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Bose-Einstein condensation of a finite number of particles trapped in one or three dimensions

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Bose-Einstein condensation (BEC) of an ideal gas is investigated for a finite number of particles. In three dimensions, we find a transition temperature which is lower than in the thermodynamic limit. Lowering the dimension increases the transition temperature and is therefore favorable for BEC. This is in contrast to the standard result obtained in the thermodynamic limit which states that BEC is not possible in, e.g., a one-dimensional (1D) harmonic potential. As a result, 1D atom traps, such as radially tightly confining magnetic traps or optical dipole traps, are promising for studying BEC. [S1050-2947(96)06807-2]

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The recent observations of Bose-Einstein condensation (BEC) in ultracold trapped atomic gases [1–3] have created a wave of renewed interest in this phenomenon. BEC is a purely quantum-statistical phase transition, characterized by a macroscopic population of the ground state below the transition temperature T_c. In most textbooks of statistical mechanics, e.g., [4], the theory of BEC is formulated for noninteracting bosons in a three-dimensional (3D) box. This treatment has been extended to power-law potentials [5,6] and lower-dimensional systems [7–9], leading to the conclusion that BEC in one- and two-dimensional systems is only possible for sufficiently confining potentials. In all these treatments either the thermodynamic limit was used, or the discrete level structure was approximated by a continuous density of states under the assumption that the level spacing was negligible compared to the temperature. Recent BEC experiments on atomic gases, however, were performed with numbers of particles N ranging from a few thousand [1] to a few million [3]. For these relatively low numbers neither of the above approximations seems *a priori* justified, and one is led to wonder whether this leads to deviations from the theoretical predictions.

In this paper, we study BEC for finite N. We focus on the harmonic potential, because of its relevance to the recent experiments and its mathematical simplicity. We indeed find marked differences from the usual treatments: a measurable correction to the transition temperature for low values of N, and, surprisingly, the occurrence of BEC in low-dimensional systems, in cases where it does not appear in the usual treatments. Furthermore, our treatment is of pedagogical value: it discusses BEC without the continuous spectrum approximation, there are no divergent integrals, and no special role is given to the ground state of the system. This work also illuminates subtleties involved in the limit of infinite N.

As a starting point we assume that the population $N(E_i)$ of a state with energy E_i is given by the Bose-Einstein distribution

$$N(E_i)=\frac{1}{e^{\beta(E_i-\mu)}-1}=\frac{ze^{-\beta E_i}}{1-ze^{-\beta E_i}}. \tag{1}$$

This result is derived from first principles of statistical mechanics, most conveniently using the grand canonical ensemble [4]. β is related to the temperature T by $\beta=1/k_BT$. The energy of the ground state has been taken to be zero. The fugacity z can be expressed by the chemical potential μ as $z=\exp(\beta\mu)$. It is determined by the constraint that the total number of particles in the system is N:

$$\sum_{i=0}^{\infty} N(E_i)=N. \tag{2}$$

Degeneracy factors are avoided by accounting for degenerate states individually. The phenomenon of BEC for noninteracting particles is fully described by Eqs. (1) and (2). The nontrivial aspect is the determination of the chemical potential as a function of N and T. Once μ is known, all thermodynamic quantities like total energy, specific heat, and compressibility follow directly from sums over the energy levels involving the occupation numbers in Eq. (1). Several authors have discussed $\mu(T)$ for finite N [5,10,11], but have not discussed the conclusions presented in this paper.

Using

$$N=\sum_{i=0}^{\infty}\sum_{j=1}^{\infty} z^j\exp(-j\beta E_i), \tag{3}$$

for a 3D isotropic harmonic potential with frequency ω we obtain

$$N=\sum_{j=1}^{\infty} z^j\left(\sum_{n=0}^{\infty}\exp(-jn\beta\hbar\omega)\right)^3=\sum_{j=1}^{\infty} z^j/(1-x^j)^3, \tag{4}$$

where $x=\exp(-\beta\hbar\omega)$. Note that no special treatment is given to the ground state, in contrast to what is necessary with the continuous spectrum approximation [6].

