CRITICAL ATOM NUMBER OF A HARMONICALLY TRAPPED ^{87}Rb BOSE GAS AT DIFFERENT TEMPERATURES

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Received July 16, 2008

We have graphically determined the critical atom number of a harmonically trapped ^{87}Rb Bose gas, for different temperature values. The critical point is defined as the intersection between the condensed atoms N_0, and the excited atoms N_{ex}, when graphically represented at the same reduced temperature. Both condensed and excited atoms are calculated using a modified density of states. This modification assures the extension of its domain of applicability. The main effects, confining potential, finite size and interatomic interaction effects, can be all simultaneously taken into consideration. The results of the modified approach are shown to coincide with purely quantum-mechanical calculations for finite size effect. Moreover, good agreement was obtained with the measured experimental results for ^{87}Rb, as reported in Gerbier *et al.* [2].

Key words: Density of states, thermodynamical properties of condensates, critical point for Bose-Einstein condensation.

1. INTRODUCTION

Recent experiments on Bose-Einstein condensation (BEC) have drawn significant attention [1–3]. In such experiments, typical values for the number of atoms and temperature at the transition are measured. They are also called critical point values. The measured data result was deviated from both the ideal gas ones and from the calculated results, based on the mean field theory or the local density approximation [4].

In our previous paper, a new accurate ansatz formula for the density of states was suggested [5]. This ansatz formula considered the finite size, the interatomic interactions and the anisotropy effect, all of them simultaneously. The calculated results for the condensed fraction, release energy and the specific heat are compatible with the experimentally measured results [6, 7]. Furthermore full agreement is obtained with other methods used in order to determine the corresponding parameters.

Surprisingly, fewer attention was payed to the critical point for the BEC phenomenon. Transition temperature T_c and the corresponding critical atoms number N_c, are still lacking [1, 3]. An efficient method for determining the critical point relevant to this experiment is the graphic representation [8]. This method is required to calculate both the condensed atoms number N_0 in the ground state, and the number of atoms in the excited state N_{ex}. An accurate method for determining these two numbers is the semiclassical approximation, which has been employed when considering the properties of Bose-condensed ideal gases trapped in power-law potentials [9]. Finite size effects on the temperature dependence of the condensate fraction in presence of an external trap, have been investigated using the semiclassical approximation, that is the density of states approach [10–12]. The advantage of the density of states approach is its simplicity, compared to quantum-mechanical calculations, while its generality makes it suitable for describing the interacting trapped Bose gas. The calculated results are taken over the effective temperature range for the experiment of Gerbier *et al.* [1], 300–600 nK. There is a significant agreement between our obtained results and the measured experimental data.

Our paper is organized as follows. The density of states approach in case of simultaneously finite size and interatomic interaction effects is presented in section two. In section three, the condensate temperature and the corresponding critical atoms number are determined. In section four, we summarize and conclude.

2. DENSITY OF STATES APPROACH

Quantitative information about the Bose-Einstein phase transition can be obtained by considering the statistical mechanics of atoms at a temperature T, obeying a Bose-Einstein energy distribution:

$$n_i(E_i) = \frac{1}{e^{\beta(E_i-\mu)}-1} = \frac{ze^{-\beta(E_i-E_0)}}{1-ze^{-\beta(E_i-E_0)}}, \quad (1)$$

where $n_i(E_i)$ is the population of atoms in the (possibly degenerate) atomic state with energy E_i; μ is the chemical potential and E_0 is the ground state energy. The fugacity z is expressed in terms of the chemical potential μ as $z = e^{\beta(\mu-E_0)}$, with $\beta = (1/K_B T)$, where K_B is the Boltzmann constant. This result can be inferred from the first principles using the grand canonical ensemble. The total number of particles N, is given by

$$N = \sum_{i=0}^{\infty} n(E_i) = \sum_{i=0}^{\infty} \frac{ze^{-\beta(E_i-E_0)}}{1-ze^{-\beta(E_i-E_0)}} \quad (2)$$

Atomic ensembles in BEC experiments are typically held in a three-dimensional harmonic potential

$$V_{ext}(\mathbf{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

with the corresponding quantized energy levels

$$E_i' = E_i - E_0 = \hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z), \tag{3}$$

where $E_0 = \frac{\hbar}{2}(\omega_x + \omega_y + \omega_z) = \frac{3}{2}\hbar\bar{\omega}$ is the zero point energy. By substituting Eq.(3) in Eq.(2), and then using the relation

$$\frac{ze^{-\beta E_i'}}{1 - ze^{-\beta E_i'}} = \sum_{j=1}^{\infty} z^j e^{-j\beta E_i'}, \tag{4}$$

we obtain

$$N = \sum_{j=1}^{\infty} z^j \left(\sum_{i=0}^{\infty} e^{-j\beta E_i'} \right) \tag{5}$$

