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Simultaneously Finite Size and Interaction Effects on a Harmonically Trapped ^{87}Rb Gas

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Abstract

In the framework of the semiclassical approximation ($K_B T >> \hbar\Omega$), an accurate ansatz formula for the density of states is suggested. This formula is able to include the finite size, interatomic interaction effects, and the role of dimensionality simultaneously. Condensed fraction, and average energy per particle for a condensed ^{87}Rb gas in anisotropic trap in 3D and 2D are calculated. The results for the above mentioned thermodynamic quantities show good agreement with the measured experimental results. Furthermore, full agreement is obtained with the other method used to calculate the same quantities.

Key Words: Bose-Einstein condensation; finite size and interaction effects; density of states approach.

1. Introduction

Bose-Einstein condensation (BEC) has been observed with ^{87}Rb, ^{23}Na, ^{7}Li, ^{1}H, ^{85}Rb, ^{4}He, ^{41}K, ^{133}Cs , ^{174}Yb and ^{52}Cr [1–10], neutral bosonic atoms. This experimental achievement has stimulated a new interest in the theoretical study of boson gases. Determination of thermodynamical quantities such as the condensate fraction, average energy per particle, specific heat, and release energy as functions of temperature are of primary interest in the study of these condensations. The nature of BEC is fundamentally affected by the finite size effects, harmonic oscillator length, inhomogeneity, and interatomic interactions. In fact the question of how these parameters affect the thermodynamic quantities of these systems have been the object of several theoretical investigations [11–14]. The above mentioned effects lead to a significant correction to the thermodynamical parameters of the system. So it is very important to study the leading corrections due to these effects simultaneously.

In doing this we will extend the previous work [15–17] on the thermodynamics of an ideal isotropic gas to the interacting anisotropic gas. The authors there studied the ideal gas of bosons trapped in a three-dimensional isotropic and/or anisotropic harmonic oscillator potential. They employed an approach where the sum over the discrete space, for the thermodynamical quantities, was replaced by an integral with an appropriate density of states [18–23]. Moreover, it has been proposed that highly anisotropic traps may freeze out one or two dimensions, so that the system to a good approximation is lower dimensional. This implies that it is of interest to study these systems also.

In this paper, an accurate ansatz formula for the density of states is suggested [24]. This ansatz formula is able to include the finite size, interatomic interaction, and anisotropicity effect simultaneously. The calculated results for the condensed fraction, and average energy per particle are compatible with the measured experimental data. Furthermore, full agreement is obtained with the other methods used to calculate the same quantities.

The plan of the present paper is as follows. In the next section we study interacting bosons in a confining anisotropic harmonic potential in three dimensions (3D) and review the density of states approach. In section three, simultaneously finite size and interaction effects on the condensate fraction, and the average energy per particle are calculated. The obtained results are compared with experimental results. In section four, we discuss the same system in one and two spatial dimensions. In section five we summarize and conclude.

2. A simple model of a trapped Bose gas

2.1. BEC in 3D anisotropic harmonic trap

For a system of N indistinguishable particles, distributed in an external anisotropic harmonic oscillator potential, $V_{\text{ext}}(\mathbf{r}) = \frac{m}{2}(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2)$, the single particle energies are given by

$$E_{n_1 n_2 n_3} = \hbar(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3) + E_0, \tag{1}$$

where $n_1, n_2, n_3 = 0, 1, 2, 3, ...$ and E_0 is the zero point energy. If the system is described using the grand canonical ensemble, the number of its particle can be obtained from the first principle of statistical mechanics. The mean number of particles in any state is given by Bose-Einstein distribution

$$n(E_{n_1 n_2 n_3}) = \frac{z e^{-\beta E_{n_1 n_2 n_3}}}{1 - z e^{-\beta E_{n_1 n_2 n_3}}}, \tag{2}$$

where $\beta = (1/K_B T)$, K_B is the Boltzmann constant. The fugacity z is given in terms of the chemical potential μ as $z = e^{\beta(\mu - E_0)}$. The chemical potential μ and the temperature T are determined from the constraints on total number N and average energy per particle E of the system particles are