In Fig. 1, the number of atoms in the ground state $N_0=z/(1-z)$, is plotted versus temperature for various values of N. z was determined numerically from Eq. (4). The reference temperature T_c^0 is given by

$$T_c^0=\left(\frac{N}{g_3(1)}\right)^{1/3}\frac{\hbar\omega}{k_B} \tag{5}$$

with the usual definition of the Bose functions $g_n(z)=\Sigma_{j=1}^{\infty}(z^j/j^n)$ [4]. Figure 1 demonstrates that the signature

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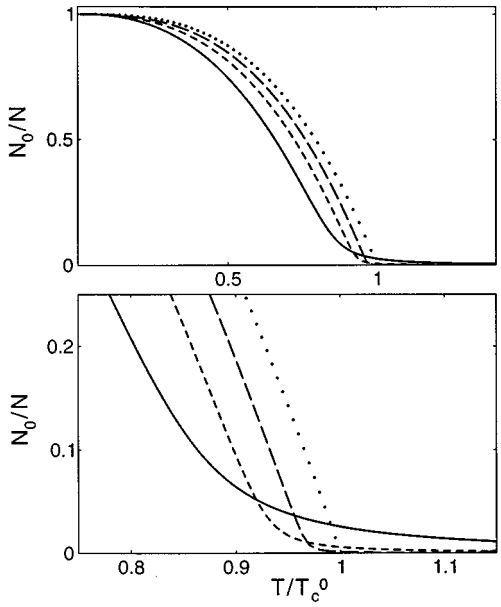

FIG. 1. The condensate fraction for a finite number N of atoms in a three-dimensional harmonic potential versus temperature. Plots are shown for $N=100$ (solid line), 1000, 10^4, and infinite (dotted). The lower plot enlarges the region around the transition temperature.

of BEC in systems with a small number of particles is very similar to the case of infinite number, the major difference being a shifted and smeared out onset of the macroscopic population of the ground state. The population of the first excited level is shown in Fig. 2. It reaches at most a few percent in systems of less than a thousand particles, and vanishes in the limit of large N. It has been argued that exchange interaction is necessary to prevent the macroscopic population of *several* states which are almost degenerate in the thermodynamic limit [12]. Figure 2 shows that, for $N\rightarrow\infty$, the population of the first excited state is negligible even in the absence of any interactions [10], provided that the limit is correctly taken by first calculating the properties for finite N and then letting N approach ∞.

To compare our results with the standard treatment, we approximate Eq. (4) for $k_BT\gg\hbar\omega$, retaining the two highest-order terms in $k_BT/\hbar\omega$. Since the sum in Eq. (4) diverges for $z\rightarrow 1$, one has to rewrite Eq. (4) as $N=z/(1-z)+\Sigma_{j=1}^{\infty}z^j([1/(1-x^j)]^3-1)$ before applying the high-temperature expansion [13]. Formally, this corresponds to splitting off the ground-state population. The result is

$$N=\frac{z}{1-z}+g_3(z)\left(\frac{k_BT}{\hbar\omega}\right)^3+\tfrac{3}{2}g_2(z)\left(\frac{k_BT}{\hbar\omega}\right)^2. \qquad (6)$$

At this point we briefly digress to describe the usual treatment of BEC in a 3D harmonic potential [6] in some more detail. Starting from Eq. (3), the ground-state population is split off, and the finite sum over the excited states is replaced by an integral

$$N-N_0=\sum_{j=1}^{\infty}z^j\int_0^{\infty}\rho(E)\exp(-j\beta E)dE \qquad (7)$$

where $\rho(E)$ is the density of states, usually taken to be $(E/\hbar\omega)^2/2$. The result is

$$N=\frac{z}{1-z}+g_3(z)\left(\frac{k_BT}{\hbar\omega}\right)^3. \qquad (8)$$

The critical temperature T_c can now be found by setting $N_0=0$ and $z=1$. The physical meaning of this is that the second term in Eq. (8) represents the maximum number of particles which can be accommodated in excited states when the fugacity z reaches its maximum value of 1. All particles exceeding this maximum number must condense in the ground state. This results in Eq. (5) for the critical temperature, and a condensate fraction given by

