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Bose–Einstein Condensation in Harmonic Oscillator Potentials

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Abstract

Bose–Einstein Condensation (BEC) of both the ideal and the weakly interacting cold alkali gases confined by anisotropic harmonic oscillator potentials is investigated in this paper. It is shown that the transition point is shifted towards lower temperatures because of the trapped potentials, and the specific heat below the transition point is no longer proportional to $T^{3/2}$. Expressions of modified condensation temperature, internal energy and the specific heat are derived for the ideal trapped gases explicitly. Moreover, the effect of interactions among the atoms on the transition temperature is also given and discussed.

The recent observation of Bose–Einstein Condensation (BEC) in ultracold trapped alkali gases [1–3] have created a wave of renewed interest in this phenomenon. BEC is a purely quantum statistical phase transition, which is characterized by a macroscopic population of the ground state below the transition point T_c. Experiments on BEC demonstrated that below T_c (about a few microkelvin), several thousand atoms are found in the ground state. Because the gases are dilute, in most textbooks of statistical mechanics, e.g. [4], the theory of BEC is formulated for noninteracting bosons in a three-dimensional box. This treatment has been extended to power-law potentials by de Groot [5], Bagnato *et al.* [6] who found that the transition temperatures and the specific heat depend on the shape of the potentials. BEC in one- and two-dimensional systems is only possible for sufficiently confining potentials [7–9]. All these investigations are based on the use of the thermodynamic limit and the assumption that the ground state energy was negligible. However, recent BEC experiments on alkali gases were performed with finite numbers of particles [1–3]. For these relatively low numbers (about 10^9), the effects caused by the above approximation are nonvanishing.

In this paper, we study BEC in anisotropic harmonic oscillator potentials, because this kind of potentials is a good approximation to the recent BEC experiments. We will derive analytical expressions of the density of states for a system of a finite number of particles in an anisotropic harmonic oscillator potential, a direct application of this result to study BEC of atoms trapped in anisotropic harmonic oscillator potentials is given, meanwhile the effect of the nonvanishing ground state energy on BEC of atomic gases in trap potentials is evaluated. We indeed find marked differences from the usual treatments: the transition point is shifted toward lower temperatures by the trap potentials, the specific heat below the onset of condensation is no longer proportional to $T^{3/2}$, the effect of the ground energy is nonvanishing, and the interactions between the atoms increase or decrease the transition temperature, according to whether the scattering length is negative or positive.

In order to express the density of states for a system of ultracold atoms trapped in a potential, we consider a range of parameters describing the BEC of atoms [3]. The potentials for the centre-of-mass motion of a single atom in the ground electronic state can be approximated as a three-dimensional anisotropic harmonic oscillator potential with frequencies $\omega_y = 235$, $\omega_z = 410$, $\omega_x = 745$ Hz in the y, z and x directions, respectively. Because the trap potential forms a finite barrier, there are several thousand energy levels within the trap. In these several thousands of energy levels about 10^9 sodium atoms are distributed, therefore, it is too low a number to use the thermodynamic limit. Nevertheless, the finite number effects on BEC can be discussed in many ways [10, 11]. In this paper, we discuss the finite number effects using the density-of-state approach [12]. The energy eigenvalues for an atom trapped in an anisotropic oscillator potential read

$$E_N = E(n_x, n_y, n_z) = \sum_{i=x,y,z} \hbar\omega_i(n_i + \tfrac{1}{2}). \tag{1}$$

Under real experimental conditions the temperature is high on the scale of the trap level spacing, namely, $k_B T \gg \hbar\omega_i$ $(i = x, y, z)$. Therefore, within the canonical ensemble, the partition function

$$Q(\beta) = \sum_N e^{-\beta E_N} = \sum_{n_x, n_y, n_z = 0}^{\infty} e^{-\beta(n_x\omega_x + n_y\omega_y + n_z\omega_z)}$$
$$= \prod_{i=x,y,z} \frac{1}{1 - e^{-\beta\omega_i}} \tag{2}$$

of such a system without interactions can be expanded as follows:

$$Q(\beta) \simeq a_2\beta^{-3} + a_1\beta^{-2} + a_0\beta^{-1} + a_{-1} + O(\beta) \tag{3}$$

