Fluctuations of Bose-Einstein Condensate

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We study the ground state occupation number and its fluctuations for the Bose-Einstein condensate of trapped atoms using the microcanonical ensemble. The analytic formulas are obtained with the help of the saddle point method. We show that microcanonical fluctuations below the critical temperature tend to zero and scale with the number of particles as $1/\sqrt{N}$. [S0031-9007(97)02871-8]

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The recent achievement of Bose-Einstein condensation (BEC) in trapped atoms of dilute gases [1–3] has been quickly followed by the quantitative measurements of the condensate's properties. In particular the dependence of the fraction of atoms in the condensate on the temperature has been found to be in agreement with the theory of the noninteracting Bose gas in a harmonic trap [4]. From the point of view of the textbook thermodynamics the atomic condensate studied by Boulder and MIT groups is an exotic system: (1) It consists of a finite number of particles. This number does not fluctuate after the complicated cooling process is over. (2) It is highly nonuniform. The trapping harmonic potential changes within the condensate.

And yet the textbook theory of the Bose-Einstein condensation is based on the thermodynamic limit of the uniform, noninteracting gas described by the grand canonical ensemble. Perhaps the first person to worry about this was Schrödinger [5], long before the present experiments. He considered, however, only the case of a finite number of noninteracting bosons in a cell. Later the grand canonical ensemble predictions for the harmonically trapped finite number of noninteracting bosons was made [6–8]. According to this theory $\langle N_0\rangle/\langle N\rangle = 1 - (T/T_c)^3$, where $\langle N_0\rangle$ is the mean number of atoms in the condensate, $\langle N\rangle$ is the mean total number of trapped atoms, T is the temperature, and T_c is the critical temperature. The recent experimental results agree with the above formula. But the fluctuations of the condensate fraction certainly do not agree with the results of the grand canonical ensemble. This last quantity suffers large relative fluctuations which approach 100% as the temperature tends to zero. Hence the theory of the harmonically trapped condensate based on a microcanonical ensemble is needed. In the recent Letter [9] these fluctuations were computed in a one dimensional model. This cannot be directly compared to the experiment, which is obviously three dimensional. Moreover, in one dimension there is no phase transition in the limit of number of particles going to infinity. It is the purpose of this Letter to estimate for the first time the fluctuations of the condensate fraction according to the microcanonical ensemble, which, we think, could be soon tested in the experiment.

The microcanonical description of a many body system is difficult because of constraints imposed on a total energy and particle number. That obstacle is traditionally overcome by applying the grand canonical description instead of the microcanonical one. In the thermodynamic limit these approaches become equivalent, in the sense that a relative grand canonical fluctuation of a mean energy and particle number vanish [10]. Therefore, expectation values are the same for different statistical ensembles. But the standard deviations may be different.

We consider the microcanonical ensemble for a system of N bosons confined by a 3D isotropic harmonic potential of frequency ω. The characteristic energy $\hbar\omega$ of the single excitation is our unit of energy. Thus, the single-particle energy is $E_n = n + 3/2$, where n is a nonnegative integer. The degeneracy of the energy E_n is equal to $(n+1)(n+2)/2$. In the case of N noninteracting atoms the total energy is simply a sum of single particle energies: $U = E + 3N/2$ with integer E. The E has the meaning of a number of excitation quanta. The microcanonical partition function $\Gamma(N,E)$ is equal to a number of completely symmetric N-particle states of a given total number of excitation quanta, E. The direct computation of the microcanonical partition function is probably not possible for $N > 1000$. In the interesting case of a large number of particles, $N \gg 1$ and excitation quanta, $E \gg 1$, we can use the approximate technique based on the saddle point method widely used in statistical physics [10].

