

Effective Width and Expansion Energy of the Interacting Condensed ⁸⁷Rb Bose Gas with Finite Size Effects

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Abstract

This work is devoted to study the temperature dependence of the effective width and expansion energy on the finite size and interaction effects (repulsive interactions). It is found that the effective size $\langle r^2 \rangle$, and expansion energy in the radial direction E_y of a Bose gas follow a characteristic temperature dependence, i.e. $\langle r^2 \rangle$, $E_y \propto (T/T_0)^4$ if $T_0 < T$ and $\langle r^2 \rangle$, $E_y \propto (T/T_0)$ if $T_0 > T$. Our results show that these two parameters increases with the number of atoms, and with increasing repulsive interaction strength at temperature less than the transition temperature, $(T < T_o)$; yet it has little effect at temperatures higher than the transition temperature $(T > T_o)$. The obtained results are compared with the available experimental data for ⁸⁷Rb directly, full agreement is obtained.

Key Words: Interacting Bose gas; Thermodynamical properties for BEC; Semiclassical approach.

1. Introduction

Trapped gases offer a new opportunity to study the interplay between quantum-statistical phenomena and interactions in Bose systems. Many properties of these trapped gases have been extensively studied and understood [1, 2]. Although several key thermodynamical properties, such as condensed fraction and average energy, are readily measurable experimentally, a detailed comparison of experiments with finite-temperature theories of the interacting cloud is to our knowledge still lacking. Surprisingly less attention has been payed to the effective width and expansion energy for condensed Bose gases [3-5].

One way of obtaining information on the properties of a Bose-Einstein condensate (BEC) is to investigate its behavior after it is released from the trap. Recent experimental realization of BEC for ⁸⁷Rb [6-9], has filled this gap. These experiments provide us an important thermodynamical parameter. Among them is the axial length and the expansion energy in the redial direction. These parameters have special behavior at temperatures greater or less than the transition temperature T_0 . These two parameters drop suddenly when the condensation

occurs, after the trapped gas temperature is lowered below the transition temperature T_0 . As a consequence, this reduction is used as a good evidence for the onset of BEC. Information about these two parameters are extracted from time-of-flight absorption imaging.

Two important quantities are calculated through a fit to absorption images: the condensed fraction and the effective temperature. The condensed number N_0 can be estimated from the effective width through the parametrization [7]

$$\langle r^2 \rangle^{1/2} = \langle r_0^2 \rangle^{1/2} (1 + \alpha N_0)^{1/5},$$

where $\langle r_0^2 \rangle^{1/2}$ is the predicted non-interacting effective width and α is extracted empirically. This procedure yields robust values of N_0 provided that the temperature is high enough that the non-condensed atoms form a distribution that is significantly broader than the sharp condensate feature. The effective temperature can be extracted from the cloud size via the relation

$$k_{\rm B}T_x = \frac{M\omega_x^2 \left\langle x^2 \right\rangle}{1 + (\omega_x \tau)^2},$$

where $\langle x^2 \rangle$ is the radial size and ω_x is the radial frequency. So, it is very important to study and investigate these parameters intuitively.

One of the efficient methods for describing these systems is the density-of-state approach. In this approach the sums over the energy levels for the thermodynamical quantities are approximated directly by ordinary integrals weighted by an appropriate density of state [10-19]. In our previous work, [20-22], an accurate ansatz formula for the density of states was suggested. This ansatz formula enabled us to study the finite size, interatomic interaction and anisotropic of the external potential effects (repulsive interactions) simultaneously. It is used to calculate condensed fraction, average energy per particle, release energy and specific heat capacity . The calculated results for the above mentioned thermodynamic parameters are compared with the available measured experimental data for ⁸⁷Rb, and full agreement is obtained [7].

In this paper we report our investigations of the temperature-dependent effective width and expansion energy of a trapped interacting ⁸⁷Rb Bose gas by using the density of states approach. We undertake this study in an effort to provide some theoretical support for the experiment by Gerbier et al. [8, 9]. Our results show that, for high temperature ($k_{\rm B}T >> \hbar\omega$), we ignored the contribution from the condensate, the axial length and radial length are proportional to T^2 for $T > T_0$, and it is proportional to $T^{1/2}$ for $T < T_0$. Expansion energy has the same behavior. This results agree with the measured experimental data. Moreover, we support the opinion this behavior is a good indication for the presence of BEC.

