Effect of a finite number of particles in the Bose-Einstein condensation of a trapped gas

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We consider a finite number of noninteracting bosons trapped in an isotropic three-dimensional harmonic oscillator. Using the grand canonical ensemble, we calculate the heat capacity of the system as a function of temperature, for several values of the number of particles. We find that a new definition of critical temperature is necessary for a finite number of trapped particles, and present a definition that is experimentally convenient and in good agreement with a recent definition given by W. Ketterle and N. J. van Druten [Phys. Rev. A **54**, 656 (1996)]. [S1050-2947(97)07305-8]

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Bose-Einstein condensation is predicted to occur when the thermal de Broglie wavelength of a sample of bosons becomes comparable to the average interparticle distance [1]. Experiments on ^{4}He [2], excitons in semiconductors [3], and, more recently, on trapped alkali-metal atoms [4–6] have showed strong evidence for the occurrence of this purely quantum phase transition. The Bose-Einstein condensates of trapped alkali-metal atoms have been achieved at temperatures as low as 100 nK, and, unlike in the case of ^{4}He, in a density regime (from 10^{12} to 10^{14} atoms/cm^3) in which the average interparticle distance is much larger than the range of the interatomic interactions. It is this weakly interacting characteristic of magnetically trapped alkali-metal atoms that has currently attracted immense attention. It is hoped that the dynamics of the Bose-Einstein condensation will be better understood by studying these weakly-interacting systems, a prospect that is hardily possible in the context of condensates, such as ^{4}He, whose dynamics is dominated by strong interactions. Moreover, the number of particles in the ground state of the traps ranged from a few thousand [4] to a few million [6]. Some of the implications of a finite number of particles in Bose-Einstein condensation have recently been considered by Ketterle and van Druten [7]. They have studied an ensemble of N noninteracting bosons trapped by a harmonic potential. Their main results are a measurable correction to the transition temperature for low values of N and the prediction of occurrence of Bose-Einstein condensation also in one- and two-dimensional systems, a possibility usually ruled out by conventional approaches [8]. In these approaches the spacing between energy levels is assumed to be much smaller than the thermal energy scale k_BT, and therefore the system is described by a continuum of energy states plus the discrete ground state. In particular, Ketterle and van Druten [7] have found a transition temperature that is lower than in this continuum limit, implying the necessity of a new definition for the critical temperature T_c. A discussion about the finite-N statistics is presented in Ref. [9]. All the calculations done in Ref. [7] are based on the grand canonical ensemble [1], as a limit of a large number of particles. In this paper we follow the approach of Ketterle and van Druten [7] and complement their analysis by calculating the heat capacity of an ensemble of a finite number N of noninteracting bosons.

A discontinuous heat capacity is one of the main characteristics of a phase transition. In the case of the Bose-Einstein condensation, the heat capacity for a fixed finite number of particles, C_N, has not yet been measured. Since in the near future we expect C_N to be measured, we feel motivated to calculate it. We begin by considering a three-dimensional isotropic harmonic external potential trapping bosons of mass m, which oscillate in the trap with a frequency ω. The energy eigenvalues E_n $(n=0,1,2,\dots)$ are given by

$$E_n=n\hbar\omega. \tag{1}$$

Since the trapping potential is three dimensional, we must take into account the degeneracy γ_n of the energy levels, which, given the isotropy of the trap, is easily found to be

$$\gamma_n=\frac{(n+1)(n+2)}{2}. \tag{2}$$

The Bose-Einstein distribution gives the average number $\eta(E_n)$ of particles in each of the energy eigenstates [1]:

$$\eta(E_n)=\frac{1}{e^{\beta(E_n-\mu)}-1}, \tag{3}$$

where $\beta\equiv 1/k_BT$, k_B is Boltzmann's constant, T is the absolute temperature, and $\mu\equiv\mu(T)$ is the chemical potential. We are assuming a fixed number N of bosons, therefore we can calculate μ by the constraint

$$N=\sum_{n=0}^{+\infty}\gamma_n\eta(E_n). \tag{4}$$

In the above summation, it is usual to separate out the possibly divergent ground-state contribution [1]. In the continuum approximation, Eq. (4) yields [1,7]

