RELEASE ENERGY AND SPECIFIC HEAT CAPACITY OF A TRAPPED ^{87}Rb GAS WITH CONCURRENT FINITE SIZE AND INTERATOMIC INTERACTION EFFECTS

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A generalization for the semiclassical approach is suggested allowing an essential extension of its region of applicability. In particular, it becomes possible to describe interacting Bose gas with finite size effects simultaneously. We parameterize a new accurate ansatz formula for the density of state to calculate the release energy and specific heat capacity of ^{87}Rb condensed gas with repulsive interaction inside a harmonic trap at finite temperature. Our results indicate that interacting bosons have similar behavior to those of an ideal system for weak interactions. The release energy drops suddenly when condensation occurs. It is shown that there are a temperature at which the specific heat has a maximum that can be identified as the temperature at which BEC occurs. There is a quantitative agreement between our results and those of the other methods. Our results recommended to use the sudden shrinking of the release energy and continuous of the specific heat at its maximum as a good evidence for the onset of BEC. As expected, this study points to be an important issue for interacting Bose gases.

Key words: thermodynamical properties of condensates, specific heat capacity for Boson gases, Boson systems.

1. INTRODUCTION

The experimental realization of *Bose-Einstein Condensation* (BEC) for ^{87}Rb [1–3], and others neutral bosonic atoms has stimulated a new interest in the theoretical study of Bose gases. This type of particles are described only by the rules of quantum mechanics and occupy a discontinuous spectrum of energy state. Only special statistics can be applied to the energy distribution in such systems. From the standpoint of the mathematics of statistical physics, the essential general constraint of quantum statistics is that: the thermodynamical parameters of quantum systems are determined as sums over energy levels rather than integrals over phase space. One of the efficient methods for describing these systems is the semiclassical approximation. In this approximation the sums over the energy levels for the thermodynamical quantities are approximated directly by ordinary integrals weighted by an appropriate density of states.

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Density of state approach has been employed for considering the properties of Bose-condensed ideal gas trapped in power-law potential [4]. The advantage of this method its simplicity, as compared to quantum-mechanical calculations. A modification is needed, which makes it more possible to essentially extend the region of its applicability. In doing this we are going to extend the previous studies [5–9]. An accurate ansatz formula for the density of states is suggested [10]. This new ansatz formula enable us to study more main effects, such as finite size and interatomic interaction effects, which can be altered the ideal Bose gas physics.

In this paper the released energy and specific heat capacity of ^{87}Rb as a function of temperature are investigated. Unfortunately it is difficult to find a reliable analytical approximation for the specific heat which allows us to study whether it has a maximum, and if it dose, at what temperature it occurs. The release energy (which is defined as the energy of the condensed particles after switching off the trapping potential $E_{rel} = E_{kin} + E_{int}$ [2, 3]) is calculated from the root mean square cloud radius and the time of flight. While the specific heat capacity is calculated by differentiating the average energy per particle. Indeed, we show that there is a temperature at which the specific heat capacity has a maximum. This temperature can be identified as the critical temperature at which BEC occurs. Full agreement is obtained with the other used method to calculate the same quantity for the release energy.

The present paper is planed as follows: Section two include a simple model for the BEC in 3D harmonic trap, and the density of state approach. Sections three and four are devoted to calculate the release energy and specific heat capacity, respectively. Section four presents a short conclusion which summarizes our results.

2. A SIMPLE MODEL OF A TRAPPED BOSE GAS

Numerous review papers [11–13] as well as a dedicated textbook are by now available on BEC detailing nearly every aspect of this topic. Here we introduce the necessary theoretical basis and the nomenclature relevant to the achievement experiments. Atomic ensembles in BEC experiments are typically held in a three-dimensional anisotropic harmonic potential

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

the single particle energies are given by

$$E_{n_x n_y n_z} = \hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z) + E_0 \tag{1}$$

where $n_x, n_y, n_z = 0, 1, 2, 3, \ldots$ and $E_0 = \frac{3}{2}\hbar\bar{\omega}$ is the zero point energy, with