with

$$a_2 = \frac{1}{\omega_x\omega_y\omega_z},$$
$$a_1 = \tfrac{1}{2}a_2(\omega_x + \omega_y + \omega_z), \tag{4}$$
$$a_0 = \tfrac{1}{12}a_2(\omega_x^2 + \omega_y^2 + \omega_z^2 + 3\omega_x\omega_y + 3\omega_y\omega_z + 3\omega_z\omega_z),$$
$$a_{-1} = \tfrac{1}{8} + \tfrac{1}{24}(\omega_x/\omega_y + \omega_x/\omega_z + \omega_y/\omega_z$$
$$+ \omega_y/\omega_x + \omega_z/\omega_x + \omega_z/\omega_y), \tag{5}$$

where, $\beta = k_B T$, k_B is the Boltzmann constant, and the contribution of the ground state was singled away for special treatment. On the other hand, by making use of

$$Q(\beta) = \sum_N \mathrm{e}^{-\beta E_N} = \int_0^\infty \mathrm{e}^{-\beta E} \rho(E)\, \mathrm{d}E \tag{6}$$

the partition function can be calculated equally, where $\rho(E)$ is the density of states. Comparing with eq. (3), it is proved that the density of states $\rho(E)$ takes the form:

$$\rho(E) = b_0 + b_1 E + b_2 E^2 + \cdots \tag{7}$$

This expansion cannot contain the terms E^r with r being negative or non-integer, since they become zero after comparison with the direct calculation given by eq. (3). Substituting eq. (7) into eq. (6), one can easily find:

$$Q(\beta) = b_0 \beta^{-1} + b_1 \beta^{-2} + 2b_2 \beta^{-3} + \cdots \tag{8}$$

Comparison of eq. (8) with the direct calculation (3) shows that

$$b_0 = a_0, \quad b_1 = a_1, \quad b_2 = 0.5 a_2 . \tag{9}$$

There is an additional constant term b_0 in the density of states in comparison with the result of Grossmann [12]. As we see below, this additional term will result in a shift of the transition point.

Now, let us consider a system of N noninteracting bosons such that the population $N(E_i)$ of a state with energy E_i is given by the Bose–Einstein distribution

$$N(E_i) = \frac{1}{\mathrm{e}^{\beta(E_i - \mu)} - 1} . \tag{10}$$

Here, we set the statistical weights corresponding to the state E_i, $g_i = 1$. μ stands for the chemical potential, which is determined by the constraint that the total number of particles in the system is N:

$$N = \sum_i^\infty N(E_i). \tag{11}$$

Around the transition point, $\mu \simeq \varepsilon_0$ is a good approximation with error $1/n_0$ (ε_0 and n_0 denote the ground state energy and ground state population, respectively). Using the density-of-state approximation [10], eq. (10) can be rewritten as follows:

$$N = n_0 + \int_{E_{\min}}^\infty \frac{\rho(E)\, \mathrm{d}E}{\exp\left[\beta(E - \varepsilon_0)\right] - 1} + n_{\min} . \tag{12}$$

Here, we single out the ground state population n_0, because we are interested in BEC where the ground state plays a key role. $n_{\min}$ denotes the population of all the other states with energies below $E_{\min}$, for the case of particles trapped in a cavity with volume $N = L^3$, $E_{\min}$ takes a value which is at least $400h^2/8ML^2$ [10] to avoid the error of converting from sum to integral. Using eq. (7), we can obtain that

$$\begin{aligned} N = n_0 + n_{\min} + \tfrac{1}{2} a_2 \Bigg[& \beta^{-3} \Gamma(3) \zeta(3) \\ & - \frac{E_{\min}^2}{\beta} \left(\frac{\lambda^2}{2} + \lambda + \ln(\lambda - 1) \right) \Bigg] \\ & - \frac{a_0}{\beta} \ln\left[\beta \varepsilon_0 (\lambda - 1)\right] + \frac{a_1}{\beta^2} \frac{\pi^2}{6} \end{aligned} \tag{13}$$

where $\lambda = E_{\min}/\varepsilon_0$, $\Gamma(n)$ and $\zeta(n)$ denote the Gamma function and the Riemann's zeta function, respectively. The ground state population n_0 can be determined by the $E_{\min}$-independent part of the r.h.s. of eq. (13), because n_0 remains unchanged when the parameter $E_{\min}$ is varied. Thus, we have:

$$n_0 = N - \tfrac{1}{2} a_2 \beta^{-3} \Gamma(3) \zeta(3) + a_0 \beta^{-1} \ln(\beta \varepsilon_0) - \frac{a_1 \pi^2}{6\beta^2} . \tag{14}$$

The first two terms in eq. (14) are just the results in the thermodynamic limit [6], whereas the last two terms are direct corrections of the finite number effects. The corrections depend on the ground state energy ε_0 and the shape of the trap potentials.

