Fluctuations of the Weakly Interacting Bose-Einstein Condensate

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We consider the role of weak interatomic interactions on the fluctuations of the number of condensed atoms within canonical and microcanonical ensembles. Unlike the corresponding case of the ideal gas this is not a clean, well-defined problem of mathematical physics. Two related reasons are the following: there is no unique way of defining the condensate fraction of the interacting system and no exact energy levels of the interacting system are known. [S0031-9007(99)09269-8]

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The recent achievement of Bose-Einstein condensation (BEC) in the collection of trapped atoms [1] has renewed interest [2] in the theory of cold bosons. In particular, statistical properties of the condensate fraction have been thoroughly investigated using the microcanonical and canonical ensembles of statistical physics. Although much more complicated than the celebrated grand canonical ensemble, these more restricted ones are necessary since grand canonical ensemble predicts unphysically large fluctuations of the number of condensed atoms. In a series of papers [3–9] the fluctuations of the condensate fraction were calculated in both ensembles by a variety of approximate methods: both numerical (based on recurrence formulas and on contour integration) and analytic (asymptotic formulas based on the notion of the Maxwell demon ensemble), for various trapping potentials and in different numbers of dimensions. All of the above results, however, were obtained for ideal Bose gas. In this case the condensed fraction is just the number of atoms in the (single particle) ground state. Also all single particle energy levels in simple trapping potentials are known. For this reason statistical properties of the ideal Bose gas require solving a well-posed combinatorial problem. In fact in one case—that of 1D harmonic potential—finding the microcanonical partition function is identical with the classical number theory problem of computing the number of unrestricted partitions of an integer, solved by mathematicians in 1918 [10].

The purpose of this Letter is to present the first results for the fluctuations of weakly interacting condensate in the perfectly isolated system of a finite number of atoms described by the microcanonical ensemble. We comment briefly on the recent Letter reporting fluctuations of the interacting Bose gas in canonical ensemble in the thermodynamic limit [11] and on the earlier attempt [12].

The problem of condensate fluctuations of the weakly interacting Bose gas is not well defined. It is not obvious how to identify a condensed subsystem in an unambiguous way for the interacting system. And yet the dependence of the condensate fraction on temperature was measured [13] and found to be in good agreement with the theory. The experimentalists use a pragmatic approach, defining the condensed subsystem by fitting a two-component formula to the measured probability distribution either in position or in momentum space. This method does not translate easily into a clear theoretical tool.

Of several possible theoretical definitions of the condensate proposed over the years [14] we favor the one based on the properties of the spectral decomposition of the single particle density matrix: $\rho(\mathbf{r_1}, \mathbf{r_2}) = \sum_j \langle n_j \rangle \varphi_j^*(\mathbf{r_1}) \varphi_j(\mathbf{r_2})$. The Bose-Einstein condensation manifests itself by the macroscopic occupation of one of the eigenmodes. It is very difficult to compute the eigenmodes. The symmetry of the Hamiltonian helps. Note, however, that in the physically most interesting case of the harmonic binding potential, even in its most regular, spherically symmetric case, symmetry determines the angular dependence of the eigenmodes, but tells nothing about their radial dependence. The exceptionally simple, and hence the best studied, is the case of the system confined in the box with periodic boundary conditions. In this case the single particle density matrix is translationally invariant and periodic, so its spectral decomposition is just the Fourier series labeled by the quantized momentum $\mathbf{p} = (2\pi\hbar/L)(n_x, n_y, n_z)$, where L is the size of the box.

We are interested in the statistics of a weakly interacting Bose gas for temperatures below the condensation temperature. In this regime, the system may be viewed as being composed of two macroscopic subsystems, a condensate of $n_0 \sim O(N)$ particles occupying the $\mathbf{p} = 0$ state, and an excited part of $N_{\rm ex} \equiv \sum_{\mathbf{p}\neq 0} n_{\mathbf{p}}$ particles. Since in our approach no distinction is made between a condensate at rest and a condensate in a state of collective motion, the label $p = 0$ refers to an effective mean momentum of the condensate, rather than a specific single-particle state. For isolated systems, particle number conservation implies $N_{\rm ex} = N - n_0$.

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After splitting the system into its condensed and excited parts we have to define the approximate dynamics. This can be done in a number of ways and one of our conclusions is that the fluctuations sensitively depend on the details of this approximation.

One commonly made assumption is to neglect the interatomic interaction within the excited subsystem. Thus, the states of the excited atoms are still single particle states in a box, since the condensate is uniform. Accordingly, the energy of the excited subsystem is given by $E_{\text{ex}}(\{n_p\}) = \sum_{\mathbf{p}\neq 0}(\mathbf{p}^2/2m)n_{\mathbf{p}}$.