$\overline{\omega}=\frac{1}{3}(\omega_x+\omega_y+\omega_z)$. 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. *Note that, it is well-known that for large number of particles N, interactions lead to suppression of fluctuation in the grand canonical ensemble* [15]. The mean number of particles in a state with energy $E_{n_x n_y n_z}$ is given by Bose-Einstein distribution,

$$n(E_{n_x n_y n_z})=\frac{ze^{-\beta E_{n_x n_y n_z}}}{1-ze^{-\beta E_{n_x n_y n_z}}}, \tag{2}$$

where $\beta=(1/K_BT)$. The fugacity z is determined in terms of the chemical potential μ as $z=e^{\beta(\mu-E_0)}$. Within the grand canonical ensemble, the chemical potential μ and the temperature T are fixed by the requirement [4, 5]

$$\begin{aligned} N &= \sum_{n_x n_y n_z} n(E_{n_x n_y n_z}) = \sum_{n_x n_y n_z}\sum_{j=1}^{\infty} z^j e^{-j\beta E_{n_x n_y n_z}} \\ <E> &= \sum_{n_x n_y n_z} E_{n_x n_y n_z} n(E_{n_x n_y n_z}) = \sum_{n_x n_y n_z}\sum_{j=1}^{\infty} z^j E_{n_x n_y n_z} e^{-j\beta E_{n_x n_y n_z}}. \end{aligned} \tag{3}$$

Here degeneracy factors are avoided by accounting for degenerate states individually. The phenomenon of BEC for ideal Bose gas is fully described by Eq.'s (1) to (3). The thermodynamical parameters of a Bose gas, such as its condensate fraction, average per particle, release energy, and specific heat are completely determined once the sum has been calculated.

2.1. DENSITY OF STATES APPROACH

It is impossible to evaluate the sum in Eq. (3) analytically in a closed form. Another possible way to do this analysis is to approximate the sum directly into ordinary integrals weighted by an appropriate density of states $\rho(E)$ [5, 6]. This approximation requires that the condition $K_BT>>\hbar\Omega$ with $\Omega=(\omega_x\omega_y\omega_z)^{1/3}$ to be satisfied. If the lowest energy state population 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 $\mu\sim E_0$), Eq. (3) can be written as

$$\begin{aligned} N &= N_0+\sum_{j=1}^{\infty} z^j\int_0^{\infty}\rho(E)e^{-j\beta E}dE \\ <E> &= E_0+\sum_{j=1}^{\infty} z^j\int_0^{\infty}E\rho(E)e^{-j\beta E}dE. \end{aligned} \tag{4}$$

The density of state $\rho(E)$ can be modified to include the main effects which can be altered the ideal Bose gas physics. So, Eq. (4) contains nearly, the number of spatial dimensions, finite size, interatomic interactions, and the confining potential effects. All these effects can be taken care of in the power law of the density of states, $\rho(E)$. For particles with mass m, $\rho(E)$ is given by

$$\rho(E)=\frac{(2m)^{2/3}}{4\pi^2\hbar^3}\int_{v_{ext}(r)<E}\sqrt{E-v_{ext}}\,d^3r,$$

where the integration has to be over the classically accessible region, vanishes for negative energies. For ideal gas confined in a three-dimensional anisotropic harmonic potential, the density of states, $\rho(E)$ is given by

$$\rho(E)=\frac{1}{2}\frac{E^2}{(\hbar\Omega)^3}.$$

Some authors have modified this formula. For finite size effect, a modified ansatz formula for $\rho(E)$ is given by Grossmann and Holthaus [5]. Based on the two leading terms in the degeneracy $g_l=\frac{1}{2}(l+1)(l+2)$, they constructed a continuous density of states as

$$\rho(E)=\frac{1}{2}\frac{E^2}{(\hbar\Omega)^3}+\gamma\frac{E}{(\hbar\Omega)^2}, \tag{5}$$

where $\Omega=(\omega_x\omega_y\omega_z)^{1/3}$ is the geometric averages of the oscillator frequencies. The coefficient γ depends on the individual oscillator frequencies. For anisotropic oscillator, $\gamma=\frac{1}{2}(\omega_x\omega_y\omega_z)^{2/3}\left[\frac{1}{\omega_x\omega_y}+\frac{1}{\omega_x\omega_z}+\frac{1}{\omega_y\omega_z}\right]$ [7]. For isotropic oscillator $\gamma=3/2$ which follows immediately from the relation $g_l=\frac{1}{2}l^2+\frac{3}{2}l+1$. Grossmann ansatz formula accounted well for finite size effect.