This paper is organized as follows. The present section provides a brief introduction. Sections two and three describe the calculations for the effective width for both an ideal and interacting trapped Bose gas respectively. We analyze the expansion energy in the radial direction of a Bose gas in section four. Section five presents a short conclusion.

2. Effective width of a trapped Bose gases

We now discuss the square width of an ideal Bose gases at finite temperature. For an ideal Bose gas, the average number of particles in a single particle state $|i\rangle$ with energy ϵ_i is given by the familiar Bose-Einstein

distribution

$$n_i = \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1} = \frac{ze^{-\beta\epsilon_i}}{1 - ze^{-\beta\epsilon_i}},\tag{1}$$

where $\beta = 1/k_{\rm B}T$, with $k_{\rm B}$ denoting the Boltzmann constant. The degeneracy factors are avoided by accounting for degenerate states individually [23, 24]. The fugacity z is determined in terms of the chemical potential μ as $z = e^{\beta(\mu - \epsilon_0)}$, with ϵ_0 being the energy of the lowest state. Within the grand canonical ensemble the chemical potential μ is determined by the conservation of the total number N

$$N = \sum_{i=0}^{\infty} n_i \tag{2}$$

The statistical properties of a Bose gas are completely determined once the sum in equation (2) is found or z is calculated.

For a spherically symmetric harmonic trap, the external harmonic potential is given by

$$V_{\rm ext}(r) = \frac{M}{2}\omega^2 r^2,$$

where ω 's is the frequency. The corresponding quantized energy levels is given by

$$\epsilon_i = i\hbar\omega + \epsilon_0,$$

where ϵ_0 is the zero point energy and $\epsilon_0 = \frac{3}{2}\hbar\omega$. The square width of a single particle state $|i\rangle$ can be obtained from the first principle of quantum mechanics: [5, 25],

$$\langle r_i^2 \rangle = \frac{\langle 2V_{\text{ext}}(r) \rangle}{M\omega^2} = \frac{\epsilon_i}{\hbar\omega} a_r^2,$$
(3)

where $a_r = \sqrt{\frac{\hbar}{M\omega}}$ is the characteristic length for the harmonic trap. The expected square width of N trapped atoms of a Bose gas is then given by

$$\langle r^2 \rangle = \sum_{i=0}^{\infty} n_i \langle r_i^2 \rangle$$

$$= \sum_{i=0}^{\infty} \frac{z e^{-\beta \epsilon_i}}{1 - z e^{-\beta \epsilon_i}} \langle r_i^2 \rangle.$$

$$(4)$$

The key point for exploring BEC within this formalism is to treat the lowest energy state separately, i.e.

$$\langle r^2 \rangle = \frac{z}{1-z} \langle r_0^2 \rangle + \sum_{i=1}^{\infty} \frac{z e^{-\beta \epsilon_i}}{1-z e^{-\beta \epsilon_i}} \langle r_i^2 \rangle$$

$$= \frac{3}{2} \frac{z}{1-z} a_r^2 + \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} z^j e^{-j\beta \epsilon_i} \langle r_i^2 \rangle$$

$$= \frac{3}{2} \frac{z}{1-z} a_r^2 + \frac{a_r^2}{\hbar \omega} \sum_{j=1}^{\infty} z^j \sum_{i=1}^{\infty} \epsilon_i e^{-j\beta \epsilon_i}.$$

$$(5)$$

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For large N, the usual approximation of changing the summation over i into an integral weighted by an accurate density of states can be taken:

$$\left\langle r^2 \right\rangle = \frac{3}{2} \frac{z}{1-z} a_r^2 + \frac{a_r^2}{\hbar\omega} \left\{ \sum_{j=1}^{\infty} z^j \int_0^\infty E\rho(E) e^{-j\beta E} dE \right\},\tag{6}$$

where $\rho(E)$ is the density of states. It plays an important role in our calculations. The main effect is the ideal Bose gas can be embodied in this density of states. However, the resulting thermodynamic properties depend crucially on the choice and contraction of the power law of the density of states. For anisotropic harmonic potential, the density of states is given by [20-22]

$$\rho(E) = \frac{1}{2} \frac{E^2}{(\hbar\omega)^3} + \frac{E}{(\hbar\omega)^2} \left\{ \gamma + \frac{\mu}{\hbar\omega} \right\}$$
(7)

