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Atomic density of an harmonically trapped ideal gas near Bose-Einstein transition temperature

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Abstract. We investigate the atomic density of a cloud confined in an isotropic harmonic trap at the vicinity of Bose-Einstein transition temperature. We show that, for an ideal gas and near this temperature, the ground-state density cannot be neglected, even at the thermodynamic limit. In particular, at the transition temperature, the value of $\rho(0)\lambda^3$ with $\rho(0)$ the total peak density and λ the thermal de Broglie wavelength, is more than two times the famous $\zeta(3/2) \approx 2.612$. We compare the exact calculations, available in an harmonic trap, to semi-classical approximations.

PACS. 03.75.Hh Static properties of condensates; thermodynamical, statistical and structural properties – 03.65.Sq Semiclassical theories and applications – 05.30.Jp Boson systems

The phenomenon of Bose-Einstein condensation (BEC) is a phase transition. Below the critical temperature T_c , the ground-state population, which is the order parameter, becomes macroscopic. This phenomenon, that happens strictly speaking only at the thermodynamic limit, is usually illustrated in textbooks with an homogenous gas. Experimentally, the Bose-Einstein condensation of dilute gases has been observed since 1995 with atoms confined in an harmonic trap. These stimulating experimental data quickly showed that two more effects were to be considered for complete interpretation: interatomic interactions and the finite atom number, typically 10^6 . This leads [1] to a shift of the transition temperature, to Bogoliubov-like excitation spectrum of the condensate, to Thomas-Fermi profile for dense condensate... Several papers address more specifically finite size effects on harmonically trapped ideal gases. Two quantities have been investigated in detail: the atom number [2,3,5,6,7,8] and the specific heat [4,6,8]. It is shown that the transition temperature associated to the atom number is shifted compared to T_c , but by a small amount, typically of few percent for atom numbers in the range 10^6 . The transition temperature for the specific heat is different but is also very close to T_c [4,8].

Surprisingly fewer attention was payed on the atomic density of an ideal gas. In an homogenous gas it is obviously equivalent to the atom number but this is no more the case in a spatially varying potential. It becomes the good parameter of the theory, in particular to perform local density approximations. One can wonder if the den-

sity will behave similarly as the atom number around the transition temperature. We will see that the answer is generally no. This point will be illustrated for an isotropic harmonic trapping and for a finite atom number. Furthermore, it implies that semi-classical approximations for the atomic density have to be derived carefully. This should be particularly true, for example, for the study of the shift of the critical temperature by the interatomic interactions, both within the mean-field approximation [5] and beyond this approximation [9]. The effect of interactions will not be addressed in this paper.

In an harmonic trap and at the transition temperature we will find that the ground-state peak density is not negligible and has the same order of magnitude as the excited states density. The Einstein criterion for BEC $\rho(0)\lambda^3 = \zeta(3/2)$ with $\rho(0)$ the *total* peak density and λ the thermal de Broglie wavelength has to be replaced by $\rho(0)\lambda^3 = \zeta(3/2) + 2\sqrt{2\zeta(2)}$. This result, obtained at the thermodynamic limit, is still valid for finite atom numbers. We will compare the exact results with semi-classical approximations. The addition of the ground-state contribution on the latter improve their accuracy. We will finally show that spatial integrations of the density, used usually for imaging, decrease the effect.

We will use finite atom number for our calculations and hence speak rather about transition temperature instead of critical temperature. It will be denoted T^* in the following. As we will discuss several models for the atomic density we will define different values of T^* . The Bose-Einstein distribution gives the population N_i of a given

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energy level ϵ_i : $N_i = (e^{\beta(\epsilon_i - \mu)} - 1)^{-1}$ with $\sum_{i=0}^{\infty} N_i = N$.

Here $\beta = 1/k_B T$ with k_B the Boltzmann's constant, μ is the chemical potential and N the total atom number. For a fixed atom number the chemical potential increases as the temperature decreases. As μ has to be smaller than ϵ_0 , the ground-state energy, the excited state population will saturate when μ approaches ϵ_0 whereas N_0 is still increasing: $N - N_0 = \sum_{i=1}^{\infty} N_i(\mu, T) \leq \sum_{i=1}^{\infty} N_i(\mu = \epsilon_0, T)$.

The transition temperature T^* is defined [1,10] as the temperature such that the saturated excited states population is equal to the total atom number :

$$\sum_{i=1}^{\infty} N_i(\epsilon_0, T^*) = N \quad (1)$$

It is important to note that at the transition temperature, the chemical potential *is not* equal to the ground-state energy. The preceding equation gives the value of the transition temperature and, adding the ground state contribution, $\sum_{i=0}^{\infty} N_i(\mu^*, T^*) = N$ gives then the value of the chemical potential at $T = T^*$.

We will first examine the thermodynamic limit case. There, things seem simple. For an isotropic harmonic trap of oscillation frequency ω , this limit means $N \rightarrow \infty$ with $N\omega^3$ kept constant. Then $\tau = \hbar\omega/(k_B T) \ll 1$ and semi-classical approximations should work. Replacing the discrete energy spectrum by a continuous one and neglecting the ground-state energy ϵ_0 , leads to the density $\rho(r) = \frac{1}{\lambda^3} g_{\frac{3}{2}}[z \exp(-\frac{\tau}{2}(r/\sigma)^2)]$ with $z = e^{\beta\mu}$ the fugacity, $\sigma = \sqrt{\frac{\hbar}{m\omega}}$ the size of the ground-state and $g_{\frac{3}{2}}()$ a Bose function [11]. With the above notation, the thermal de Broglie wavelength is $\lambda = \sigma\sqrt{2\pi\tau}$. Similarly, the atom number would be $N = g_3(z)/\tau^3$. Obviously these expressions neglect the population of the ground-state. As $\tau \ll 1$, eq.1 leads then to $z_c = 1$ and $N = \zeta(3)/\tau^3$, with T_c the critical temperature. The critical peak density would then be given by $\rho_c(0)\lambda_c^3 = g_{\frac{3}{2}}(z_c) = \zeta(3/2) \approx 2.612$.