The grand canonical partition function, $\Xi(z,\xi)$, is, by its definition, related to the microcanonical sum $\Gamma(N,E)$:

$$\Xi(z,\xi) = \sum_{N=0}^{\infty} z^N \sum_{E=0}^{\infty} \xi^E \Gamma(N,E), \tag{1}$$

where ξ is the Boltzmann factor, $\xi = \exp(-\beta) \equiv \exp(-\hbar\omega/k_BT)$, and z is the fugacity related to the chemical potential μ by the standard formula, $z = \exp[\beta(+3/2)]$. On the other hand, the relatively compact

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expression for the grand canonical partition function,

$$\Xi(z,\xi) = \prod_{E=0}^{\infty}\left(\frac{1}{1 - z\xi^E}\right)^{(E+1)(E+2)/2}, \tag{2}$$

allows us, at least in principle, to find $\Gamma(N,E)$ by expanding $\Xi(z,\xi)$ into power series in z and ξ what can be done by analytic continuation of the function $\Xi(z,\xi)$ and the Cauchy integral formula

$$\Gamma(N,E) = \frac{1}{(2\pi i)^2}\oint_{\Gamma_z} dz \oint_{\Gamma_\xi} d\xi\,\frac{\Xi(z,\xi)}{z^{N+1}\xi^{E+1}}, \tag{3}$$

where contours of integration Γ_z and Γ_ξ have to go around points $z = 0$ and $\xi = 0$, respectively. It is convenient to rewrite the function under the integral in Eq. (3) in the form of $\exp[\varphi(z,\xi)]$. Then the function $\varphi(z,\xi)$ is

$$\varphi(z,\xi) = \ln\Xi(z,\xi) - (N + 1)\ln z - (E + 1)\ln\xi\,. \tag{4}$$

Taking the contours through the extrema (saddle points) z_0 and ξ_0 of $\varphi(z,\xi)$ we get for $N\to\infty$, $E\to\infty$ the following asymptotic formula:

$$\Gamma(N,E) = \frac{1}{[2\pi D(z_0,\xi_0)]^{1/2}}\,\frac{\Xi(z_0,\xi_0)}{z_0^{N+1}\xi_0^{E+1}}, \tag{5}$$

where $D(z_0,\xi_0)$ is the determinant of the second derivatives of the function $\varphi(z,\xi)$ evaluated at the saddle points. The equations for the saddle points take the form

$$N + 1 = z\frac{\partial}{\partial z}\ln\Xi(z,\xi), \tag{6}$$

$$E + 1 = \xi\frac{\partial}{\partial\xi}\ln\Xi(z,\xi). \tag{7}$$

The presented method, although quite technical, has also its physical interpretation. The grand canonical partition function is, in fact, a weighted sum of microcanonical partitions. However, for a given value of the fugacity z_0 and Boltzmann factor ξ_0, practically only a few terms contribute to the whole sum in Eq. (1). The function $\Xi(z,\xi)$ is sharply peaked at z_0 and ξ_0 which relates us to the grand canonical expectation values: $N + 1 = \langle N\rangle$ and $E + 1 = \langle E\rangle$. The determinant in Eq. (5) is a measure of width of the partition function $\Xi(z,\xi)$ and it also has a simple interpretation in the grand canonical ensemble. The determinant $D(z_0,\xi_0)$ is related to the grand canonical fluctuations:

$$D(z_0,\xi_0) = [\delta_N^2\delta_E^2 - \delta_{NE}^2]/(z_0^2\xi_0^2), \tag{8}$$

where δ_E and δ_N are fluctuations of the total energy and particle number, respectively, and δ_{NE} is the second order correlation function: $\delta_{NE}^2 = \langle NE\rangle - \langle N\rangle\langle E\rangle$.

The microcanonical partition function can be written in the form

$$\Gamma(N,E) = \sum_{N_e=1}^{N} P_E(N_e), \tag{9}$$

where $P_E(N_e)$ is the number of completely symmetric N-particles states (of the total energy E) of *exactly* N_e particles in excited levels. Remaining $N_0 = N - N_e$ particles are simply spectators occupying the ground state. $P_E(N_e)$ can be expressed in terms of the microcanonical partition function: $P_E(N_e) = \Delta\Gamma(N_e,E) = \Gamma(N_e,E) - \Gamma(N_e - 1,E)$. Therefore, the system with N_0 particles in the ground state appears in the microcanonical ensemble with the probability $p_E(N_0\,|\,N)$ which is given by