The constant $\gamma = \frac{3}{2}$ [12]. This approximation requires the condition $k_{\rm B}T >> \hbar\Omega$. Equation (6) includes all the main effects of the density of states [12, 20-22].

From equation (6) and equation (7), the temperature dependent square width is given by

$$\langle r^2 \rangle = a_r^2 \left\{ \frac{3}{2} \frac{z}{1-z} + 3 \left(\frac{k_{\rm B}T}{\hbar \omega} \right)^4 g_4(z) + 2 \left(\frac{k_{\rm B}T}{\hbar \omega} \right)^3 g_3(z) \left[\gamma + \frac{\mu}{\hbar \omega} \right] \right\}$$

$$= a_r^2 \left\{ \frac{3}{2} N_0 + 3 \left(\frac{k_{\rm B}T}{\hbar \omega} \right)^4 g_4(z) + 2 \left(\frac{k_{\rm B}T}{\hbar \omega} \right)^3 g_3(z) \left[\gamma + \frac{\mu}{\hbar \omega} \right] \right\}.$$

$$(8)$$

Here, $g_n(z) = \sum_{j=1}^{\infty} (z^j/j^n)$ is the usual Bose function, $N_0 = 0$ for $T_0 > T$ and $N_0 = \{1 - (T/T_0)^3\}$ for $T_0 < T$, and $T_0 = (\frac{\hbar\omega}{k_B})(N/\zeta(3))^{(1/3)}$ is the transition temperature for ideal Bose gas. Bracket in equation (8) takes a familiar form with the first term denoting the square width for the ground state (condensate), while the second term gives the excited states (the thermal component). The last term includes the correction due to finite size and interaction effects as we shall see later.

It is convenient to introduce a dimensionless parameter η [1]:

$$\frac{\mu(N_0,T)}{k_{\rm B}T_0} = \frac{\mu(N,T=0)}{k_{\rm B}T_0} (\frac{N_0}{N})^{2/5} = \eta (1-t^3)^{2/5}$$

Parameter η is a scaling parameter that gives the scaling behavior of all thermodynamic quantities due to interaction. In terms of the scattering length a, the scaling parameter η is given by $\eta = 1.57 \left(N^{1/6} \frac{a}{a_r}\right)^{2/5}$ [26-29].

The approximation made here involve two energy scales: $k_{\rm B}T_0$ and $\hbar\omega$. In most of the traps, the former is about 2 orders of magnitude greater than the latter, so semiclassical approximation is expected to work well in these systems over a wide range of temperatures. Moreover, as pointed by W. Zhang et al. [5], at high temperatures $k_{\rm B}T >> \hbar\omega$, as normally is the case, the contribution from the condensate can be ignored. We thus have the following two cases. 1. For temperature $T < T_0$:

$$\langle r^2 \rangle \approx 3a_r^2 \left(\frac{k_{\rm B}T}{\hbar\omega}\right)^4 g_4(z) + 2\gamma a_r^2 \left(\frac{k_{\rm B}T}{\hbar\omega}\right)^3 g_3(z) + 2a_r^2 \left(\frac{k_{\rm B}T}{\hbar\omega}\right)^3 g_3(z) \frac{\mu}{\hbar\omega}$$
$$= r_c^2 t^4 + r_c^2 \frac{\zeta(3)}{\zeta(4)} \left[\left(\frac{\zeta(3)}{N}\right)^{1/3} + \frac{2}{3}\eta(1-t^3)^{2/5} \right] t^3.$$

