Scaling and thermodynamics of a trapped Bose-condensed gas

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Abstract

We investigate the thermodynamics of a Bose gas interacting with repulsive forces and confined in a harmonic trap. We show that the relevant parameters of the system (temperature, number $N$ of atoms, harmonic oscillator length, deformation of the trap, $s$-wave scattering length) fix its large $N$ thermodynamic behaviour through two dimensionless scaling parameters. These are the reduced temperature $t = T/T_0$ and the ratio $\eta$ between the $T = 0$ value of the chemical potential, evaluated in the Thomas-Fermi limit, and the critical temperature $T_c$ of the non-interacting model. The scaling functions relative to the condensate fraction, energy, chemical potential and moment of inertia are calculated within the Popov approximation.

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First measurements of relevant thermodynamic properties in gases of alkali atoms confined in magnetic traps have been recently become available [1,2]. These include the temperature dependence of the fraction of atoms in the condensate and the release energy. On the theoretical side the study of non uniform interacting Bose gases has a long history, starting from the works by Gross, Pitaevskii and Fetter [3] and the first approaches to thermodynamics developed in ref. [4]. More recently several theoretical papers have focused on the problem of the thermodynamic behaviour of such systems [5–10], and first calculations of the temperature dependence of the condensate have become available [7–9].

The properties of these trapped Bose gases at a given temperature are fixed by a large number of parameters: total number of atoms in the trap, atomic mass, harmonic oscillator length, deformation of the trap and strength of the interaction, which in a dilute gas is fixed by the s-wave scattering length. This makes these systems very rich for both experimental and theoretical investigations, but at the same time difficult to study in a systematic way. For example the deformation of the trap in the experiments carried out at MIT [1] and at Jila [2] as well as the corresponding number of atoms are quite different and it is not always easy to compare the experimental results. The purpose of this letter is to point out the occurrence of a scaling behaviour in the thermodynamics of these many-body systems. This permits to compare very different experimental situations, provided they correspond to the same value of the scaling parameters.

A first natural scaling parameter is given by the reduced temperature $t = T/T_0^c$, where $k_BT_0^c = \hbar\omega(N/\zeta(3))^{1/3}$ [11], with $\zeta(3) \simeq 1.202$, is the critical temperature predicted by the noninteracting harmonic oscillator model in the large $N$ limit and $\omega = (\omega_x\omega_y\omega_z)^{1/3}$ is the geometrical average of the oscillator frequencies characterizing the confining potential $V_{ext} = \frac{1}{2}m(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2)$.

In addition to the reduced temperature $t$ we introduce a second scaling parameter accounting for the role of the two-body repulsive interaction. This parameter is fixed by the ratio $\eta$ between the $T = 0$ value of the chemical potential, calculated in the Thomas-Fermi approximation, and the critical temperature $k_BT_0^c$. In the Thomas-Fermi approximation
the ground state density of a Bose gas takes the form \[ n_0(r) = (\mu_0^{TF} - V_{ext}(r))/g, \]
where \( g = 4\pi\hbar^2a/m \) is the coupling constant fixed by the (positive) s-wave scattering length \( a \) and the chemical potential is given by \( \mu_0^{TF} = \frac{1}{2}\hbar\omega(15Na/a_{HO})^{2/5} \), where \( a_{HO} = (\hbar/m\omega)^{1/2} \) is the harmonic oscillator length. The parameter \( \eta \) then takes the useful form

\[
\eta = \frac{\mu_0^{TF}}{k_B T_0} = \alpha \left( N^{1/6} \frac{a}{a_{HO}} \right)^{2/5},
\]

with \( \alpha = \xi(3)^{1/3}15^{2/5}/2 \approx 1.57 \). Note that \( \eta \) exhibits a very smooth dependence on \( N \) \( (\eta \sim N^{1/15}) \) and its value in the presently available experiments ranges from 0.38 to 0.45 even if \( N \) varies by orders of magnitude in the different experiments. The ratio (1) can be also written in the form \( \eta = 2.24(a^3n_0(r = 0))^{1/6} \), where \( n_0(r = 0) \) is the density of the atomic cloud in the center of the trap evaluated at zero temperature. With the above values of \( \eta \), the gas parameter \( a^3n_0(r = 0) \) turns out to be extremely small \( (10^{-4}-10^{-5}) \) so that the system is always very dilute.