$$\begin{aligned} N &= \sum_{n_1 n_2 n_3} n(E_{n_1 n_2 n_3}) = \sum_{n_1 n_2 n_3} \sum_{j=1}^{\infty} z^j e^{-j\beta E_{n_1 n_2 n_3}}, \\ E &= \sum_{n_1 n_2 n_3} E n(E_{n_1 n_2 n_3}) = \sum_{n_1 n_2 n_3} \sum_{j=1}^{\infty} z^j E e^{-j\beta E_{n_1 n_2 n_3}}. \end{aligned} \tag{3}$$

Degeneracy factors are avoided by accounting for degenerate states individually. The phenomenon of BEC for noninteracting particles is fully described by equations (1) to (3). The condensed fraction, average energy per particle, and the critical temperature for ideal Bose gas in the thermodynamic limit $N \to \infty$, are given by

$$\begin{aligned} \frac{N_0}{N} &= (1 - t^3) \\ \frac{E}{N K_B T_0} &= 3\frac{\zeta(4)}{\zeta(3)} t^4 + \frac{E_0}{N_0 K_B T_0} \\ T_0 &= \frac{\hbar\Omega}{K_B} \left(\frac{N}{\zeta(3)}\right)^{1/3}, \end{aligned} \tag{4}$$

respectively. In equation (4), N_0 is the ground state occupation number, ζ is the Riemann zeta function, $t = \left(\frac{T}{T_0}\right)$ is the reduced temperature, and $\Omega = (\omega_1 \omega_2 \omega_3)^{1/3}$ is the geometric averages of the oscillator frequencies. The thermodynamic quantities given in equation (4) contains no free parameters and is not fit to experimental measured data.

2.2. Density of states method

The sum in equation (3) cannot evaluated analytically in a closed form. Another possible way to do this analysis is to approximate the sums by integrals. This approximation required that the condition $K_BT >> \hbar\Omega$ must be satisfied. A crucial feature in obtaining a reliable semiclassical approximation is to use an appropriate density of states $\rho(E)$ [15–23]. In equation (3), if the lowest energy E_0 is separated out from the sum, the number of particles in this state is N_0 (this number can be macroscopic, i.e. of the order of N, when $\mu \approx E_0$) leads to

$$\begin{aligned} N &= N_0 + \sum_{j=1}^{\infty} z^j \int_0^{\infty} \rho(E) e^{-j\beta E} dE \\ E &= E_0 + \sum_{j=1}^{\infty} z^j \int_0^{\infty} E\rho(E) e^{-j\beta E} dE \end{aligned} \tag{5}$$

Equation (5) contains nearly all the main effects which can be altered for the ideal Bose gas physics. The number of spatial dimensions, finite size, interatomic interactions, and the confining potential effects , are all taken care of in the power law of the density of states, $\rho(E)$. Some of thermodynamic quantities can be calculated without difficulty.

A better approximation for the density of states is given by Grossmann and Holthaus [15]. They constructed a continuous density of states, for isotropic trap, as

$$\rho(E) = \frac{1}{2}\frac{E^2}{(\hbar\Omega)^3} + \gamma\frac{E}{(\hbar\Omega)^2}, \tag{6}$$

where the coefficient γ depends on the individual oscillator frequencies and it is given by [18–22]

$$\gamma = \frac{1}{2}(\omega_1\omega_2\omega_3)^{2/3}[\frac{1}{\omega_1\omega_2} + \frac{1}{\omega_1\omega_3} + \frac{1}{\omega_2\omega_3}]$$

for isotropic oscillator $\gamma = 3/2$, which follows immediately from the relation $g_l = \frac{1}{2}l^2 + \frac{3}{2}l + 1$.