Minguzzi *et. al* [14] employed a mean field, semiclassical two-fluid model to study the interacting Bose gas. This work provides semianalytical expressions for the density distribution for both condensed particles and the thermal component. A modified formula for the density of state is derived. In spite of the formula appears more complicated, it is used in calculating the chemical potential from Eq. (4). The obtained results for the chemical potential is used in the numerical solution of the self-consistent model.

2. SIMULTANEOUSLY FINITE SIZE, AND INTERATOMIC INTERACTION

It is a straightforward generalization to include the main three effects within the density of states. In doing this we are going to evaluate a modified formula for the density of state. In the semiclassical approximation we can introduce a coordinate system defined by the three variables $E_{n_x,n_y,n_z} = = \hbar(\omega_{x,y,z} n_{x,y,z})$ in terms of which the surface of the constant energy given in Eq. (1) is the plane

$$(E_{n_x,n_y,n_z} - E_0) \equiv (E+\mu) = E_{n_x} + E_{n_y} + E_{n_z}.$$

In this case the number of states $N(E)$ is proportional to the volume in the first octant bounded by this plane, *i.e.*

$$N(E) = \frac{1}{(\hbar\Omega)^3}\int_0^{E+\mu} dE_{n_x} \int_0^{E+\mu-E_{n_x}} dE_{n_y} \int_0^{E+\mu-E_{n_x}-E_{n_y}} dE_{n_z} = \frac{1}{6}\frac{(E+\mu)^3}{(\hbar\Omega)^3}.$$

The density of state is defined by

$$\rho(E) = \frac{\partial N(E)}{\partial E} = \frac{1}{2}\frac{(E+\mu)^2}{(\hbar\Omega)^3}. \tag{6}$$

Eq. (6) contains a constant term, $\frac{\mu^2}{2(\hbar\Omega)^3}$, it is independent on E. This term will produce $\zeta(1)$ in the critical temperature T_c formula, which would lead to the conclusion that $T_c \to 0$. Recently Yukalove solve this problem [21]. However, we will drop this term and consider only the linear term in μ. Finally, in order to obtained the anisotropic effect of the trap, the second term will be multiplied by $\left(\frac{\overline{\omega}}{\Omega}\right)$. Gathering Grossmann ansatz formula, Eq. (5), with the calculated formula in Eq. (6) one have

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

In the following, and when we use this ansatz formula in calculating the thermodynamical parameters, it is convenient to introduce a dimensionless parameter η [11]. It is defined such that

$$\frac{\mu(N_0,T)}{K_B T_0} = \frac{\mu(N,T=0)}{K_B T_0}\left(\frac{N_0}{N}\right)^{2/5} = \eta(1-t^3)^{2/5}.$$

The parameter η is a scaling parameter gives the scaling behavior of all thermodynamic quantities due to interatomic interaction. In terms of the scattering length a, the scaling parameter η is given by $\eta = 1.57\left(N^{1/6}\frac{a}{a_r}\right)^{2/5}$ with $a_r = \sqrt{\frac{\hbar}{m\Omega}}$ is a characteristic length for the harmonic trap [17].

Substitution from Eq. (7) in Eq. (4) one have the total number of condensed atoms and the average energy per particle as,

$$N_0 = N\left\{1-t^3-\frac{\zeta(2)}{\zeta(3)}\left[\gamma\left(\frac{\zeta(3)}{N}\right)^{1/3}+\left(\frac{\overline{\omega}}{\Omega}\right)\eta(1-t^3)^{2/5}\right]t^2\right\}$$
$$\frac{<E>}{NK_BT_0}=3\frac{\zeta(4)}{\zeta(3)}t^4+2\gamma\left(\frac{\zeta(3)}{N}\right)^{1/3}t^3+\frac{1}{7}\eta\left(1-t^3\right)^{2/5}\left(5+14\left(\frac{\overline{\omega}}{\Omega}\right)t^3\right), \tag{8}$$

where $t=T/T_0$ is the reduced temperature, with T_0 is the transition temperature for ideal condensed gas, its given by $T_0=\frac{\hbar\Omega}{K_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}$, and ζ is the Riemann zeta function. The relation $\frac{E_0}{NK_BT_0}=\frac{5}{7}\eta(1-t^3)^{2/5}$ is used [11]. Eq. (8) gives simultaneously the finite size, and interatomic interaction correction effects. The same results is obtained by semi-ideal model, mean field theory approximation, and canonical statistics approach as obtained in Thomas-Fermi approximation [11, 16, 13]. Eq. (8) contains two free parameters, γ and η, these two parameters are accounted for finite size and interatomic interaction effects respectively. So, it provides a detailed test for the system.