Here, r_c^2 denotes the square width of a Bose condensate at the transition temperature T_0 :

$$r_c^2 = 3a_r^2 \zeta(4) [N/\zeta(3)]^{4/3},$$

where $t = T/T_0$ is the reduced temperature, $\zeta(n)$ is the Riemann zeta function. The dimensionless square width is given by

$$\frac{\langle r^2 \rangle}{r_c^2} = t^4 + \frac{\zeta(3)}{\zeta(4)} \left[\left(\frac{\zeta(3)}{N} \right)^{1/3} + \frac{2}{3} \eta (1 - t^3)^{2/5} \right] t^3$$
$$= t^3 \chi_1(t), \tag{9}$$

where

$$\chi_1(t) = t + \frac{\zeta(3)}{\zeta(4)} \left[\left(\frac{\zeta(3)}{N}\right)^{1/3} + \frac{2}{3}\eta(1-t^3)^{2/5} \right]$$

In the thermodynamic limit $(N \to \infty \text{ and } \eta \to 0) \ \chi_1(t) \to t$

2. On the other hand, for $T \ge T_0$, we found

$$\langle r^2 \rangle \approx 3a_r^2 N\left(\frac{k_{\rm B}T}{\hbar\omega}\right) \frac{g_4(z)}{g_3(z)} + 2\gamma a_r^2 \left(\frac{N}{g_3(z)}\right) g_3(z) + 2a_r^2 \left(\frac{N}{g_3(z)}\right) g_3(z) \frac{\mu}{\hbar\omega} \}$$
$$= \alpha r_c^2 t + \frac{\zeta(3)}{\zeta(4)} \left[\left(\frac{\zeta(3)}{N}\right)^{1/3} + \frac{2}{3}\eta (1-t^3)^{2/5} \right],$$

where $\alpha = g_4(z)\zeta(4)/[g_3(z)\zeta(4)] \approx 1$ has a very weak dependence on T. The dimensionless form is given by

$$\frac{\langle r^2 \rangle}{r_c^2} = \chi_1(t). \tag{10}$$

Therefore there is a qualitative as well as quantitative difference between the ideal Bose gas and a system of interacting Bose gases. The width of a Bose gas $\langle r^2 \rangle^{1/2}$ is proportional to T^2 for $T < T_0$ and to $T^{1/2}$ for $T \ge T_0$. This result is consistent with earlier experimental reports, that the area of absorption image of a Bose gas is proportional to its temperature in the absence of a condensate [7-9].

In Figure 1, the temperature dependence effective width, $\langle r^2 \rangle^{1/2} / r_c$, of a Bose gas in a spherically symmetric harmonic trap is given. In this figure we consider the interatomic interaction effect on the ideal



Figure 1. The temperature-dependent width of a Bose gas in spherically symmetric harmonic trap. The trap parameters are $\gamma' s = 2\pi \times 65$ and the number of particles is taken to be 4×10^4 . Note that both T_c and r_c depend on N.

trapped Bose gas. The solid, dashed and dotted lines denote, respectively, the case of width with $\eta = 0, 0.5$, and 1.0; the number of particles is taken to be $N = 1 \times 10^6$.

We now come to our analysis of equations (9) and (10), and the fundamental difference between our results and the ideal Bose gas (thermodynamic limit) [5]. An interesting feature we note is that the repulsive interaction causes the width of a Bose gas to increase at temperatures lower than the transition temperature $(T < T_o)$, yet it has little effect on the width at temperatures higher than the transition temperature $(T > T_o)$. The low temperature phenomenon is easy to understand in terms of a repulsive-interaction induced expansion of a Bose gas [3, 4]. First, a condensate with repulsive interaction is larger in its size due to atom-atom repulsion. Second, the presence of a condensate pushes the thermal non-condensed cloud out, further increasing the size of a gas [29]. At high temperatures $(T > T_o)$ the effect of repulsive interaction becomes negligible as the density of a Bose gas decreases dramatically with increasing temperatures.

3. Axial and radial width, and effective area

One of the key parameters for describing an expanding condensate is its effective area, which is normally defined as a square root of the condensate widths along the two symmetric axes. In general, for the magnetic traps that are used in the experiment the axes are parallel to the axial and the radial direction, respectively. The effective area is given by

$$S(t) = \sqrt{\langle z^2 \rangle \langle x^2 \rangle},$$

where $\langle z^2 \rangle$ and $\langle x^2 \rangle$ is the effective width in the axial and radial direction respectively.