Substitution of equation (6) into equation (5), after performing the integral, we have the finite size correction for the condensed fraction and average energy per particle as follows [15, 18–22]:

$$\begin{aligned} \frac{N_0}{N} &= (1 - t^3) - \gamma\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}t^2 \\ \frac{E}{NK_BT_0} &= 3\frac{\zeta(4)}{\zeta(3)}t^4 + 2\gamma\left(\frac{\zeta(3)}{N}\right)^{1/3} t^3 + \frac{E_0}{N_0K_BT_0}. \end{aligned} \tag{7}$$

The same result of equation (7) is obtained by Ketterle and Druten [25]. They suggested that the behavior of the finite number of particles given in equation (7) is similar to the thermodynamic limit ($N \to \infty$), even for $N > 10^4$. However, the contribution of the last term in equation (7) is important. These approximation methods in which the sum is replaced by integrals, have been criticized by Kristen and Toms [18–22]. Instead, they propose to evaluate the sum directly by contour integration. In spite of that, this method is difficult to use in the transition region, it gives results similar to those of equation (7). Moreover, Kristen and Toms give a more modified form for the density of states $\rho(E) \approx (1/2)c_1E^2 + c_2E + c_3$, where c_i's is a constant defined in terms of ω's. The last term in this formula, c_3 term, will produce $\zeta(1)$ function in the condensation fraction and T_c formula. Since, $\zeta(1) = \infty$, then T_c and N/N_0 are undefined at onset of the condensation.

From the above results one can see that the role of interatomic interaction is not predicted in equation (7). However, effect of interaction is considered by other method and for isotropic oscillator. Naraschewski and Stamper-Kurn calculated the effect of interaction on the condensed fraction by using the semi-ideal model approach [26]. A more convenient analysis is considered by Dalfovo et al [14]. They give the same expression for the condensed fraction and average energy per particle. Also Giorgini et al develop the formalism of mean field theory approach [11–13]. By employing the WKB semiclassical approximation for the excited states they drive systematic results for the temperature dependence of various thermodynamical quantities. The results is given by

$$\begin{aligned} \frac{N_0}{N} &= (1-t^3) - \eta\frac{\zeta(2)}{\zeta(3)}(1-t^3)^{2/5}t^2 \\ \frac{E}{NK_bT_0} &= 3\frac{\zeta(4)}{\zeta(3)}t^4 + \frac{1}{7}\eta\left(1-t^3\right)^{2/5}\left(5+16t^3\right). \end{aligned} \tag{8}$$

The second term in equation (8) describes the influence of the interaction effect to lowest order in η. The parameter eta is a scaling parameter gives the scaling behavior of all thermodynamic quantities due to interatomic interaction. It is defined as [14]

$$\frac{\mu(N_0,T)}{K_BT_0} = \frac{\mu(N,T=0)}{K_BT_0}(\frac{N_0}{N})^{2/5} = \eta(1-t^3)^{2/5}.$$

This is the usual semiclassical approximation founded in the literature. In the next section an expressions for the condensed fraction, and the average energy per particle will be obtained. These two effects are considered simultaneously.

3. Simultaneously finite size and interaction effects

The accurate density of states for simultaneously finite size and interaction effects can be obtained by gathering the Grossmann ansatz formula [15] and interaction effect calculated in our previous paper [24]. Equation (7) provides us by the finite size correction, second term. Then we will fix the coefficient of E^2 as given in equation (7). A new term will be add to the constant γ. This new term, $\frac{\mu}{\hbar\Omega}$, gives a correction due to the interatomic interaction effect as obtained by semi-ideal model, mean field theory approximation, and canonical statistics approach [14, 26, 27]. Finally, in order to obtained the anisotropic effect, the interacting term will be multiplied by $\frac{\bar{\omega}}{\Omega}$. The new ansatz formula becomes

$$\rho(E) = \frac{1}{2}\frac{E^2}{(\hbar\Omega)^3} + \frac{E}{(\hbar\Omega)^2}\{\gamma + (\frac{\bar{\omega}}{\Omega})\frac{\mu}{\hbar\Omega}\}, \tag{9}$$

where $\bar{\omega} = \frac{1}{3}(\omega_1+\omega_2+\omega_3)$ is the arithmetic averages of the oscillator frequencies. Substitution from equation (9) into equation (5), after performing the integral, the condensed fraction, and the average energy per particle are given by