$$N_0/N=1-(T/T_c)^3. \qquad (9)$$

It is in fact possible to obtain the last term in Eq. (6) using this traditional approach: since the degeneracy of the state with energy $n\hbar\omega$ is $(n+1)(n+2)/2$, a better approximation for the density of states is $\rho(E)=\frac{1}{2}[(E/\hbar\omega)^2+3(E/\hbar\omega)]$. Inserting this expression into Eq. (7) yields Eq. (6). This shows that there is no fundamental difference between the use of discrete sums or a continuous spectrum if the density of states is correctly approximated. In Fig. 3, several approximations to the exact result are compared. Already for $N=1000$, results obtained with Eq. (6) are almost indistinguishable from the exact result [Eq. (4)]. However, the contribution of the last term in Eq. (6) is important.

Strictly speaking, phase transitions only occur in the thermodynamic limit (e.g., for infinite N). That is why we have so far avoided using the term ''phase transition,'' but rather concentrated on the fraction of atoms in the ground state which can be exactly calculated even for the finite-N system. However, as was shown above, the behavior of the finite-N system is very similar to the thermodynamic limit, even for N as low as 10^4. Phase transitions are usually defined by singularities and critical behavior. In the case of BEC, the phase transition is characterized by the appearance of a complex order parameter (which can be identified with the condensate wave function) and the onset of off-diagonal long-range order [14]. For the finite-N system, we adopt the treatment described above [6], and take the macroscopic occupation of the ground state as the defining characteristic of the BEC phase transition. Note that in the recent experiments

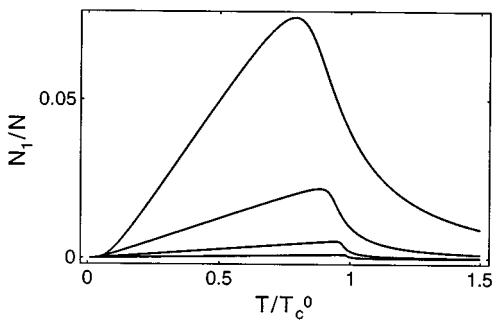

FIG. 2. The fraction of atoms in the (threefold degenerate) first excited level versus temperature for 100 (upper curve), 1000, 10^4, and 10^5 (lower curve) atoms.

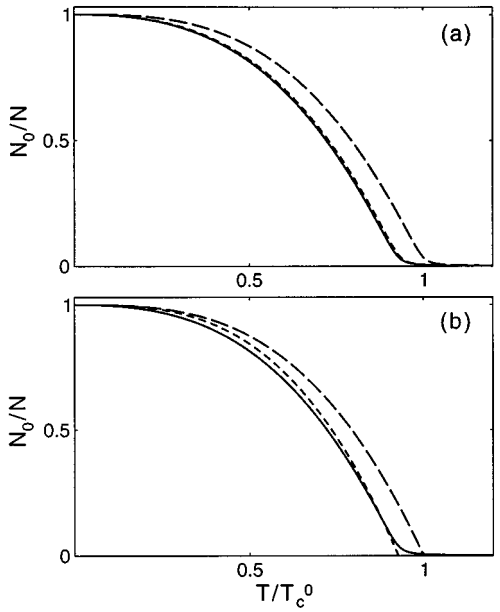

FIG. 3. Various approximations for the condensate fraction versus temperature for $N=1000$ atoms. (a) The exact result (solid line) is compared to the result obtained using Eq. (6) (short dashes) and Eq. (8) (long dashes). (b) Comparison with Eq. (9) (short dashes) and Eq. (9) with T_c replaced by T_c^0 (long dashes).

[1–3], the appearance of a macroscopic occupation of the ground state was also regarded as evidence for BEC. We thus define the transition temperature T_c for a finite-N system by

$$\sum_{i=1}^{\infty} \frac{1}{e^{E_i/k_BT_c}-1} = N. \tag{10}$$

Using approximation (6) results in a transition temperature

$$\frac{T_c}{T_c^0} = 1 - \frac{g_2(1)g_3(1)^{-2/3}}{2} N^{-1/3} = 1 - 0.7275N^{-1/3}. \tag{11}$$

For $N=1000$, the transition temperature is lowered by 7% compared to the usual result [Eq. (5)] extrapolated from $N=\infty$. To measure this finite-N effect is in reach of current experiments [1–3]. Equation (9) describes the condensate fraction very well even for finite N; however, it is important to use T_c [Eq. (11)] and not T_c^0 (Fig. 3).