To fully define the problem, we need to specify the relation between the total energy of the system E and E_{ex}. This may be done in a number of ways as various approaches are being used in the literature. Each of them has both advantages and drawbacks. Therefore, it is very hard to judge *a priori* which one is better suited for studying fluctuations.

If we assume the standard contact interaction between condensed atoms and between condensed atoms and excited atoms, then the single excited orbital version of the Hartree-Fock theory [15] gives

$$E = \alpha(N^2 - N_{\text{ex}}^2) + E_{\text{ex}}(\{n_p\}), \qquad (1)$$

where $\alpha = (2\pi a \hbar^2/mV)$, and a is the scattering length. A nice feature of this approximation is the exact orthogonality of the excited orbitals to the condensate wave function, given by the solution of the Gross-Pitaevski equation also in more realistic, harmonic potential. Its drawback is the instability as the number of atoms increases. For the sufficiently large system, the transition to the excited part becomes energetically favorable—so this model is not suitable for the study of thermodynamic limit.

If we assume a two-gas model obtained by the reduction of the Bogolubov approximation [16], then the relation takes the form

$$E = \alpha(N^2 + 2NN_{\text{ex}} - 3N_{\text{ex}}^2) + E_{\text{ex}}(\{n_p\}). \qquad (2)$$

This has an obvious weakness: the wave functions describing the quasiparticles for the harmonic potential are not orthogonal to the condensate wave function. Hence, counting them as particles must incur some error.

If we use the lowest order perturbation theory [17] in its simplified form again neglecting the terms proportional to the product of excited occupation numbers:

$$E = \alpha(N^2 + 2NN_{\text{ex}} - N_{\text{ex}}^2) + E_{\text{ex}}(\{n_p\}), \qquad (3)$$

we obtain a model which does have a gap in the thermodynamic limit, which disappears if higher order corrections are taken into account [17]. However, in the case of the finite system and in the weak interaction limit these higher order terms can be neglected.

In all three cases we may compute now the microcanonical partition function, $\Gamma(N,E) = \sum_0^N \Gamma_{\text{ex}}(N, N_{\text{ex}}, E)$, where $\Gamma_{\text{ex}}(N, N_{\text{ex}}, E)$ is the number of microstates with N_{ex} particles being distributed over single particle states $\mathbf{p} \neq 0$, $n_0 = N - N_{\text{ex}}$ particles residing in the condensate, the totality of particles sharing an energy E. Apart from normalization this is just a probability of finding N_{ex} excited atoms or $N - N_{\text{ex}}$ atoms in the condensate. Hence the microcanonical fluctuations are just a second moment of this distribution.

Computation of $\Gamma_{\text{ex}}(N, N_{\text{ex}}, E)$ for any given N_{ex} is easy, since we have $\Gamma_{\text{ex}}(N, N_{\text{ex}}, E) = \Gamma_{\text{ex}}^0(N_{\text{ex}}, E_{\text{ex}})$, where $\Gamma_{\text{ex}}^0(N_{\text{ex}}, E_{\text{ex}})$ is the microcanonical partition function of the excited subsystem of an ideal Bose gas. Useful numerical techniques based on the recurrence relations were developed in connection with the ideal Bose gas for computation of the microcanonical partition function. They are easily applied to systems with several hundred particles.

The results are compared to the noninteracting case in Fig. 1 for the temperature dependence of the absolute value of fluctuations $\delta^2 N_0 \equiv \langle (n_0 - \langle n_0 \rangle)^2 \rangle$ of the number of condensed atoms. The inset displays the mean number $\overline{N}_0 \equiv \langle n_0 \rangle$ of atoms in the condensate. The temperature is measured in units given by the spacing between two lowest levels in the 3D box: $\Delta = (2\pi\hbar)^2/(2mL^2)$ and the scattering length a is in units of the box length L. We see that all three simplified models give markedly different results. On the basis of these results, it is not even possible to say if the correction coming from the interatomic interaction decreases or increases the microcanonical fluctuations with respect to the ideal gas case. Condensate fluctuations unlike the mean occupation and critical temperature seem to be much more sensitive to the model assumptions. In the case of the harmonic trap the latter computed out of the mean-field two-gas model [18], agree remarkably well with experimental data of [13]. Theoretical models of the condensate