$$\begin{aligned} \frac{N_0}{N} &= (1-t^3) - \{\gamma\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}t^2 + (\frac{\bar{\omega}}{\Omega})(\frac{\mu}{K_BT})\frac{\zeta(2)}{\zeta(3)}t^3\} \\ \frac{E}{NK_BT_0} &= 3\frac{\zeta(4)}{\zeta(3)}t^4 + \{2\gamma\left(\frac{\zeta(3)}{N}\right)^{1/3}t^3 + 2(\frac{\bar{\omega}}{\Omega})(\frac{\mu}{K_BT})t^4\} + \frac{E_0}{N_0K_BT_0}. \end{aligned} \tag{10}$$

Using the relations $\frac{\mu}{K_BT} = \eta(1-t^3)^{2/5}/t$ and $\frac{E_0}{N_0K_BT_0} = \frac{5}{7}\eta(1-t^3)^{2/5}$ [11,12,26,27], the last term in equation (10) gives exactly the usual lowest-order modification due to interatomic interaction effect as obtained in equation (8):

$$\begin{aligned} \frac{N_0}{N} &= (1-t^3) - \{\gamma\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}t^2 + \eta(\frac{\bar{\omega}}{\Omega})\frac{\zeta(2)}{\zeta(3)}(1-t^3)^{2/5}t^2\} \\ \frac{E}{NK_BT_0} &= 3\frac{\zeta(4)}{\zeta(3)}t^4 + 2\gamma\left(\frac{\zeta(3)}{N}\right)^{1/3}t^3 + \frac{1}{7}\eta\left(1-t^3\right)^{2/5}\left(5+14(\frac{\bar{\omega}}{\Omega})t^3\right). \end{aligned} \tag{11}$$

Equation (11) gives the corrections due to the interatomic interaction and finite number of particles of the system simultaneously. Moreover, equation (11) contain two free parameters, so it provides a detailed test for the system. It is obtained that these two parameters are accounted for finite size and interatomic interaction effects [15,24]. In our approach these two effects can be studied simultaneously. The same results of equation (11) is obtained by Xiong et al via the canonical statistics approach for the condensed fraction [27].

In Figure 1 we represent the condensed fraction N_o/N as a function of the reduced temperature $t = T/T_o$. We choose our scaling temperature to be T_o as given in equation (4). For $\gamma = 1.66$ and $\eta = 0.45$, these two effects lead to a reduction in the condensed fraction comparing to equation (4) by about 10%. Our results agree well with the measured experimental data [28].

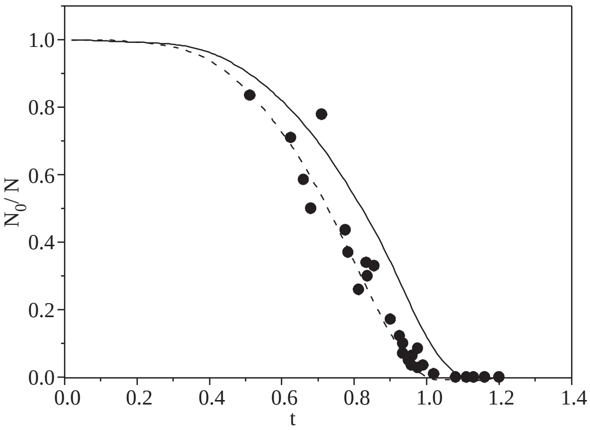

Figure 1. Condensed fraction, N_o/N, as a function of reduced temperature $t = T/T_o$. Black circles are the experimental results of Ensher et al. [28]. The dashed line shows the results calculated from equation (11) for $\eta = 0.45$ and $\gamma = 1.66$, The value of γ is calculated from ω's as given in [28]. The solid line shows the condensed fraction,$N_o/N = 1 - t^3$, of the ideal gas in a harmonic potential.