The second sum in Eq. (5) cannot be analytically expressed as a closed form. An approximation is required. Another possible way to perform this analysis, is to approximate the second sum in Eq. (5) directly with an integral

$$N - N_0 = \sum_{j=1}^{\infty} z^j \int_0^{\infty} \rho(E) e^{-j\beta E} dE, \tag{6}$$

where $\rho(E)$ is the density of states. 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 would be

$$\rho(E) = \frac{1}{2}\frac{E^2}{(\hbar\Omega)^3} + \gamma\frac{E}{(\hbar\Omega)^2} \tag{7}$$

Introducing this expression for the density of states into Eq. (6), yields to

$$N = N_0 + g_3(z)\left(\frac{K_B T}{\hbar\Omega}\right)^3 + \gamma g_2(z)\left(\frac{K_B T}{\hbar\Omega}\right)^2, \tag{8}$$

where the coefficient γ depends on the individual oscillator frequencies, $\gamma = \frac{3}{2}\frac{\bar{\omega}}{\Omega}$ [12], and $\Omega = (\omega_x \omega_y \omega_z)^{1/3}$ represents the geometric average of the oscillator frequencies. A similar result with Eq. (8) is obtained by Ketterle and Druten [13]. They suggested that the behavior of the finite number of particles given in Eq. (8) is similar to the thermodynamic limit ($N \to \infty$), even for $N > 10^4$. However, the contribution of the last term in equation Eq. (8) is important. *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*. The same formula for the density of states can be found in [10] and it is calculated in [12].

For an ideal Bose gas in the thermodynamic limit $N \to \infty$, the condensed fraction and the transition temperature respectively, are given by

$$\frac{N_0}{N} = (1 - t^3)$$
$$T_0 = \frac{\hbar\Omega}{K_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}, \tag{9}$$

Where $\zeta(n)$ is the Riemann zeta function and $t = (T/T_0)$ represents the reduced temperature. These results can be directly obtained from Eq. (5), if we use $\rho(E) = \frac{1}{2}\frac{E^2}{(\hbar\Omega)^3}$. The thermodynamic quantities given in Eq. (9) contain no free parameters and they do not fit with experimentally measured data. Finally, Eq. (8) can be written in terms of the reduced temperature $t = T/T_0$ as,

$$\frac{N_0}{N} = (1 - t^3) - \gamma\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}t^2 \tag{10}$$

The second term in Eq. (10) depends on *N*, thus characterizing the finite size effect. The correction for the transition temperature due to finite-size effects has shown to be

$$T_c = T_0\left[1 - \gamma\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}t^2\right]^{\frac{1}{3}} = T_0(1 - 0.48\gamma N^{-1/3}) \tag{11}$$

This critical temperature shift given in Eq. (11), is reported by many authors [10, 11, 13]. From the above results, it is obvious that the role of interatomic interaction is not predicted in Eq. (11).

Generally, the second sum in Eq. (5) is converted directly into an ordinary integral, with a density of states given by [5, 6],

$$\rho(E) = \frac{1}{2}\frac{E^2}{(\hbar\Omega)^3} + \frac{E}{(\hbar\Omega)^2}\left\{\frac{3}{2} + \frac{\mu}{\hbar\Omega}\right\} \tag{12}$$

For later convenience, let us introduce the scaling interaction parameter η, defined as [14–16]

$$\eta = \frac{\mu}{K_B T},$$

which describes the strength of the atomic interactions within the condensate. The parameter η is independent of the system size, when the thermodynamic limit is taken as $N \to \infty$, $\Omega \to 0$, $N\Omega \to$ constant. By substituting from Eq. (12) into Eq. (5), and after performing the integration, the number of condensed atoms can be expressed as

$$N_0 = N\left\{(1-t^3) - \left[\frac{3}{2}\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}} + \eta\frac{\zeta(2)}{\zeta(3)}\right]t^2\right\} \tag{13}$$

This result for the condensed atoms number takes into account all the perturbing effects which appear in the ideal Bose gas physics. The number of spatial dimensions, finite size, interatomic interactions and the confining potential effects are all described using the power law of the density of states. Moreover, it provides a detailed test for the system through the free parameter, η. The first term on the right hand side of Eq. (13), $N(1-t^3)$, gives precisely the number of condensed atoms for the ideal gas, while the second term, $\left(\frac{3}{2}\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}\right)$, accounts for the finite size effect. This effect is always negative and vanishes in the large N limit. The last term gives the correction due to interatomic interactions.