$$p_E(N_0\,|\,N) = \Delta\Gamma(N - N_0,E)/\Gamma(N,E). \tag{10}$$

Having this probability, the microcanonical expectation value $\bar{N}_0$ and standard deviation $\delta\bar{N}_0$ of the ground state occupation number can be easily found:

$$\bar{N}_0 = \sum_{N_0=0}^{N} N_0 p_E(N_0\,|\,N), \tag{11}$$

$$\delta^2\bar{N}_0 = \sum_{N_0=0}^{N}(N_0 - \bar{N}_0)^2 p_E(N_0\,|\,N). \tag{12}$$

We solved numerically Eqs. (6) and (7) and analyzed the behavior of $\bar{N}_0$ and $\delta\bar{N}_0$ for a finite number of particles. However, the approximate analytic formula for the probability $p_E(N_0\,|\,N)$ can also be obtained. Equation (2) is not very useful for the detailed analysis. Instead, in the interesting limit of $z\to 1$ and $\beta\to 0$ the asymptotic expression can be found with the help of the Euler summation formula [11]:

$$\ln\Xi(z,\xi) = -\ln(1 - z) + \frac{g_4(z\xi)}{\beta^3} + \frac{5}{2}\frac{g_3(z\xi)}{\beta^2} + 3\frac{g_2(z\xi)}{\beta} + \frac{3}{2}g_1(z\xi) + R, \tag{13}$$

where $g_k(x) = \sum_{l=1}^{\infty} x^l/l^k$ are the Bose-Einstein functions, and R is the remainder which in the limit of $(1 - z)/\beta \ll 1$ has the following asymptotic form:

$$R = \ln\sqrt{2\pi} - 1 - \frac{5}{24}g_1(z\xi) + 4\beta\frac{z\xi}{1 - z\xi} + r, \tag{14}$$

and r is given by the infinite series and according to our numerical evaluations its value can be approximated by $r \approx 0.37/720$. In the opposite limit of $(1 - z)/\beta \gg 1$ the asymptotic expression for R is given by

$$R = -\frac{5}{24}g_1(z\xi) + 6\beta\frac{z\xi}{1 - z\xi}. \tag{15}$$

Because of the analogy with the grand canonical ensemble, Eqs. (6) and (7) may be solved in the standard way [8] in the limit of an infinite number of particles. It can be easily shown that in this case the fugacity z_0 obtained from the saddle point equations reaches the value one at the critical energy E_c:

$$E_c = 3\zeta(4)\,[N/\zeta(3)]^{4/3}, \tag{16}$$

where $\zeta(n) = g_n(1)$ are Riemannian zeta functions. If $E < E_c$ most of the atoms occupy the ground state. The most striking feature of the BEC is the fact that it occurs when the excitation per particle is proportional to $N^{1/3}$ and hence goes to infinity for large systems.

The higher order corrections to the approximate solutions of Eqs. (6) and (7) can be found by expansion of all terms into the powers of the parameter $z_1(N)$:

$$z_1(N) \approx \left[N - \frac{\zeta(3)}{\beta_0^3}\left(1 + \frac{3\zeta(2)}{2\zeta(3)}\beta_0\right)\right]^{-1}. \tag{17}$$

The approximate expressions for the saddle points have the form

$$z_0 = 1 - z_1(N) + z_1^2(N) + z_1^3(N) \times \frac{\zeta(3)}{\beta_0^3}\left(\frac{\zeta(2)}{\zeta(3)} + \frac{3\zeta(3)}{4\zeta(4)} - \frac{5\beta_0 \ln \beta_0}{2\zeta(3)}\right), \tag{18}$$

$$\beta_0 = \left(\frac{3\zeta(4)}{E}\right)^{1/4}\left[1 + \frac{\zeta(3)}{4\zeta(4)}\left(\frac{3\zeta(4)}{E}\right)^{1/4}\right]. \tag{19}$$

These solutions are obtained with the assumption that $z_0 \approx 1$ and $\beta_0 \approx 0$; i.e., they correspond to the condensed phase.