All experiments on BEC of atomic gases were done in anisotropic parabolic potentials. The generalization of the above treatment to a potential with three different frequencies ω_i is straightforward, and yields the exact result

$$N = \sum_{j=1}^{\infty} z^j \Big/ \prod_{i=1}^{3} (1-x_i^j), \tag{12}$$

with $x_i = \exp(-\beta\hbar\omega_i)$, and

$$N = \frac{z}{1-z} + g_3(z)\left(\frac{k_BT}{\hbar}\right)^3 \frac{1}{\prod \omega_i} + \frac{g_2(z)}{2}\left(\frac{k_BT}{\hbar}\right)^2 \frac{\sum \omega_i}{\prod \omega_i} \tag{13}$$

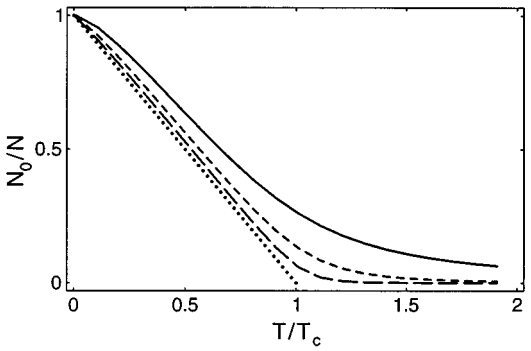

FIG. 4. The condensate fraction for a finite number N of atoms in a one-dimensional harmonic potential versus temperature. Plots are shown for $N=100$ (solid line), 10^4, 10^8, and infinite (dotted).

for $k_BT \gg \hbar\omega_i$.

The correction term to the transition temperature in (11) has to be multiplied by $\frac{1}{3}\Sigma\omega_i/(\Pi\omega_i)^{1/3}$, which is $\geqslant 1$, i.e., anisotropy enhances the low-N decrease of the transition temperature.

A nice feature of the exact result Eq. (12) is that it is valid for arbitrary ω_i. It is therefore possible to study the freezing out of degrees of freedom and the transition from a 3D system to systems of lower dimensions. The 1D case is particularly interesting because the standard result is that BEC is not possible, based on the use of the continuous spectrum [7]. Assuming $k_BT \ll \hbar\omega_i$ for $i=1$ and 2, from Eq. (12) with $\omega=\omega_3$ and $x=\exp(-\beta\hbar\omega_3)$, we obtain

$$N = \sum_{j=1}^{\infty} z^j/(1-x^j) = \frac{z}{1-z} + \sum_{j=1}^{\infty} \frac{z^j x^j}{1-x^j}. \tag{14}$$

Figure 4 shows the fraction of ground-state atoms versus temperature for various N. Qualitatively, the ''condensation phenomenon'' looks very similar to the 3D case, clearly indicating that BEC exists in a 1D harmonic potential in contrast to previous predictions [7].

For $\varepsilon = \hbar\omega/k_BT \ll 1$, Eq. (14) is approximated by [15]

$$N = \frac{z}{1-z} + \frac{1}{\varepsilon}\sum_{j=1}^{\infty} \frac{[z\exp(-\varepsilon/2)]^j}{j} = \frac{z}{1-z} - \frac{k_BT}{\hbar\omega}\ln\left[1 - z\exp\left(-\frac{\hbar\omega}{2k_BT}\right)\right]. \tag{15}$$

This approximation is already excellent for $N=100$. Equation (15) can also be obtained from Eq. (7) using $\rho(E)=1/\hbar\omega$, and introducing $\hbar\omega/2$ as the lower limit of the integral to avoid the unphysical low-frequency divergence.