In the following we will show that the relevant thermodynamic properties of the system exhibit, when expressed in their natural units, a scaling behaviour in terms of the parameters \( t \) and \( \eta \). Scaling is actually achieved only if \( N \) is sufficiently large and finite size corrections to the asymptotic behaviour of the various thermodynamic functions can be ignored. We will show that scaling is reached with very good accuracy for most thermodynamic properties not only in the experimental conditions of ref. (1) where \( N \) is of order of \( 10^6 - 10^7 \), but also in the ones of ref. (2) where \( N \) is much smaller \( (10^4 - 10^5) \).

The scaling behaviour can be exploited by investigating the thermodynamic behaviour of these systems within the Popov approximation (13-15). This approximation provides coupled equations for the condensate density and the thermal density of the system. In this letter we will use the semiclassical approximation for the excited states and hence we will always consider temperatures much larger than the oscillator temperature \( \hbar\omega/k_B \). The equation for the condensate is given by

\[
-\frac{\hbar^2}{2m} \nabla^2 \Phi(r) + [V_{ext}(r) - \mu + g(n_0(r) + 2n_T(r))] \Phi(r) = 0,
\]

(2)
and the dispersion law of the elementary excitations takes the Bogoliubov-type form \[8\]

\[
\epsilon(p, r) = \sqrt{\left(\frac{p^2}{2m} + V_{ext}(r) - \mu + 2gn(r)\right)^2 - g^2n_0^2(r)}. \tag{3}
\]

In eqs. (2), (3) \(n_0 = \Phi^2\) is the density of the condensate, \(n = n_T + n_0\) is the total density of the system and the thermal density \(n_T\) is defined by \(n_T(r) = \int dp/(2\pi\hbar)^3(-\partial \epsilon/\partial \mu)f(\beta \epsilon)\) where \(f(\beta \epsilon) = (\exp(\beta \epsilon) - 1)^{-1}\) is the quasi-particle distribution function. The semiclassical approximation (3) to the excitation spectrum is accurate only if the non-condensate density \(n_T\) varies smoothly on the scale of the oscillator length \(a_{HO}\), and if the relevant values of \(p\) satisfy the condition \(p \gg \hbar/a_{HO}\), which also implies \(\epsilon \gg \hbar \omega\). The above approximation, called Popov approximation, coincides with the Bogoliubov approach at very low temperatures, while at high \(T\) it coincides with the finite temperature Hartree-Fock theory for Bose systems \[4\] (for further details on the Popov approximation see refs. \[6,8\]). Equations (2)-(3) are solved \[8\] using a self consistent procedure, the value of the chemical potential \(\mu\) being determined by the normalization condition \(\int d\mathbf{r}(n_0(r) + n_T(r)) = N_0 + N_T = N\).

The scaling behaviour of the Popov equation is exhibited in the Thomas-Fermi limit, which is reached when the ratio \(\mu_0^{TF}/\hbar \omega = 0.94 N^{1/3}\eta\) is much larger than unity. In this limit, which is formally achieved taking \(N \to \infty\) with \(\eta\) fixed, the kinetic energy term in the Schrödinger equation (2) for the condensate can be neglected. By introducing the dimensionless quantities \(\tilde{p}_i = \sqrt{1/2mk_BT_0^0p_i}, \tilde{r}_i = \sqrt{m/2k_BT_0^0}\omega_i r_i, \tilde{\mu} = \mu/k_BT_0^0, \tilde{\epsilon} = \epsilon/k_BT_0^0, \tilde{n}_T = n_T(2k_BT_0^0/m\omega^2)^{3/2}/N\) and \(\tilde{n}_0 = n_0(2k_BT_0^0/m\omega^2)^{3/2}/N\), one can rewrite the Popov equations in the reduced form

\[
\tilde{n}_0(\tilde{r}) = \frac{1}{g} \left(\tilde{\mu} - \tilde{r}^2 - 2g\tilde{n}_T\right) \theta(\tilde{\mu} - \tilde{r}^2 - 2g\tilde{n}_T), \tag{4}
\]

\[
\tilde{\epsilon}(\tilde{p}, \tilde{r}) = \sqrt{\left(\tilde{p}^2 + \tilde{r}^2 - \tilde{\mu} + 2g(\tilde{n}_0 + \tilde{n}_T)\right)^2 - g^2\tilde{n}_0^2}, \tag{5}
\]