Theoretically, the expansion of a condensate width and its effective area, as a function of temperature, can be found in special cases. So, it can be used as a direct test of the validity of the density of state approach when it is applied to a dilute atomic Bose gases.

For cylindrically symmetric trap with frequencies $\omega_x = \omega_y$ and $\omega_z = \lambda \omega_{x,y}$, the external potential in this case is given by

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

The temperature dependence of the three squared width are the same as in a spherically symmetric trap discussed above. The normalization factors become, respectively,

$$z_{\rm c}^2 = a_z^2 \lambda^{-2/3} \zeta(4) \left[N/\zeta(3) \right]^{4/3} = \frac{\lambda^{-2/3}}{M\omega_z^2} \frac{\zeta(4)}{\zeta(3)} N k_{\rm B} T_0$$
$$x_{\rm c}^2 \equiv y_c^2 = a_{x,y}^2 \lambda^{1/3} \zeta(4) \left[N/\zeta(3) \right]^{4/3} = \frac{\lambda^{1/3}}{M\omega_{x,y}^2} \frac{\zeta(4)}{\zeta(3)} N k_{\rm B} T_0 \tag{11}$$

for the axial and transverse directions, respectively. Note that $\gamma = \frac{3}{2}(\frac{\bar{\omega}}{\Omega}) = \frac{1}{2}(2+\lambda)\lambda^{-1/3}$, and the characteristic lengths for the harmonic trap is given by $a_{x,y,z} = \sqrt{\hbar/M\omega_{x,y,z}}$.

The axial length is given by

$$\frac{\langle z^2 \rangle}{z_c^2} = t^4 + \frac{1}{3} \frac{\zeta(3)}{\zeta(4)} \left[(\lambda + 2) \lambda^{-1/3} \left(\frac{\zeta(3)}{N} \right)^{1/3} + 2\eta (1 - t^3)^{2/5} \right] t^3$$

$$= \chi_2(t) t^3, \quad T \le T_0$$

$$= \chi_2(t), \quad T \ge T_0, \tag{12}$$

while the transverse length is given by

$$\frac{\langle x^2 \rangle}{x_c^2} \equiv \frac{\langle y^2 \rangle}{y_c^2} = t^4 + \frac{1}{3} \frac{\zeta(3)}{\zeta(4)} \left[(\lambda + 2) \lambda^{-1/3} \left(\frac{\zeta(3)}{N} \right)^{1/3} + 2\eta (1 - t^3)^{2/5} \right] t^3$$

$$= \chi_2(t) t^3, \quad T \le T_0$$

$$= \chi_2(t), \quad T \ge T_0, \tag{13}$$

with

$$\chi_2(t) = t + \frac{1}{3} \frac{\zeta(3)}{\zeta(4)} \left[(\lambda + 2)\lambda^{-1/3} \left(\frac{\zeta(3)}{N}\right)^{1/3} + 2\eta (1 - t^3)^{2/5} \right]$$

In the thermodynamic limit, $N \to \infty$ and $\eta \to \text{zero}, \chi_2(t) \to t$

The effective area is given by

$$S(t) \approx \sqrt{\langle z^2 \rangle \langle x^2 \rangle}$$

= $S_c \chi_2(t) t^3, \quad T \le T_0$
= $S_c \chi_2(t), \quad T \ge T_0.$ (14)

Once again, this is clearly consistent with earlier experimental observations that the effective area is proportional to the temperature above BEC and drops suddenly below the condensation temperature.

4. Expansion energy

Another important quantity to discuss is the expansion energy in the redial direction (release energy). This energy is defined as the sum of the kinetic and interaction energy released at the trap cutoff and available for the expansion of the whole cloud. Experimentally it is measured from time of flight of the condensed gas. In an anisotropic trap such as considered by Gerbier et al. $(\omega_{x,y}/\omega_z = 51)$, all the interaction energy converts into radial expansion velocity [9]. The radial expansion of the cloud is observed in the y-direction and fixed by the expansion energy

$$E_y = \frac{1}{2} M \left\langle v_y^2 \right\rangle_{\tau \to \infty} = \frac{1}{2\tau^2} M \left\langle y^2 \right\rangle_{\tau \to \infty}$$
(15)

with τ as the time of flight.