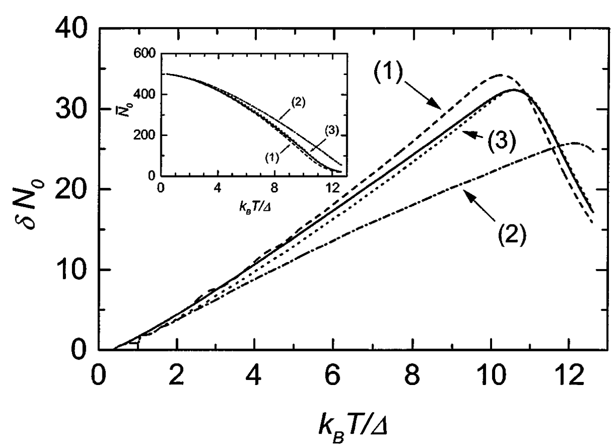

FIG. 1. Root-mean-square fluctuations of the ground state occupation for various models of interaction in the microcanonical ensemble. The total number of particles $N = 500$ and scattering length $a/L = 0.0004$. Curves are labeled (1), (2), and (3) in correspondence to Eqs. (1)–(3). The solid line refers to the ideal Bose gas. Note the large discrepancy between different models. Inset: Mean number of particles in the condensate.

fluctuations do not provide any systematic method of evaluations of the quality of different approaches. Verification of their predictions in the experiment is the only and ultimate test. We hope that two-point correlation function $g_2(\mathbf{r_1}, \mathbf{r_2})$ [19], which depends on fluctuations, would be soon available to the experimental measurement.

We turn now to the canonical ensemble. For models discussed here we go several steps towards analytic results for the canonical ensemble. To this end note, that if the interaction energy depends only on the total number of atoms N and total number of excited atoms N_{ex} (or equivalently N and n_0) and not on the detailed distribution among excited states, as in the cases discussed above, then the canonical partition function of the system composed of N atoms, of which exactly N_{ex} are excited may be written as

$$Z_{\mathrm{ex}}(N, N_{\mathrm{ex}}, \beta) = \sum_{\sum n_{\mathbf{p}} = N_{\mathrm{ex}}} e^{-\beta E_{\mathrm{int}} - \beta E_{\mathrm{ex}}(\{n_p\})}, \qquad (4)$$

where, in principle, function $E_{\mathrm{int}}(N, N_{\mathrm{ex}})$ could be any of the interaction terms in Eqs. (1)–(3). In the detailed calculation we shall restrict ourselves to the perturbative expression (3), for which the thermodynamic limit exists. We see that (4) may be easily expressed in terms of the canonical partition function of the excited subsystem of noninteracting atoms:

$$Z_{\mathrm{ex}}(N, N_{\mathrm{ex}}, \beta) = \exp^{-\beta E_{\mathrm{int}}(N, N_{\mathrm{ex}})} Z^0_{\mathrm{ex}}(N_{\mathrm{ex}}, \beta), \qquad (5)$$

for which a good approximate asymptotic formula is well known [8,9]. Now imposing the constraint $N = n_0 + N_{\mathrm{ex}}$ to eliminate N_{ex} we obtain the probability of finding exactly n_0 atoms in the condensate:

$$P_{CN}(n_0|N) = Z_{\mathrm{ex}}(N, N - n_0, \beta)/Z(N, \beta). \qquad (6)$$

The mean value $\overline{N}_0$ and the mean square fluctuations $\delta^2 N_0$ can be calculated directly from (6) in any regime. Below the critical temperature and for a large number of atoms, the distribution is strongly peaked around its most probable value. Assuming that the mean value and the most probable value coincide, and utilizing a Gaussian approximation for the distribution (6), we find the following implicit equation for $\overline{N}_0$,

$$N - \overline{N}_0 = V/(\lambda_T)^3 g_{3/2}(e^{\mu \overline{N}_0}), \qquad (7)$$

where the Bose-Einstein function $g_n(s) = \sum_{l=1}^{\infty} s^l/l^n$, $\lambda_T = (2\pi\hbar^2\beta/m)^{1/2}$ can be related to the thermal wavelength and $\mu = -2\alpha\beta$. In the same approximation the fluctuations are given by

$$\delta^2 N_0 = \left[\left(\sum_{\mathbf{p} \neq 0} \frac{1}{4\sinh^2(\frac{\beta}{2}\frac{\mathbf{p}^2}{2m} - \frac{\mu \overline{N}_0}{2})} \right)^{-1} + \mu \right]^{-1}. \qquad (8)$$

This formula, which is the direct generalization of the expression for the ideal Bose gas found in [9], is our main result. Two limiting cases are of special interest: the limit of ultraweak interaction $a \to 0$, and the thermodynamic limit. As expected, these limits do not commute. In the limit of ultraweak interaction we find the well-known expression of the ideal Bose gas

$$\delta^2 N_0(a \to 0) \sim 15.578(7)\,[k_B T/\Delta]^2 \qquad (9)$$

while for fixed a not too small, the thermodynamic limit of Eq. (8) reads

$$\delta^2 N_0 \sim V/(\lambda_T)^3 [g^{-1}_{1/2}(e^{\mu \overline{N}_0}) - 2a/\lambda_T]^{-1}. \qquad (10)$$

Note that this expression becomes invalid in the limit of ultraweak interaction. Indeed, according to (10) the fluctuations are normal, that is they are proportional to the volume, while for the ideal gas they are anomalous with proportionality $\sim V^{4/3}$. The different scaling of fluctuations with the size of the system results in the fact that thermodynamic limit does not commute with the limit of zero interactions. Our two first models are not well suited for studying the thermodynamic limit as they neglect interaction in excited states which makes the ground state unstable in this case.