3. CONDENSATION TEMPERATURE AND THE CRITICAL ATOM NUMBER

One of the main objectives of this paper is to simultaneously study both the effect of finite size and that of repulsive interactions on the condensation temperature as a function of the critical atoms number (critical point), and then comparing the results with the experimental data. These critical points correspond to the threshold atom number and its corresponding temperature of BEC. If the atom number is increased beyond this point at constant temperature, or if the temperature is reduced for constant atom number, (N_c, T_c) define the value of the atom number and its corresponding temperature where a bimodal distribution appeared.

Gerbier *et al.* have measured the critical point (N_c, T_c). When considering the mean-field correction for the ideal gas transition temperature, a much better agreement with the experimental data resulted. Gerbier assumed that the interactive shift in the critical temperature T_c can be written as $T_c = T_0(1-\alpha N^{1/6})$, with a free coefficient α. A fit to the experimental data yields $\alpha = -0.009$.

Unfortunately, it is difficult to find a reliable approximation for the condensed atom number and the corresponding condensation temperature. In our approach, the condensation temperature is obtained as a function of the condensation number, by using a graphical representation [8]. In this method, the critical point is obtained as follows. We plotted the condensed atoms number, N_0, *versus* the reduced temperature, for different values of N. On the same graph we represented the excited atoms, N_{ex}, *versus* the same reduced temperature. The intersection point of the N_{ex} with the group of N_0 curves gives the critical point.

For a boson system consisting of many energy states E_0, E_1, E_2, …, the total number of bosons is determined from Eq. (5). The total number can be further divided into two terms: the number N_0 in the ground state with energy E_0 and the number N_{ex} in the excited states with energies E_1, E_2, …,

$$N = N_0 + N_{ex}\,, \tag{14}$$

$$N_{ex} = \sum_{j=1}^{\infty} z^j \left(\sum_{i=1}^{\infty} e^{-j\beta E_i'} \right) \tag{15}$$

When the energy levels are closely spaced,

$$N_{ex} = \sum_{j=1}^{\infty} z^j \int_{E_1}^{\infty} \rho(E) e^{-j\beta E} dE\,. \tag{16}$$

The above integral (16) can be expressed as

$$N_{ex} = \sum_{j=1}^{\infty} z^j \int_0^{\infty} \rho(E) e^{-j\beta E} dE - \sum_{j=1}^{\infty} z^j \int_0^{E_1} \rho(E) e^{-j\beta E} dE \tag{17}$$

For a very large number, $N > 10^4$, $E_1 \to 0$, the second term on the right hand side (RHS) of Eq. (17) almost vanishes. We then have

$$N_{ex} = \sum_{j=1}^{\infty} z^j \int_0^{\infty} \rho(E) e^{-j\beta E} dE = N - N_0\,, \tag{18}$$

by using Eq. (13) we have,

$$N_{ex} = N - N_0 == N \left\{ t^3 + \left[\frac{3}{2} \frac{\zeta(2)}{\zeta(3)^{2/3}} \frac{1}{N^{1/3}} + \eta(1-t^3)^{2/5} \frac{\zeta(2)}{\zeta(3)} \right] t^2 \right\} N \tag{19}$$

The calculated results from Eqs. (13) and (19) for N_0 and N_{ex}, respectively, are represented in Fig. 1. The critical points are obtained from the intersection of a series of curves.

The extracted results from Fig. 1 are represented in Fig. 2. This figure shows that the critical temperature increases monotonically and very fast with the increase of the critical number. The experimental data obtained to Gerbier *et al.* [1], is also shown for comparison. There is a considerably agreement between our results and these experimental data.

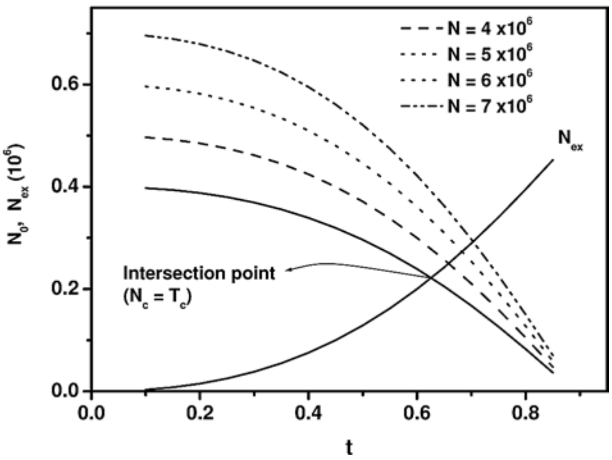

Fig. 1 – Condensed atoms N_0 and the atoms in the excited states *vs.* reduced temperature for a different total number of Rb atoms.