The second result we present in equation (11), is the total energy per a particle. In Figure 2 we report the obtained results as a function of reduced temperature t. At high temperature the behavior is given by the classical law $E/NK_BT_0 = 3t$ [13]. The average energy per particle is increased by about 5% due to finite size and interatomic interaction effects with respect to the ideal gas case. Our results are compatible with the results calculated in reference [13] for $\gamma = 1.7$ and $\eta = 0.45$.

4. Role of dimensionality

All BEC-experiments on trapped Bose gases reported so far are performed on three-dimensional systems. Though the trapping frequencies in each direction can be quite different, nevertheless the relevant results for the temperature dependence of the condensate have been obtained assuming that $K_BT >> \hbar(\omega_1\omega_2\omega_3)^{1/3}$. In order to observe effects of reduced dimensionality, one should remove such a condition in one or two directions.

In one dimension, the situation is particularly interesting because the standard results is that BEC is not possible [29]. In our calculation thermodynamic quantities relevant to BEC in one dimension cannot predicted, even in the presence of the harmonic potential, since in our approach $\rho(E) \sim E^{d-1}$. However, for ideal Bose gas in one dimension the condensed fraction and the critical temperature are given by Ketterle and Druten [25].

In two dimensions, the same method for the three dimensions can be used. We start by examining the case of a highly anisotropic three-dimensional system, and demonstrate the effective reduction to two dimensions when one of the oscillator frequency is much higher than the other two oscillator frequencies.

Excitations in a given direction of the trap will be suppressed when the temperature is below the energy scale set by the corresponding oscillator strength. Assuming $K_BT << \hbar(\omega_1\omega_2\omega_3)$ for $\omega_3 >> \omega_{1,2}$, then the highly anisotropic trap should therefore effectively be two dimensions.

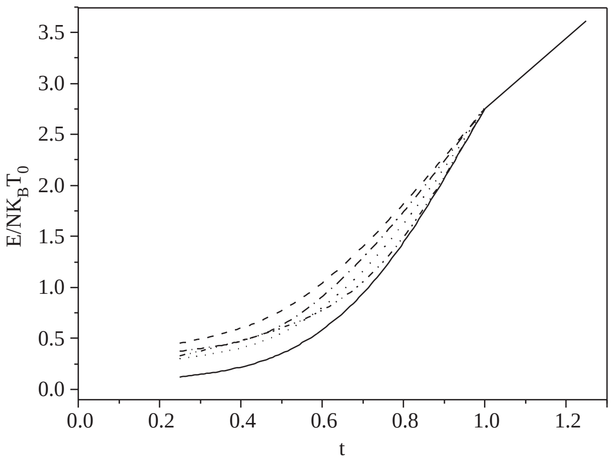

Figure 2. Average energy per particle, $\frac{E}{NK_BT_0}$, as a function of the reduced temperature, $t = T/T_0$ for three values of scaling parameter η. Dashed line: $\eta = 0.45$; the dashed dot line: $\eta = 0.39$; dotted line: $\eta = 0.31$ [13]. The boled dashed dot dot line is the results calculated from equation (11) for $\eta = 0.45$ and $\gamma = 1.7$. The total number of particles is taken to be 50000. The solid line refer to the noninteracting model in the large N limit (ideal gas).

4.1. Reduction to two dimensions

Since $\rho(E) \sim E^{d-1}$, consequently the integral for the condensed fraction in equation (5) divergence in 2D, also. we can avoid this divergence by introducing $\hbar\omega$ as the lower limit of the integral, with $\omega = (\omega_1\omega_2)^{1/2}$. For ideal Bose gas in two dimensions, the condensed fraction, and the average energy per particle are given by [30, 31]

$$\begin{aligned}\frac{N_0}{N} &= (1 - t'^2)\\ \frac{E}{NK_BT_0T_0^{2d}} &= 2\frac{\zeta(3)}{\zeta(2)}t'^3 + \frac{E_0}{N_0K_BT_0^{2d}}\\ T_0^{2d} &= \frac{\hbar\omega}{K_B}\left(\frac{N}{\zeta(2)}\right)^{1/2},\end{aligned} \tag{12}$$

with $t' = \frac{T}{T_0^{2d}}$ being the reduced temperature in two dimensions.