Finally we have defined all quantities which are necessary for a microcanonical description of the condensate. We do not present here solutions for z_0 and ξ_0 corresponding to the normal phase above the critical point. However, we want to stress that some contribution to the microcanonical fluctuations originates at that region of parameters and, therefore, our approximate expression presented below has some systematic error in the vicinity of the critical point. After some algebra the microcanonical partition function can be approximated by

$$\ln \Gamma(N,E) = 4\zeta(4)\left(\frac{E}{3\zeta(4)}\right)^{3/4} + \frac{3}{2}\zeta(3)\left(\frac{E}{3\zeta(4)}\right)^{1/2} - z_1(N)\gamma_1 - z_1^2(N)\gamma_2\,, \tag{20}$$

where functions γ_1 and are γ_2 are defined in the following way:

$$\gamma_1 = 1 + \frac{\zeta(3)}{8\zeta(4)}\left[1 + \beta_0\left(\frac{8\zeta(2)}{\zeta(3)} - \frac{15\zeta(3)}{2\zeta(4)}\right)\right], \tag{21}$$

$$\gamma_2 = \frac{\zeta(3)}{\beta_0^3}\left(\frac{\zeta(2)}{\zeta(3)} - \frac{3\zeta(3)}{4\zeta(4)} - \frac{5\beta_0 \ln \beta_0}{2\zeta(3)}\right). \tag{22}$$

The above expression does not have an asymptotic character. We left only leading terms proportional to $E^{3/4}$ and $E^{1/2}$ neglecting terms of the order of $E^{1/4}$ and smaller. Although terms containing $z_1(N)$ are rather small compared to the neglected ones, we have to keep them as they are the largest corrections depending on the number of particles. The range of validity of Eq. (20) is defined approximately by the condition $E < E_c$.

It can be easily checked that the microcanonical temperature defined through the condition $\hbar\omega/(k_B T_{\rm mic}) = \beta_{\rm mic} = \partial \ln \Gamma(N,E)/\partial E$ is almost equal to the grand canonical one $T_{\rm mic} = T$ (or $\beta_{\rm mic} = \beta_0$). Equations (16) and (19) allow us to introduce the microcanonical critical temperature $k_B T_c = \hbar\omega[N/\zeta(3)]^{1/3}$ for the infinite system. The differences between grand canonical and microcanonical temperatures become significant in the limit of small energies $E/N \ll 1$. We want to add that there is also an experimental ambiguity in measuring condensate temperature at very low temperature [4]. Nevertheless, being aware of all the difficulties related to the notion of temperature, we express the ground state occupation probability $p_E(N_0 \,|\, N)$ in terms of β_0 (as it is related to the microcanonical temperature) instead of energy E. Denoting this function by $p_\beta(N_0 \,|\, N)$ we have

$$p_\beta(N_0 \,|\, N) = [\gamma_1 z_1^2(N_e) + 2\gamma_2 z_1^3(N_e)] e^{\gamma_1[z_1(N) - z_1(N_e)]} \times e^{\gamma_2[z_1^2(N) - z_1^2(N_e)]}, \tag{23}$$

where $N_e = N - N_0$ is the number of excited particles.

In Fig. 1 we present the microcanonical population of the ground state as a function of the microcanonical temperature measured in units of T_c for the relatively small system of $N = 1000$ and $N = 10\,000$ particles. There is perfect agreement between the numerically obtained occupation number and the results based on the probability function $p_\beta(N_0 \,|\, N)$. The microcanonical mean values are almost undistinguishable from the grand canonical averages, i.e., in the limit of the infinite system mean number of particles in the condensate follows again the law $\bar{N}_0/N = 1 - (T/T_c)^3$.