If one introduces a temperature

$$T_c^0 = \frac{1}{k_B} \left(\frac{2N}{a_2 \zeta(3) \Gamma(3)} \right)^{1/3}, \tag{15}$$

which denotes the critical temperature of an infinite number atoms trapped in anisotropic oscillator potentials [6], then the critical temperature T_c for a finite number of atoms takes the form

$$\begin{aligned} T_c = T_c^0 \Bigg[& 1 - \frac{1}{3} \frac{b_1}{b_2} \frac{\pi^2}{3} \frac{k_B T_c^0}{\Gamma(3)\zeta(3)} \\ & + \frac{2}{3} \frac{b_0}{b_2} \frac{\ln(k_B T_c^0 \varepsilon_0)}{\zeta(3)\Gamma(3)} T_c^{0\,2} k_B^2 \Bigg]. \end{aligned} \tag{16}$$

The last term in square brackets is negative, since $(\varepsilon_0 / k_B T_c^0) \ll 1$. Hence, for a finite number of atoms trapped in anisotropic harmonic potentials, the temperature at which the BEC occurs is lower than T_c^0. To measure this effects is in reach of current experiments [1–3]. Equation (16) demonstrates that the tighter the confinement (larger $\omega_x, \omega_y, \omega_z$), the lower the critical temperature.

Generally speaking, the specific heat is more interesting from the experimental point of view, since the low-temperature behavior of the specific heat c_V is generally treated as the hallmark of onset of BEC. It is well known that the specific heat can be derived from the internal energy, which is expressed by

$$\begin{aligned} \beta U = {} & n_0 \beta \varepsilon_0 + \beta U_{\min} \\ & + \beta \int_{E_{\min}}^\infty \frac{E \rho(E)}{\exp\left[\beta(E - \varepsilon_0)\right] - 1} \mathrm{d}E. \end{aligned} \tag{17}$$

The first term on the right-hand side is the ground state energy, the second term stands for the energy of the other state below $E_{\min}$, the third term denotes the energy of the states above $E_{\min}$. Substituting eq. (7) into eq. (17), one easily finds

$$\begin{aligned} \beta U = n_0 \beta \varepsilon_0 + \frac{a_2}{2} \Bigg[& \beta^{-3} \Gamma(4) \zeta(4) + \frac{\varepsilon_0^2 \lambda^3}{3\beta(\lambda - 1)} \\ & + \varepsilon_0^3 (0.5\lambda^2 + \lambda + \ln(\lambda - 1)) \Bigg] \\ & + a_1 [\beta^{-2} \Gamma(3) \zeta(3) - \varepsilon_0^2 (0.5\lambda^2 + \lambda + \ln(\lambda - 1))] \\ & + \frac{a_0}{\beta} \left[\frac{\pi^2}{6} - \beta E_{\min} - \beta \varepsilon_0 \ln\left[\beta \varepsilon_0 (\lambda - 1)\right] \right]. \end{aligned} \tag{18}$$

The λ-dependent terms can be dropped, because λ appears only in the higher order terms [10]. In T_c^0 term, the specific heat $c_V = (1/N)(\partial U/\partial T)$ below T_c is given by

$$c_V = k_B \Gamma(4)\zeta(4)\left(\frac{a_2}{N}\right)^2 \Gamma(3)\zeta(3)\left(\frac{T}{T_c^0}\right)^3 + 3k_B[\Gamma(3)\zeta(3)]^{5/3}\left(\frac{a_2}{2}\right)^{2/3} a_1\left(\frac{1}{N}\right)^{5/3}\left(\frac{T}{T_c^0}\right)^2 + \frac{\pi^3}{3} k_B[\Gamma(3)\zeta(3)]^{1/3}\left(\frac{a_2}{2}\right)^{1/3} a_0\left(\frac{1}{N}\right)^{4/3} \frac{T}{T_c^0}. \quad (19)$$