3. RELEASE ENERGY FOR SPHERICAL SYMMETRY TRAP

In the experiments setup, the condensed Bose gas is produced at thermal equilibrium. When the trapping potential switches off suddenly, the cloud expands ballistically, and after a time long enough that the expansion velocity has reached a steady state value the kinetic energy of the expanding cloud is measured. This measured energy is known as the release energy.

By using the new ansatz formula we also calculate the release energy directly from the root mean square cloud radius and the time-of-flight. Since the release energy is a pure kinetic energy. After long expansion time it can be related to the value of thesquare radii of the system $<r^2>$ through the relation [19, 20]

$$E_{rel}=E_{kin}=\frac{m}{2}<v^2>_{\tau\to\infty}=\frac{m}{2\tau^2}<r^2>_{\tau\to\infty}, \tag{9}$$

where τ is the time of flight.

For simplicity we consider first a spherically symmetric harmonic trap ($\gamma = 3/2$ and $\omega_{x,y,z}\equiv\omega=\overline{\omega}=\Omega$) with potential

$$V_{ext}(\mathbf{r})=\frac{m}{2}\omega^2r^2, \tag{10}$$

the width of a state $|i>$ with energy $E_{n_x n_y n_z}$ is obtained from the first principle of quantum mechanics [19]

$$<r_i^2> = \frac{<2V_{ext}(\mathbf{r})>}{m\omega^2} = \frac{E}{\hbar\omega} a_r^2,$$

where $a_r = \sqrt{\frac{\hbar}{m\omega}}$. The width of N trapped atoms of a Bose gas is given by [18]

$$<r^2> = \sum_{n_1 n_2 n_3} n(E_{n_x n_y n_z}) <r_i^2>.$$

For large N we take the usual approximation of changing the summation into an integral weighted by the density of states. So from Eq. (3), and (4) this width becomes

$$<r^2> = \frac{a_r^2}{\hbar\omega}\left\{N_0 E_0 + \sum_{j=1}^{\infty} z^j \int_0^{\infty} E\rho(E) e^{-j\beta E} dE\right\}. \tag{11}$$

This expression 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 (thermal component), this term include the correction due to finite size and interaction effects. Substitution from Eq. (7) into Eq. (11) one have,

$$<r^2> = a_r^2\left\{\frac{3}{2}N_0 + 3\zeta(4)\left(\frac{N}{\zeta(3)}\right)^{4/3} t^4 + 3N\left(\frac{\zeta(3)}{N}\right)^{1/3} t^3 + 2N\eta\left(1-t^3\right)^{2/5} t^3\right\}, \tag{12}$$

where $\gamma = \frac{3}{2}$ for spherical trap, and $E_0 = \frac{3}{2}\hbar\omega$ for condensed gas in the off trap. Substituting in Eq. (9) the square radii of the condensate, we have the release energy as a function of time of flight for spherical symmetry trap.

$$\frac{E_{rel}}{NK_B T_0} = \\ = \frac{3}{2\omega_r^2\tau^2}\left\{\frac{(1-t^3)}{2}\left(\frac{\zeta(3)}{N}\right)^{1/3} + \frac{\zeta(4)}{\zeta(3)}t^4 + \left(\frac{N}{\zeta(3)}\right)^{1/3} t^3 + \frac{2}{3}\eta(1-t^3)^{2/5} t^3\right\}. \tag{13}$$

In Eq. (13) the finite size effects, which is accounted by the 3^{rd} term is proportional to the ratio $N^{-1/3}$ as obtained by many authors [5–8]. The last term in Eq. (13) gives the correction due to interatomic interaction effect which depends on N. In fact, the non-interacting model predicts a released energy independent of N. Conversely, the observed release energy per particle depends strongly on N. In the thermodynamic limit, Eq. (13) gives the results of the ideal gas.