Theoretically in the present formalism the expansion energy can be calculated from the root mean-square cloud size $\langle y^2 \rangle$ [5, 28]. Assumed that on average the kinetic and interaction energy are equal to the measured quantity, the expansion energy is given by

$$E_y = \frac{1}{2\tau^2} M \langle y^2 \rangle_{\tau \to \infty}$$

= $\frac{1}{6\tau^2} M y_c^2 \left\{ 3t^4 + \frac{\zeta(3)}{\zeta(4)} \left[(\lambda + 2)\lambda^{-1/3} \left(\frac{\zeta(3)}{N} \right)^{1/3} + 2\eta (1 - t^3)^{2/5} \right] t^3 \right\},$ (16)

which, if its scaled by the characteristic energy scale, $Nk_{\rm B}T_0$, becomes a universal function of interaction strength parameter η and the reduced temperature t. It is given by

$$\frac{E_y}{Nk_{\rm B}T_0} = \frac{\lambda^{1/3}}{6\tau^2\omega_y^2} \left\{ \frac{\zeta(4)}{3\zeta(3)} t^4 + \left[(\lambda+2)\lambda^{-1/3} \left(\frac{\zeta(3)}{N}\right)^{1/3} + 2\eta(1-t^3)^{2/5} \right] t^3 \right\} \quad T \le T_0$$

$$= \frac{\lambda^{1/3}}{6\tau^2\omega_y^2} \left\{ 3\frac{\zeta(4)}{\zeta(3)} t + \left[(\lambda+2)\lambda^{-1/3} \left(\frac{\zeta(3)}{N}\right)^{1/3} + 2\eta(1-t^3)^{2/5} \right] \right\} \quad T \ge T_0.$$
(17)

The calculated results from equation (17) are illustrated in Figure 2. In this figure the temperature dependence of the expansion energy $\frac{E_y}{Nk_{\rm B}T_0}$ (released energy) is compared with the measured data of Gerbier et al. [8]. The trap parameters are taken to be $\omega_{x,y}/2\pi = 413$ Hz, $\omega_z/2\pi = 8.69$ Hz, the number of ⁸⁷Rb atoms is taken to be 1.2×10^6 , the time of flight is $\tau = 24.27$ ms and the interaction parameter $\eta = 0.49$. This figure reveals that the behavior of the expansion energy is similar to the behavior for the square size. The difference between the expansion energy of an interacting Bose gas and an ideal gas decreases when the temperature increases and becomes negligible for $T > T_o$. We also note that the main feature of the expansion energy at high temperatures again follow the characteristic temperature dependence, i.e. $E_y \propto (T/T_0)^4$ if $T < T_o$ and $E_y \propto (T/T_0)$ if $T > T_o$.

5. Conclusion

The analytical approach adopted in the present paper would be effective to study interacting condensed Bose gas. We have investigated theoretically the temperature dependence of the effective width and the



Figure 2. Expansion energy in the radial y direction as a function of temperature. The interaction parameter is taken to be $\eta = 0.49$, while the anisotropic parameter is equal to 3.66, and $N = 1.2 \times 10^6$.

expansion energy of a trapped interacted ⁸⁷Rb gas. Our approach provides a direct comparison between the calculated results and the measured experimental data. We have investigated primarily two quantities: the effective width and the radial expansion (release energy). The data display without ambiguity an interacting gas behavior, and is in agreement with the experimental data.

Our results summarize as follows. A sudden drop for the effective width and expansion energy occur when temperature is lowered below the transition temperature. For the effective area, and the expansion energy, equations (14) and (17) reveal that the difference between an ideal gas and an interacting one increases with the number of atoms, and with increasing repulsive interaction strength for $T < T_o$. Sudden decrease in the reduced width near the transition temperature has little dependence on the number of atoms. The effective width can serve as a good indication for the presence of BEC. In view of this, our results provide a solid theoretical foundation for the experiment. Finally, in contrast to the previous work, this approach involves only analytical calculations without technical complication.

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