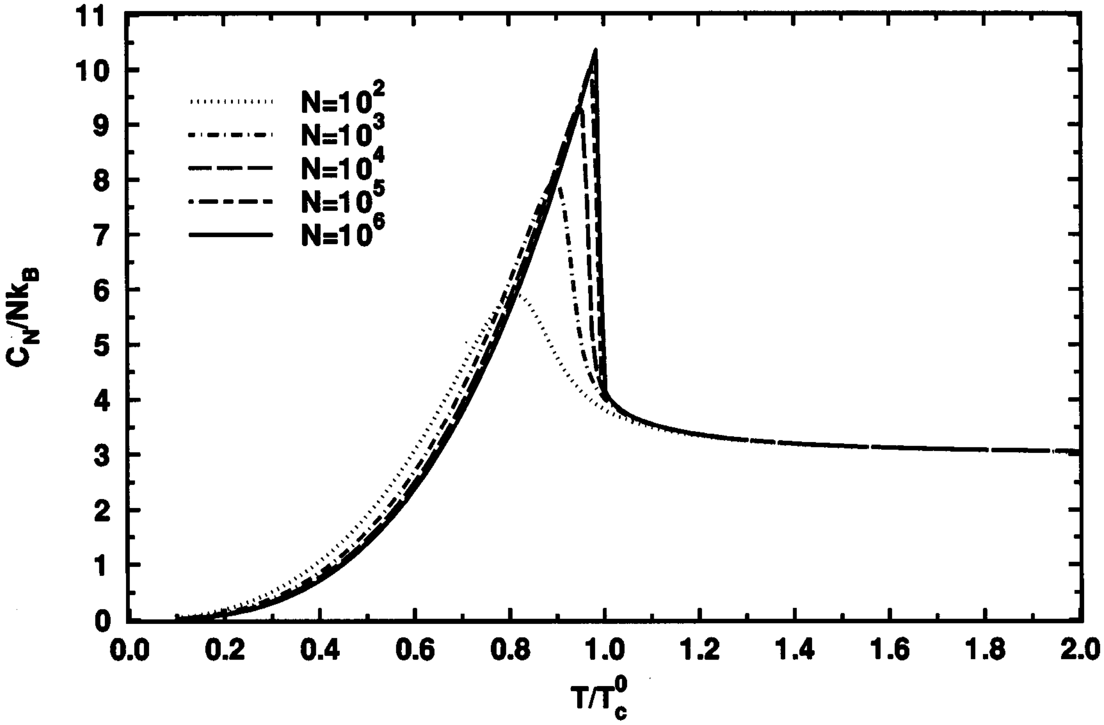

FIG. 1. Heat capacity as a function of temperature for several values of the number of noninteracting bosons.

$$N=\frac{z}{1-z}+g_3(z)\left(\frac{k_BT}{\hbar\omega}\right)^3, \tag{5}$$

where the Bose function $g_3(z)$ is defined by [1]

$$g_3(z)\equiv\sum_{j=1}^{+\infty}\frac{z^j}{j^3}, \tag{6}$$

and the quantity z is the fugacity given by

$$z=e^{\beta\mu}.$$

For fixed N, Eq. (5) shows that the ground state will be macroscopically populated if T is lower than a reference temperature T_c^0 defined as in Ref. [7], namely,

$$T_c^0\equiv\left(\frac{N}{g_3(1)}\right)^{1/3}\frac{\hbar\omega}{k_B}, \tag{7}$$

where, according to Eq. (6), $g_3(1)\approx 1.202057$. In Fig. 1 we have scaled the temperatures to T_c^0 [9]. Once we have calculated $\mu(T)$, we can immediately determine the average energy $E(N,T)$ of the system by

$$E(N,T)=\sum_{n=0}^{+\infty}\gamma_n\eta(E_n)E_n. \tag{8}$$

The heat capacity at fixed N is straightforwardly calculated by taking the partial derivative of $E(N,T)$ in Eq. (8) with respect to T:

$$C_N(T)\equiv\frac{\partial E(N,T)}{\partial T}. \tag{9}$$

Because μ is a function of T, in carrying out the differentiation above, we obtain

$$C_N(T)=\beta\sum_{n=0}^{+\infty}\frac{\gamma_nE_ne^{\beta(E_n-\mu)}}{(e^{\beta(E_n-\mu)}-1)^2}\left(\frac{E_n-\mu}{T}+\frac{\partial\mu}{\partial T}\right), \tag{10}$$

where use has been made of Eqs. (3) and (8). By implicitly differentiating Eq. (4) with respect to T, using Eq. (3), and isolating $\partial\mu/\partial T$, we get

$$\frac{\partial\mu}{\partial T}=-\frac{\sum_{m=0}^{+\infty}g_m(E_m-\mu)e^{\beta(E_m-\mu)}[\eta(E_m)]^2}{T\sum_{n=0}^{+\infty}\gamma_ne^{\beta(E_n-\mu)}[\eta(E_n)]^2}. \tag{11}$$