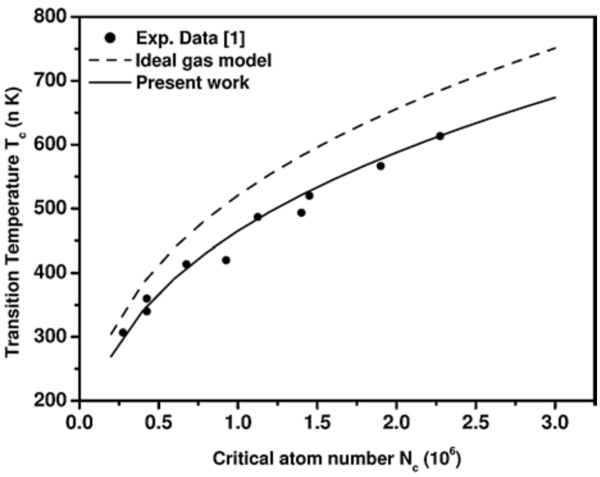

Fig. 2 – Critical temperature at the transition as a function of the critical atom number. The measured experimental data are represented by a solid circles. Results of the present work (solid line) are consistent with the measured experimental data. The dashed line represents the ideal gas model. The interaction parameter is taken to be $\eta = 0.49$.

4. CONCLUSION

A modified density of states for harmonically trapped Bose gas is suggested, which makes possible to essentially extend the region of its applicability. The main effects on the thermodynamical properties of BEC are embodied in this ansatz formula. The thermodynamic properties of the trapped Bose gas depend crucially on the choice and construction of the density of states. Indeed, it was shown that the modified formula yields the results obtained by experimental measurements [1]. In this experiment, a well defined critical point was identified, which separates the high-temperature normal state characterized by a single component density distribution, and the low-temperature state characterized by a bimodal (condensed and excited atoms). In conclusion, graphical representation can be used in determining some important thermodynamical parameters.

REFERENCES

1. F. Gerbier, J. H. Thywissen, S. Richard, M. Hugbart, P. Bouyer, A. Aspecr, Phys. Rev. Lett. **92**, 030405, (2004); Phys. Rev. A **70**, 013607 (2004).
2. F. Schreck *et al.*, Phys. Rev. Lett. **87**, 080403 (2001).
3. Z. Hadzibabic, P. Kruger, M. Cheneau, S. P. Rath, J. Dalibard, arXiv: 0712.1265V1 (2007).
4. M. J. Davis, P. B. Blakie, Phys. Rev. Lett. **96**, 060404 (2006).
5. Ahmed S. HASSAN, Azza M. El-Badry, *Turk J Phys* **32** (2008).
6. Ahmed S. HASSAN, Hassab Eldyeam HADI, *Turk J of Phys* **32**, 31 (2008).
7. Ahmed S. HASSAN, Hassab Eldyeam HADI, *Rom. Journ. Phys.*, **53**, *7–8*, 817 (2008) (to be published).
8. Ching-Fuh Lin, Chin. J. of Phys. **44**, 79 (2006).
9. V. Bagnato, D. E. Pritchard, D. Kleppner, Phys. Rev. A**35**, 4354 (1987).
10. S. Grossmann, S., M. Holthaus, Phys. Lett. A **208**, 188 (1995); S. Grossmann, S., M. Holthaus, Z. Phys. B. **97**, 319, (1995).
11. H. Haugerud, T. Haugset, F. Ravndal, 1997, Phys. Lett. A **225**, 18, (1997); T. Haugset, H. Haugerud, J. O. Andersen, Phys. Rev. A **55**, 2922, (1997).
12. K. Kirsten, D. J. Toms, Phys. Rev. E **59**, 158, (1999); K. Kirsten, D. J. Toms, Phys. Lett. A **222**, 148, (1996); K. Kirsten, D. J. Toms, Phys. Rev. A **54**, 4188, (1996); K. Kirsten, D. J. Toms, Phys. Lett. B **368**, 119, (1996); K. Kirsten, D. J. Toms, Phys. Lett. A **243**, 137, (1998).
13. W. Ketterle, N. J. Van Druten, Phys. Rev. A**5**4, 656, (1996).
14. F. Dalfovo, S. Giorgini, L. P. Pitaevskii, S. Stringari, Rev. of Mod. Phys. **71**, 463, (1999).
15. S. Giorgini, S. Stringari, Phys. Rev. A **53**, (1996), 2477; W. Krauth, Phys. Rev. Lett. **77**, 3695, (1996).
16. M. Naraschewski, D. M. Stamper-Kurn, Phys. Rev. A **58**, 2423, (1998).