Fig. 1 illustrates the temperature dependence of the release energy for spherical harmonic trap. The number of particle is taken to be $N = 5 \times 10^5$, $\omega = (2\pi)65$ Hz, and the time of flight is taken to be 50 ms. W. Zhang *et al.* [18] (solid line in the graph) pointed that the release energy for interacting ^{87}Rb gas have a characteristic temperature dependence, $E_{rel} \propto t^4$ if $t < 1$ and $E_{rel} \propto t$ if $t < 1$. Our calculated results from Eq. (13) (dotted line in the graph), with $\eta = 0.5$ and $\gamma = 1.5$ are agreement with this behavior for interacting ^{87}Rb gas. The ideal gas results is represented by a dashed line.

Finite size effect on the temperature dependence release energy is illustrated in Fig. 2. At reduced temperature $t < 1$, the released energy have the same behavior for interacting Bose gas for all N. Increasing the number of

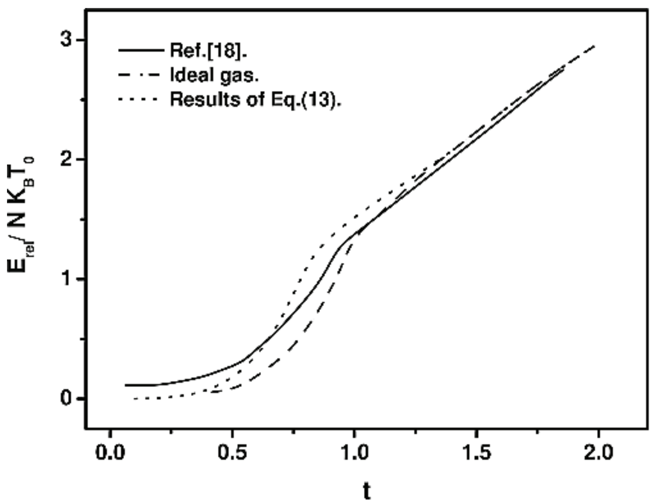

Fig. 1 – Release energy of the system as a function of reduced temperature t. The solid line is the results of W. Zhang [18], dotted line is the results of Eq. (13), and dashed line is results for the ideal gas.

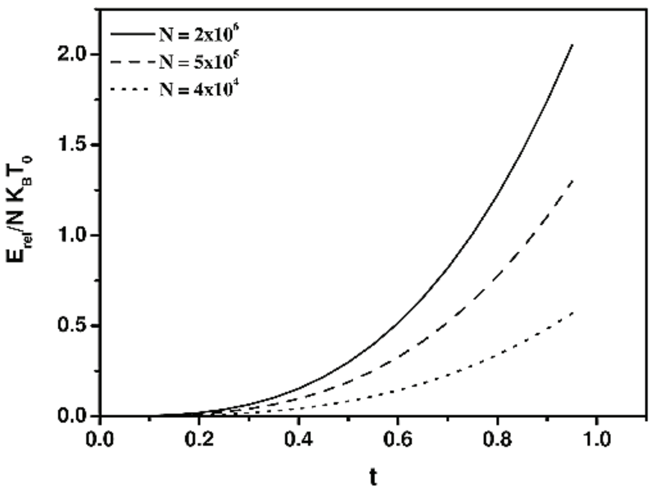

Fig. 2 – Release energy of the system as a function of reduced temperature t for three values of number of particles N. These results are calculated from of Eq. (13), for $\eta = 0.5$, $\omega's = 65(2\pi)$ Hz and $\tau = 50$ ms.

particles in the trap, leads to an increasing in the released energy. This feature has been confirmed by the experimental results on the temperature dependency of the release energy [2].