The crossover from anomalous to normal scaling occurs if the scattering length drops below a certain value a_c which is obtained by equating Eqs. (9) and (10). The result scales $a_c \sim V^{1/3}/N_0$. Noteworthy, for $a \leq a_c$ the pair interaction energy per particle, $\sim \alpha N_0$, is smaller than the kinetic energy spacing $\Delta \sim V^{-2/3}$ which governs the statistics of the ideal Bose gas, i.e., for $a \leq a_c$ the gas is effectively ideal.

In Fig. 2 we plot Eq. (10) as a function of temperature for 10^5 particles and $a/L = 4 \times 10^{-4}$. For this choice of parameters $a_c/L = 10^{-5}$, i.e., we are well into the interacting regime. Also shown are the predictions of [11], Eq. (8), which are derived within a nonnumber conserving Bogolubov approach. Again we see big differences. Note, however, that for a small number of

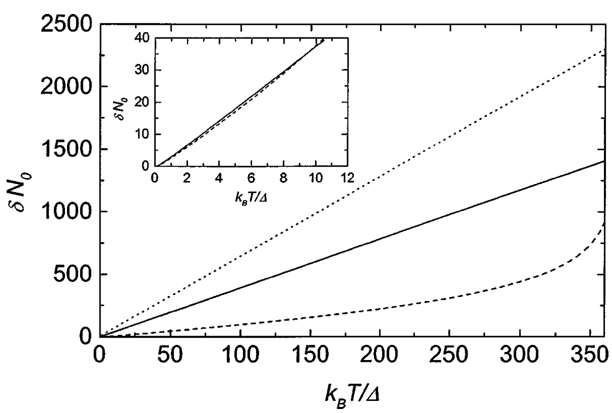

FIG. 2. Root-mean-square fluctuations of the ground state occupation in the canonical ensemble for $N = 10^5$ and $a/L = 0.0004$. Displayed are (i) our result (dashed line), (ii) Eq. (8) of Ref. [11] (dotted line), and the ideal Bose gas (full line). Inset: Our result for $N = 500$, a as above, indistinguishable from the ideal gas.

particles $N = 500$ (see inset in Fig. 2) the result of the present calculation is extremely close to the ideal gas case.

Noteworthy, our result (10) is in sharp disagreement with the predictions in [11] where it is argued that within the Bogolubov approach the fluctuations of the weakly interacting Bose gas in the box remain anomalous [20]. This approximation predicts phononlike spectrum of the lowest excitations of the condensate, however, as shown in [21], in the case of soluble 1D model it is only a certain subset of excited states. The phonon spectrum plays a crucial role in the approach of [11] because authors claim that an excitation of a single long wavelength phonon depletes the condensate. In our opinion phonons are collective excitations which do not necessarily change the number of condensated particles. Such an excitation is rather a specific distortion of the finite condensate than its depletion. Therefore, the absence of phonon states in our approach should not result in substantial error in estimation of condensate fluctuations. On the other hand, the Bogolubov method does not conserve the number of particles, and configurations with different numbers of excited atoms coincide with the same condensate, so, in particular, the interaction energy of the condensed atoms remains constant for all members of the ensemble.

However, as we have seen in the present Letter, the changing interaction energy of the condensate (αN_0^2) is crucial for the fluctuations. Although our results were obtained for the system confined in the box a similar method can be used for the harmonic trap. In this case the mutual interaction leads to some effective mean field potential felt by excited particles. The lowest energy levels of this effective potential can be computed exactly while higher states might be described within, for instance, semiclassical approximation.

To summarize: Different ways of describing approximately the weakly interacting Bose gas lead to vastly different predictions concerning the fluctuations of the condensate both in the microcanonical and the canonical ensembles. Therefore we consider the problem as open and unsolved because none of the presented approaches to this difficult many body problem treat all essential ingredients of the real physical situation with equal care. More work is needed, perhaps, on the soluble 1D chain of interacting bosons [21]. Fortunately, nature, which does not know about the theoretical ambiguities, might be very helpful. The experimental measurement of the $g_2(\mathbf{r_1}, \mathbf{r_2})$ (as shown in [22] the refractive index of a condensate is directly related to the two-point spatial correlation function) which we hope will come soon, could resolve the problem allowing for better understanding of the interacting quantum systems.

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