number of condensed atoms, which is only valid provided the average number of condensate particles is much larger than its variance; (ii) with the energy spectrum dependent on the average number of condensed atoms, which is valid for temperatures except too near the critical point; (iii) with the energy spectrum dependent on the actual number of condensed atoms with inclusion of interaction between thermal atoms, which may hold even for small systems near the critical region within the microcanonical ensemble.

In particular we have pointed out the importance of the strict constraint on the particle number conservation and of the interactions between excited atoms. The effects of interactions between out of condensate atoms have shown to be significant for temperatures near the critical point.

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