The last two terms on the right-hand side are caused by the finite number of atoms effect. It is thus absent in the thermodynamic limit [6]. At the onset of BEC, the relative importance of the three distributions is about $1 : N^{-4/3}a_2^{-4/3}a_1 : N^{-4/3}a_2^{-5/3}a_0$, in all current experiments on BEC of atomic alkali gases, the number of atoms trapped in a potential is at least 10^4, the frequency of the oscillator potential is taken to be about 0.5×10^3 Hz, therefore, the last two terms in eq. (19) can be dropped and the T^3-law can be treated as a hallmark of the atomic BEC in harmonic oscillator potentials.

It is worth noting that there are not only effects due to the thermodynamic limit but also effects caused by the interactions between the atoms. In the end of this paper, we will discuss the effect of the interactions between the atoms on the transition temperature in details. The atoms contained in anisotropic oscillator potentials interact with one another through binary collisions, which are characterized by the s-wave scattering length a. Using the mean-field approximation, the interaction energy between the atoms is $\gamma n(\mathbf{r})$ proportional to the local density $n(\mathbf{r})$ [6]. γ denotes the interaction constant which depends only on the s-wave scattering length a at low temperature, $\gamma = 2\pi\hbar^2 a/M$, where M is the mass of an atom. Under the local density approximation (LDA) [13], the density of the gas is given by

$$n(\mathbf{r}) = \exp[-\beta V(\mathbf{r})]/\lambda^3 \quad (20)$$

where $\lambda = \hbar/\sqrt{2\pi M k_B T}$ is the thermal de Broglie wavelength. $V(\mathbf{r})$ stands for the trapped potentials. The LDA is a good approximation when $k_B T \gg \hbar\omega_i$ $(i = x, y, z)$ [14]. Because the gas is weakly interacting, $n(\mathbf{r})$ can be expanded in powers of γ. Retaining the first term, the density of states takes the form

$$\rho(E) = a_0\left(1 + 0.5\frac{\gamma}{\lambda k_B T}\right) + a_1\left(1 + \frac{\gamma}{\lambda k_B T}\right)E + 0.5a_2\left(1 + 1.5\frac{\gamma}{\lambda k_B T}\right)E^2. \quad (21)$$

In first order approximation, the effects of the interactions between the atoms are only to modify the parameter in the expression of $\rho(E)$. The modified results are equal to increasing or decreasing of the frequency for the light field used to trap the atoms, according to whether the scattering length is negative or positive. Following the above procedure, the transition temperature is given by

$$T_c = T_c^{\gamma=0} - \frac{\gamma}{\lambda_0}\frac{1}{k_B T_c^0} T_c^{\gamma=0}, \qquad \lambda_0 = \frac{\hbar}{2\pi M k_B T_c^0} \quad (22)$$

where T_c^0 was represented by eq. (15), $T_c^{\gamma=0}$ stands for the transition temperature for $\gamma = 0$. Equation (22) shows that if the scattering length is negative, T_c is larger than $T_c^{\gamma=0}$. As expected, the correction is proportional to the ratio γ/λ_0. In most textbooks of statistical mechanics, the problem of BEC of imperfect Bose gases was discussed with the assumption that the scattering length a is positive. For alkali atoms, however, the problem is much more complex, since the molecular potential curves which can typically support many bound states are not known precisely. Some of the atoms (e.g. cesium) are believed to have a positive a [15], and others (e.g. lithium) to have a negative a [16]. In this paper we show that binary collisions with negative a increase the critical temperature. With the same procedure, we can derive the specific heat below the critical temperature, the correction of the interactions between the atoms to the specific heat is also proportional to γ/λ_0.

In conclusion, we have discussed the BEC of atomic gases trapped in anisotropic oscillator potentials, it was shown that corrections due to the effect of finite atoms and the ground state energy are small, but observable. The transition point was shifted toward lower temperature in comparison with the case in the thermodynamic limit. The T^3-law for the low-temperature behavior of c_V may still be used to detect the onset of BEC.

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