Effects of finite size and interatomic interaction are expected to modify in a deep way the nature of the condensation described by equation (12). In particular, interacting Bose systems exhibit the well-known Berezinsky-Kosterlitz-Thouless transition in 2D [32, 33]. However, for the interacted gas in a 2D harmonic trap with the fundamental frequencies ω_1, ω_2, the condensate fraction, $\frac{N_0}{N}$, and the average energy per particle, $\frac{E}{NK_BT_0^{2d}}$, can be calculated from the two equations

$$\begin{aligned}N &= N_0 + \sum_{j=1}^{\infty} z^j \int_{\hbar\omega}^{\infty} \rho(E)e^{-j\beta E}dE\\ E &= E_0 + \sum_{j=1}^{\infty} z^j \int_{0}^{\infty} E\rho(E)e^{-j\beta E}dE\end{aligned} \tag{13}$$

and

$$\rho(E) = \frac{E}{(\hbar\omega)^2} + \frac{1}{(\hbar\omega)}\{\gamma + (\frac{\bar{\omega}}{\omega})\frac{\mu}{\hbar\omega}\}, \tag{14}$$

where $\bar{\omega} = \frac{1}{2}(\omega_1 + \omega_2)$. The expressions for the condensed fraction and average energy per particle are given by

$$\begin{aligned} \frac{N_0}{N} &= 1 - \frac{g_2(e^{-(\frac{\zeta(2)}{N})/t'})}{\zeta(2)}t'^2 - \{[\gamma + \eta(\frac{\bar{\omega}}{\omega})(1-t'^2)^{2/5}] + 1\}\frac{g_1(e^{-(\frac{\zeta(2)}{N})/t'})}{\zeta(2)^{1/2}}\frac{1}{N^{1/2}}t' \\ \frac{E}{NK_BT_0} &= 2\frac{\zeta(3)}{\zeta(2)}t'^3 + \gamma\left(\frac{\zeta(2)}{N}\right)^{1/2}t'^2 + \frac{1}{7}\eta\left(1-t'^2\right)^{2/5}\left(3 + 14(\frac{\bar{\omega}}{\omega})t'^2\right)\}t'^2, \end{aligned} \tag{15}$$

where the relations $\frac{\mu}{K_BT} = \eta(1-t'^2)^{2/5}$ and $\frac{E_0}{N_0K_BT_0} = \frac{5}{7}\eta(1-t'^2)^{2/5}/t'$ are used. $g_n(e^{-(\frac{\zeta(2)}{N})/t'}) = \sum_{j=1}^{\infty}\frac{(e^{-(\frac{\zeta(2)}{N})/t'})^j}{j^n}$ is the usual Bose function. In the thermodynamic limit, $N \to \infty$, equation (15) leads to the same results given in equation (12). The Q2D will be consider in detail elsewhere.

5. Conclusion

In this paper, a new ansatz formula for the density of states is suggested. This formula is used to calculate the condensed fraction and the average energy per particle. It was shown that the corrections due to the finite size, and interatomic interaction can be calculated simultaneously.

Finite size effect and Interatomic interaction effect lead to a reduction in the condensed fraction. While the average energy per particle is increased. However, the measured internal energy is found higher in the BEC phase than predicted by the ideal Bose gas model. Increasing of the average energy per particle is understood as a consequence of the interatomic repulsion force. A quantitative estimate is still lacking.

In conclusion, we have discussed BEC in anisotropic system with finite size and interaction effects. It was shown that the corrections due to these three effects can be observed simultaneously. The results for the thermodynamical quantities are in agreement with those of the other methods mentioned in the text. The new ansatz formula for the density of states allows one, in a very clear fashion, to see how the thermodynamic quantities are affected simultaneously by finite size and interaction effects. In contrast to the other methods, density of state approach involves only analytical calculation without technical complication. The method we have outlined can be extend to many other situations of interest, such as the critical temperature, release energy and specific heat, and we will present a more complete discussion elsewhere.

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