4. SPECIFIC HEAT CAPACITY

When the temperature T is below the BEC transition temperature T_0, the chemical potential $\mu = E_0$, and only the condensed component of the Bose gas has a contribution to the specific heat capacity. At $T < T_0$, the specific heat capacity can be calculated from the relation

$$C(T) = \frac{\partial < E(T) >}{\partial T} = \frac{\partial}{\partial T}\left\{ E_0 + \sum_{j=1}^{\infty} z^j \int_0^{\infty} E\rho(E)e^{-j\beta E}dE \right\} \quad (14)$$

by using Eq. (8) one have,

$$\frac{C(t)}{NK_B} = 12\frac{\zeta(4)}{\zeta(3)}t^3 + 9\left(\frac{\zeta(3)}{N}\right)^{1/3} t^2 + 6\eta\left(1-t^3\right)^{2/5} t^2 \left\{ 1 - \frac{\frac{6}{7} + \frac{12}{5}t^3}{1-t^3} \right\}. \quad (15)$$

Results calculated from Eq. (15) show that there is a temperature at which the specific heat capacity has a maximum value. This temperature can be identified as the temperature at which BEC occurs, we will refer to it by critical temperature T_c. At temperature greater than T_c the specific heat capacity falls rapidly over a temperature range of about $t = 0.04$. According to the value η, the specific heat capacity has a maximum value less than the semiclassical value of ideal gas at the transition temperature, $\left(\frac{C(t)}{NK_B}\right)_{T=T_0} \approx 10.8$. Table 1 summarizes the calculated maximum values for the specific heat capacity and the corresponding values of t_c for different η.

Fig. 3 presents the dependence of $C(t)/NK_B$ on the reduced temperature, t for three different values of η. These η values are chosen to be relevant to the experimental values, and N is taken to be 4×10^4. At very low temperature,

Table 1

The maximum values for the specific heat capacity and the corresponding values of t for different η, and $N = 40000$

γ	$\eta = 0.3$	$\eta = 0.4$	$\eta = 0.5$
	t_c	t_c	t_c
1.5	0.75	0.725	0.70

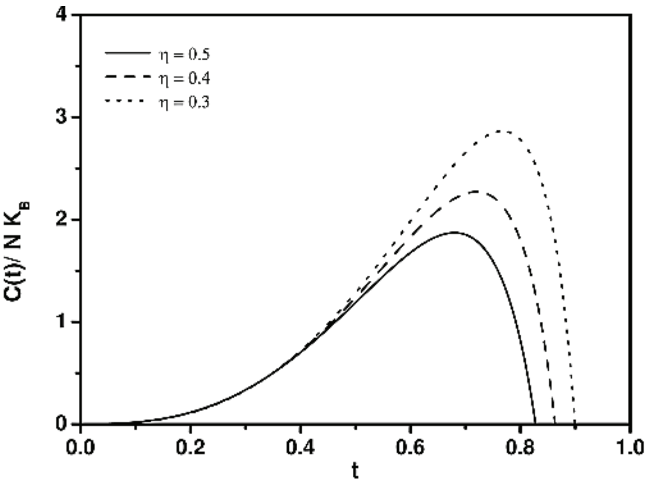

Fig. 3 – Specific heat capacity of the system as a function of reduced temperature t for three values of number of η. These results are calculated from of Eq. (9), for $N = 5 \times 10^4$, and $\omega's = 65(2\pi)$ Hz.

$t < 0.4$, effect of η is very weak. For $t > 0.4$, effect of η is very clear. The specific heat capacity increases monotonically with t, and reach its maximum value at $T = T_c$. At $T_0 > T > T_c$ the specific heat capacity decreases very fast, where $t_c = T_C/T_0$ is the reduced critical temperature at $T = T_c$. As it can be seen in the table, increasing η leads to monotonic decreasing in the value of the critical temperature. This dependence of $C(t_c)/NK_B$ on η is of major importance for the effect of interaction on the shift of the critical temperature from its ideal gas value T_0. Increasing the interacting parameter η leads to a shift in the critical temperature toward lower values 1.

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 release energy and specific heat capacity of a trapped interacted ^{87}Rb gas. Our approach allows for a careful comparison between the calculated results and the measured experimental data. Finally we summarize our conclusion as follows: There is a qualitative as well as a quantitative difference between the free boson gas and a system of bosons confined in a harmonic oscillator potential. It is interesting to notice that finite size effects, are still visible even in the presence of the interaction. But they are strongly quenched. In contrast to the previous work this approach involves only analytical calculations without technical complication. The new ansatz formula for the density of states allows one in a very clear fashion how the thermodynamical parameters affected simultaneously by, the finite size and interaction effects.

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