The situation is completely different in the case of fluctuations. It can be shown using Eq. (23) that fluctuation of the ground state occupation number below the critical temperature is proportional to $[z_1(N)\gamma_1 + z_1^2(N)\gamma_2]^{1/2} \approx 1/\sqrt{N}$. Therefore, in the limit of an infinite particle number the microcanonical fluctuations vanish. A similar scaling law in the case of a canonical description has been reported recently [12]. In Fig. 2 we present the microcanonical fluctuations based on the numerical solutions of

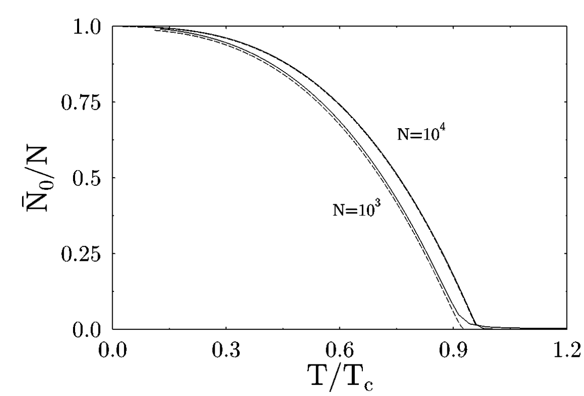

FIG. 1. Relative occupation of the ground state $\bar{N}_0/N$ as a function of the microcanonical temperature for the system of $N = 1000$ and $N = 10\,000$ particles. Full lines represent the numerical results while the dashed lines correspond to the analytic formula. The saddle point method does not allow us to determine the ground state population for very low temperatures.

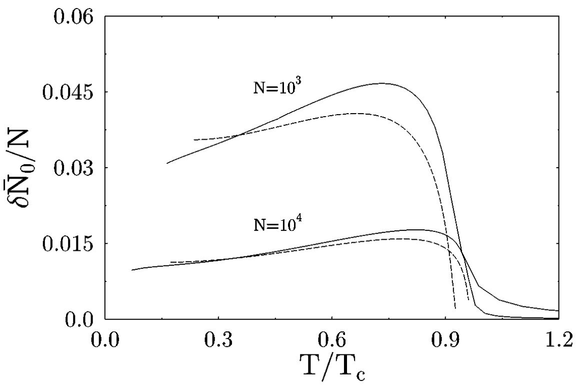

FIG. 2. Relative fluctuations of the ground state occupation number $\delta \bar{N}_0/N$ as a function of the microcanonical temperature for the system of $N = 1000$ and $N = 10\,000$ particles. The full lines represent the numerical results while the dashed lines correspond to the analytic formula. The saddle point method does not allow us to determine fluctuations for very low temperatures.

the saddle point equations (6) and (7) for $N = 1000$ and $N = 10\,000$ and compare them with those calculated from Eq. (23). The small disagreement seen in Fig. 2 is due to the fact that the formula for the function $p_\beta(N_0 \,|\, N)$ can be used only if $N - N_0 > \zeta(3)\,[E/3\zeta(4)]^{3/4}$. The opposite case corresponds to the region above the critical point and has been neglected in our approach. However, the way the fluctuations scale with the particle number agrees with our analytical estimation. The saddle point method fails in the case of small energy E or particle number N as the Gaussian approximation to the integrand in Eq. (3) becomes incorrect. We estimate that the range of applicability of the saddle point method is limited to the total energies of the system larger than the number of particles, $E > N$, i.e., to temperatures $T/T_c > N^{-1/12}$. The regime of very low temperatures has to be treated separately because the double integral in Eq. (3) has to be computed exactly. We are currently investigating this problem.

In conclusion, we have computed the fluctuations of the number of condensed particles for finite size BEC. We found that for 1000 particles these relative fluctuations are of the order of 4.5%. The fluctuations decrease as $1/\sqrt{N}$. In our approach we considered the ideal Bose gas neglecting the weak repulsive interaction between trapped atoms. This interaction is lowering the critical temperature and the fraction of condensed atoms by the amount of a few percent [13]. The qualitative estimation of condensate fluctuations can be found in [12]. This estimation shows that interatomic repulsion would enforce smaller fluctuations if the interaction is sufficiently strong. In real experiments there are other sources of fluctuations. In particular, if the results are collected from many different realizations of the BEC, then the total number of particles N cannot be treated as constant. The microcanonical fluctuations can therefore be regarded as the lower bound of fluctuations in the experiments with BEC.

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