The transition temperature T_c is determined by

$$N = \frac{k_BT_c}{\hbar\omega}\ln\left(\frac{2k_BT_c}{\hbar\omega}\right), \tag{16}$$

and the condensate fraction is $N_0/N=1-[T\ln(2k_BT/\hbar\omega)/T_c\ln(2k_BT_c/\hbar\omega)]$ with the logarithmic terms becoming negligible for large N.

In the limit of large N, the relation between the number of atoms and the transition temperature T_c in 1D is given by (16), in 2D it is [7] $N=(k_BT_c/\hbar\omega)^2 g_2(1)$, and in 3D $N=(k_BT_c/\hbar\omega)^3 g_3(1)$. This demonstrates that the general rule [implied by (10)], the tighter the confinement the higher the transition temperature for a given N, is still valid when degrees of freedom freeze out and the system becomes two or one dimensional. It is only the usual thermodynamic limit in d dimensions, which assumes $N\to\infty$ with $N\omega^d$ finite [5], which incorrectly predicts that BEC is not possible in a 1D harmonic potential.

A 2D box has the same density of states $\rho(E)\propto E$ as a 1D harmonic potential, and should therefore show identical behavior around the BEC transition. Using (7) with the energy of the first excited state as the low-frequency limit of the integral, we obtain the relation between N and T_c in a 2D box $N=2(L/\Lambda_t)^2\ln(L/\Lambda_t)$, compared to $N=(L/\Lambda_t)^3 g_{3/2}(1)$ in a 3D box of linear size L. $\Lambda_t=(2\pi\hbar^2/mk_BT)^{1/2}$ is the thermal de Broglie wavelength. Again, the number of atoms N needed to reach BEC at a given temperature T_c is lower in 2D than in 3D. However, the thermodynamic limit in d dimensions assumes $N\to\infty$ with N/L^d finite, resulting in a transition temperature of zero (or the absence of BEC) in 2D in this limit.

Our result on the possibility of observing BEC in a 1D atom trap is important for current experimental efforts. To achieve BEC in alkali vapors requires tight confinement in a magnetic trap. This was achieved using time-dependent magnetic fields [1], permanent magnets [2], or an optically plugged magnetic trap [3]. All these solutions entail quite some inflexibility for future experiments. The tightest confinement in a more conventional magnetic trap is achieved in the Ioffe-Pritchard configuration [16,17] with a very tight radial confinement. Transverse gradients of 500 G/cm and a bias field of 0.1 G result in a radial field curvature of 2.5×10^6 G/cm^2 corresponding to an oscillation frequency for Na atoms in the $F=2$ hyperfine state of 4 kHz. The separation between radial oscillator levels is 200 nK. We therefore expect the radial oscillations to freeze out at temperatures which have been reached by evaporative cooling [1]. Below 100 nK the systems behaves as a 1D harmonic oscillator, but will still undergo BEC. For example, with an axial frequency of 5 Hz, one-dimensional BEC would happen at 50 nK with $N=1060$. Another example of a highly anisotropic atom trap is the optical dipole trap [18,19]. In this case, transverse oscillation frequencies can be tens of kHz resulting in a transition from 3D to 1D dynamics at a temperature of about 1 μK.

In conclusion, we have discussed BEC in systems with a finite number of particles. It was shown that corrections due to the finite number are small, but observable in the case of a 3D harmonic oscillator. Highly anisotropic trapping configurations may correspond to a 1D harmonic oscillator or to a 2D or 1D box. In these configurations, BEC was predicted not to happen. We were able to show that this conclusion is only an artifact of the usual thermodynamic limit which does not apply to the situation realized in atoms traps where a finite number of atoms is given (instead of a linear density or a surface density).

We have restricted the discussion in this paper to the case of the ideal gas. It is well known that the inclusion of interactions between the particles profoundly changes the nature of the BEC phase transition [4], and is important for the occurrence of a macroscopic phase (i.e., of a broken symmetry). It would be very interesting to study how such interactions would affect the results presented here.

Note added: After submission of this work we learned that Eqs. (6) and (11) were derived independently by Grossmann and Holthaus using the density-of-state approach [20]. These authors have also discussed finite-N effects on BEC in a box potential [21,22]. For the case of the 1D harmonic potential, similar results were obtained by W. J. Mullin (private communication).

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