where \(\tilde{n}_T(\tilde{r}) = 1/(\pi^3\zeta(3)) \int d\tilde{p}(-\partial \tilde{\epsilon}/\partial \tilde{\mu})f(\beta \tilde{\epsilon}), \tilde{g} = 8\pi\eta^{5/2}/15 = 5.2N^{1/6}a/a_{HO}\) and \(\theta(x)\) is the step function. The normalization condition for the reduced densities reads: \(\int d\tilde{r}(\tilde{n}_0 + \tilde{n}_T) = 1\). Equations (4)-(5) exhibit the anticipated scaling behaviour in the variables \(t\) and
η. Starting from their solutions one can calculate the condensate and the thermal densities as well as the excitation spectrum. This gives access to all the relevant thermodynamic quantities of the system. For example the condensate fraction is given by

\[
\frac{N_0}{N} = 1 - \frac{1}{\pi^3 \zeta(3)} \int d\tilde{r} d\tilde{p} \left( - \frac{\partial \tilde{\epsilon}}{\partial \tilde{\mu}} \right) f(\tilde{\epsilon}/t) . \tag{6}
\]

In particular the vanishing of the right hand side of eq. (6) fixes the value of the critical temperature \( t_c = T_c/T_c^0 \). To the lowest order in the renormalized coupling constant \( \tilde{g} \) one finds \( t_c \simeq 1 - 0.43\eta^{5/2} = 1 - 1.3N^{1/6}a/a_{HO} \). The energy of the system can be calculated starting from the standard thermodynamic relation in terms of the entropy. In units of \( Nk_B T_c^0 \) one finds:

\[
\frac{E}{Nk_B T_c^0} = \frac{5}{7} \eta + \int_0^t dt' \frac{\partial s}{\partial t'} , \tag{7}
\]

where the entropy per particle \( s \) is given by the combinatorial expression

\[
s(t, \eta) = \frac{k_B}{\pi^3 \zeta(3)} \int d\tilde{r} d\tilde{p} [(1 + f(\tilde{\epsilon}/t)) \log(1 + f(\tilde{\epsilon}/t)) \right.

\[
- f(\tilde{\epsilon}/t) \log f(\tilde{\epsilon}/t)] . \tag{8}
\]

Another important quantity is the normal (non superfluid) density given by the natural generalization

\[
\rho_n(\mathbf{r}) = - \int \frac{d\mathbf{p}}{(2\pi \hbar)^3} \frac{p^2}{3} \frac{\partial f(\beta \epsilon)}{\partial \epsilon} \tag{9}
\]

of the Landau formula \([15]\) to the case of non uniform systems. Note that in general the normal density \( \rho_n \) differs from the non condensate density \( n_T \). Only at temperatures larger than the chemical potential one has \( \rho_n \simeq mn_T \). In terms of \( \rho_n \) one can calculate the moment of inertia, defined as the linear response function to a cranking rotational field \([16]\). In the case of an axially symmetric trap one finds the result

\[
\Theta = \int d\mathbf{r} (x^2 + y^2) \rho_n(\mathbf{r}) . \tag{10}
\]

Deviations of \( \Theta \) from the rigid value \( \Theta_{\text{rigid}} = m \int d\mathbf{r} (x^2 + y^2) n(\mathbf{r}) \) provide a signature of the superfluid behaviour of the system. Above \( T_c \) one has \( \rho_n = mn_T = mn \) and \( \Theta = \Theta_{\text{rigid}}. \)
In Fig. 1 we explicitly show the accuracy of the scaling behaviour, by plotting the scaling function (3) calculated with $\eta = 0.45$ and the results obtained from the full solution of the Popov equations (2)-(3), with different choices of $N$ and of the other parameters, yielding the same value $\eta$. The open circles have been obtained with the choice: $a/a_{HO} = 7.35 \times 10^{-3}$, $\lambda = \omega_z/\omega_x = \sqrt{8}$, $N = 5 \times 10^4$, which corresponds to the experimental conditions of ref. [2], while the solid circles have been calculated with the choice: $a/a_{HO} = 2.55 \times 10^{-3}$, $\lambda = 18/320$, $N = 2.9 \times 10^7$, which is close to the experimental situation of ref. [1]. This example shows how extremely different experimental conditions give rise to the same thermodynamic behaviour. The figure clearly shows that scaling is very well verified for these configurations. Only very close to $T_c$ the $N = 5 \times 10^4$ points exhibit small deviations from the scaling behaviour. In fact close to $T_c$ the scaling law (3) is approached more slowly with increasing $N$. In the same figure we also plot the predictions for the same configurations obtained switching off the two-body interaction. Deviations from the non-interacting result $1 - t^3$ are due to finite size effects, whose importance, in the presence of the interaction, turns out to be strongly quenched. The scaling behaviour has been verified also for the other values of the parameter $\eta$ and for all the other thermodynamic properties considered in this work.