We have numerically calculated $C_N(T)$ as a function of T for different values of N by the following procedure. First, we take a certain number of levels, say, Q. Then, we evaluate the quantity

$$S(\mu,T)\equiv\sum_{n=0}^{Q}\gamma_n\eta(E_n)-N. \tag{12}$$

For each fixed value of T, we treat S as a function of μ alone, and find its root. Thus, $\mu(T)$ is obtained by imposing $S[\mu(T),T]=0$. To check for convergence, we increase Q and repeat the procedure to obtain a new value of $\mu(T)$; if this new value differs from the previous one within a specified small quantity, then the population of the levels higher than Q is small enough not to contribute appreciably to the sum in Eq. (4), and $\mu(T)$ is converged. We keep on increasing Q until convergence is reached. Once $\mu(T)$ is found, we can use Eq. (11) to calculate $\partial\mu/\partial T$, and Eq. (10) to obtain

$C_N(T)$. Figure 1 shows the results of our numerical calculations for different values of N. The first feature to notice in Fig. 1 is that there is a discontinuity in C_N in the thermodynamic limit ($N \rightarrow +\infty$). Usually one would define the critical temperature at this discontinuity. However, there is no discontinuity for finite numbers of particles. As N decreases, C_N as a function of temperature gets smoother and smoother. One would be tempted to define a critical temperature T_c at the maximum of the curve of C_N for finite N, that is,

$$\left(\frac{\partial C_N(T)}{\partial T} \right)_{T=T_c} = 0. \tag{13}$$

Such a definition coincides with the temperature at which C_N becomes quasidiscontinuous in the large-N limit. The maxima of the curves in Fig. 1 are at $T_c/T_c^0 = 0.813$, 0.898, 0.946, 0.974, and 0.984 for $N = 100$, 1000, 10^4, 10^5, and 10^6, respectively. These maxima are the second feature to notice in Fig. 1: as N decreases, T_c is shifted to values lower than T_c^0, in agreement with the behavior of the critical temperature T_c^{KvD}, defined by Ketterle and van Druten [7], approximately given by

$$\frac{T_c^{\mathrm{KvD}}}{T_c^0} \approx 1 - \frac{0.7275}{N^{1/3}}. \tag{14}$$

This lowering of the critical temperature for decreasing number of particles is due to the fact that a smaller system has a larger available effective volume [8]. Even the numerical values of Eq. (14) are not too different from the definition in Eq. (13): $T_c^{\mathrm{KvD}}/T_c^0 = 0.843$, 0.927, 0.966, 0.984, and 0.993 for $N = 100$, 1000, 10^4, 10^5, and 10^6, respectively. Therefore our definition of the critical temperature T_c, Eq. (13), incorporates all the important features of Eq. (14), and the convenience of being easily obtained from eventual experimental data showing C_N as a function of T. It should be mentioned that, strictly speaking, a finite system does not undergo a phase transition, but, as Ketterle and van Druten [7] remark, the behavior of the finite system is very similar to the one expected in the large-N limit, as we can also see in Fig. 1 for $N > 10^3$. In conclusion we notice that the numerical procedure we describe here is straightforwardly generalized to the case of an anisotropic harmonic oscillator, that is, a harmonic potential whose frequencies of oscillations along the x, y, and z axes are not the same, or to the case of one- or two-dimensional oscillators. Again we can use Eq. (13) to define the critical temperature with results analogous to those for the isotropic three-dimensional case detailed here. It is important to point out that, from a purely experimental point of view, the signature of a phase transition is more naturally depicted as a discontinuity in the heat capacity curve, hence the convenience of adopting Eq. (13) as the new definition of critical temperature. Variations in the heat capacity with the number of particles is an important issue to be understood to avoid confusion with variations due to interactions.

Notice in Fig. 1 that the heat capacity saturates to $3Nk_B$, as it should be for the ergodic dynamics of a three-dimensional harmonic oscillator. At low temperature, the quantum formulas display the usual *freezing* of the degrees of freedom, and at intermediate temperatures one gets the signature of the phase transition. Some recent results of many-dimensional Hamiltonian dynamics offer interesting insights when contrasted to the quantum formulas: it is known for several models that lack of ergodicity at low energies can produce transitions where the time to equipartition becomes infinite and the dynamics restricted to the lowest frequency vibration mode [10,11].

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