In Fig. 2 we present results for the condensate fraction $N_0/N$ as a function of the reduced temperature $t$ for three different values of the scaling parameter $\eta$, covering the presently available experimental conditions. The open diamonds with the error bars are the results of the Monte-Carlo simulation of ref. [4] which correspond to the value $\eta = 0.33$ and which are in good agreement with our predictions. The dots are the experimental results of ref. [2]. In the experiments the number of particles $N$ varies with $T$, with the value of $\eta$ ranging from 0.45 to 0.39. The experiments exhibit smaller deviations from the non-interacting curve with respect to the theoretical predictions. One should however keep in mind that the measured value of $T$ corresponds to the temperature of the thermal cloud after expansion. The identification of this temperature with the one of the system before expansion ignores the interaction with the condensate which is expected to produce an acceleration of the thermal cloud. A preliminary estimation shows that for $T \approx 0.5T_c^0$ the final kinetic energy
of the thermal cloud is about 10\% larger than its value before the expansion.

In Fig. 3 we present the results for the chemical potential in units of $k_B T_c^0$ corresponding to the same values of $\eta$. Notice that for $t \to 0$ the plotted quantity coincides with $\eta$ (see eq. (1)). In the classical limit, $T \gg T_c^0$, the dependence on the interaction parameter $\eta$ disappears and one finds the classical ideal gas prediction $\mu/k_B T_c^0 = t \log(\zeta(3)/t^3)$.

In Fig. 4 we report the results for the total energy $E$. At high temperature the behaviour is given by the classical law $E/k_B T_c^0 = 3t$. In Fig. 4 (inset) we also show our predictions for the release energy $E_R$, defined as the energy of the system after the trap potential has been switched off. In the classical non-interacting limit one has $E_R = 3Nk_B T/2$. First experimental results for the release energy have been obtained in ref. [2] and are shown in the figure.

Finally in Fig. 5 we show our predictions for the moment of inertia. We find that, differently from the other quantities discussed above, the ratio $\Theta/\Theta_{\text{rig}}$ does not exhibit any significant dependence on $\eta$. In the same figure we also show the moment of inertia calculated in the non-interacting model for two different values of $N$ and deformation $\lambda$. It is worth noting that in the absence of interaction the value of $\Theta/\Theta_{\text{rig}}$ depends rather crucially on $N$ and $\lambda$.

In conclusion we have explored the scaling behaviour of the thermodynamic properties of a trapped Bose gas. The new key parameter which permits to discuss the role of two-body interactions is the scaling parameter (1), given by the value of the zero-temperature chemical potential in units of $k_B T_c^0$. Scaling is predicted to work very well in the typical conditions of available experiments.

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FIGURES

FIG. 1. Condensate fraction as a function of $T/T_c^0$ for $\eta = 0.45$ (solid line). The open circles refer to $N = 5 \times 10^4$ Rb atoms in the JILA-type trap. The solid circles correspond to $N = 2.9 \times 10^7$ Na atoms in the MIT-type trap. The dotted line is the $1 - t^3$ curve of the non-interacting model in the large $N$ limit. The open and solid triangles correspond to $N = 5 \times 10^4$ and $N = 2.9 \times 10^7$ non-interacting particles in the JILA and MIT-type traps respectively.

FIG. 2. Condensate fraction as a function of $T/T_c^0$ for three values of the scaling parameter $\eta$. Solid line: $\eta = 0.45$, long-dashed line: $\eta = 0.39$, short-dashed line: $\eta = 0.31$. Open diamonds: PIMC results of ref. [7]. Solid circles: experimental results from ref. [2]. The dotted line refers to the non-interacting model in the large $N$ limit.

FIG. 3. Chemical potential as a function of $T/T_c^0$ for three values of the scaling parameter $\eta$ (see Fig. 2). The dotted line refers to the non-interacting model in the large $N$ limit.

FIG. 4. Total energy of the system as a function of $T/T_c^0$ for three values of the scaling parameter $\eta$ (see Fig. 2). (inset) Release energy for the same values of $\eta$. The solid circles are the experimental results of ref. [2].

The dotted lines refer to the non-interacting model in the large $N$ limit.

FIG. 5. Ratio $\Theta/\Theta_{\text{rigid}}$ as a function of $T/T_c^0$ for three values of the scaling parameter $\eta$ (see Fig. 2). The three curves coincide almost exactly and are represented by the solid line. The dotted line refers to $N = 5 \times 10^4$ atoms in the JILA-type trap in the non-interacting model. The dot-dashed line refers to $N = 2.9 \times 10^7$ atoms in the MIT-type trap in the non-interacting model.
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