These statements are wrong, however. The thermodynamic limit has to be taken at the end of the calculation, meaning that we are not allowed to neglect the ground-state population from the beginning. The above expression for the density and atom number are in fact approximations for the excited states. Adding the ground-state contribution leads to $\rho(r) = \frac{1}{\lambda^3} g_{\frac{3}{2}}[z e^{-\frac{\tau}{2}(r/\sigma)^2}] + \rho_0(r)$ and $N = \frac{1}{\tau^3} g_3(z) + N_0$ with $\rho_0(r) = \frac{N_0}{(\sqrt{\pi}\sigma)^3} e^{-(r/\sigma)^2}$ and $N_0 = \frac{z}{1-z}$. The value of the critical temperature is unchanged as it is defined by the excited states saturation, but the critical fugacity z_c is now different from 1. Using $g_3(z_c) \approx \zeta(3) - \zeta(2)x_c$ with $z_c = e^{-x_c}$ ($x = \beta(\epsilon_0 - \mu) > 0$), leads to $x_c \approx \tau_c^{3/2}/\sqrt{\zeta(2)}$ [8]. The ground-state population is $\sim 1/x_c$ and, as expected, vanishingly small as $\tau_c \rightarrow 0$ compared to the excited-state population $\zeta(3)/\tau_c^3$. The ground-state peak density is $\sim \frac{1}{(\sqrt{\pi}\sigma)^3 x_c}$ whereas the ex-

cited state peak density is $\zeta(3/2)/\lambda_c^3$. As $\lambda_c = \sigma\sqrt{2\pi\tau_c}$, the two quantities have the same order of magnitude ! The degeneracy parameter is then $\rho_c(0)\lambda_c^3 = \zeta(3/2) + 2\sqrt{2}\zeta(2) \approx 6.24$. This means that the ground-state population is extremely small but the size of its wavefunction is also extremely small compared to the atomic cloud size. For an harmonic trap both depends on the same small parameter at also the same power. So, even at the thermodynamic limit, the traditional criterion for BEC is modified.

We will now address the case of finite atom numbers and the comparison between semi-classical approximations and exact results. It is well known that the transition temperature will be shifted compared to T_c for finite atom numbers [2,3,6]. The above semi-classical approximation is then inaccurate. A better approximation, which takes into account the ground-state energy to first order, is: $\rho(r) = \frac{1}{\lambda^3} \{g_{\frac{3}{2}}[\tilde{z}(r)] + \frac{3\tau}{2} g_{\frac{1}{2}}[\tilde{z}(r)]\}$ where $\tilde{z}(r) = z e^{-\frac{\tau}{2}(r/\sigma)^2}$. Then $N = \frac{1}{\tau^3} [g_3(z) + \frac{3\tau}{2} g_2(z)]$. This is the usual semi-classical approximation found in the literature. Note that $g_{\frac{1}{2}}(z)$ diverges at $z = 1$. This means that this approximation is intrinsically bad near the center of the trap for the transition temperature. This divergence is however weak, and any spatial integration will give finite result.

We can cure this defect by adding, as before, the ground-state contribution. We obtain then

$$\begin{cases} \rho_{sc}(r) = \frac{1}{\lambda^3} \{g_{\frac{3}{2}}[\tilde{z}(r)] + \frac{3\tau}{2} g_{\frac{1}{2}}[\tilde{z}(r)]\} + \frac{z}{1-z} \frac{e^{-(\frac{r}{\sigma})^2}}{(\sqrt{\pi}\sigma)^3} \\ N = \frac{1}{\tau^3} [g_3(z) + \frac{3\tau}{2} g_2(z)] + \frac{z}{1-z} \\ T_{sc}^* \text{ such that } N = \frac{1}{\tau_{sc}^3} [\zeta(3) + \frac{3}{2}\zeta(2)\tau_{sc}^*] \end{cases} \quad (2)$$

We will use this semi-classical approximation in the following. The harmonic trap is specific because one knows exactly the eigen-energies and eigen-functions of the Hamiltonian. Semi-classical approximations can then be tested accurately. The expressions of the atomic density and atom number [12] are :

$$\begin{cases} \rho_{ex}(r) = \frac{1}{(\sqrt{\pi}\sigma)^3} \sum_{l=1}^{\infty} \frac{z^l}{(1-e^{-2\tau l})^{3/2}} e^{-\tanh(\frac{\tau l}{2})(\frac{r}{\sigma})^2} \\ N = \sum_{l=1}^{\infty} \frac{z^l}{(1-e^{-\tau l})^3} \\ T_{ex}^* \text{ such that } N = \sum_{l=1}^{\infty} \left(\frac{1}{(1-e^{-\tau_{ex}^* l})^3} - 1 \right) \end{cases}$$

where, here $z = e^{\beta(\mu - \epsilon_0)}$. The semi-classical models correspond to a Taylor expansion in τ of these last expressions.

The semi-classical model *sc* is a very good approximation of the exact solution [13]. They only differ slightly near the transition temperature. Figure 1 shows the relative deviations of T_c and T_{sc}^* from T_{ex}^* in function of the atom number. As expected the different values are very similar. The value T_{sc}^* deviates less than 1% for $N > 400$ and the relative shift is $\sim 10^{-4}$ for typical experimental atom numbers. This is well below actual experimental uncertainties. The thermodynamic value T_c is significantly higher than T_{ex}^* , typically 1 % [2,3,6,8]. This discrepancy

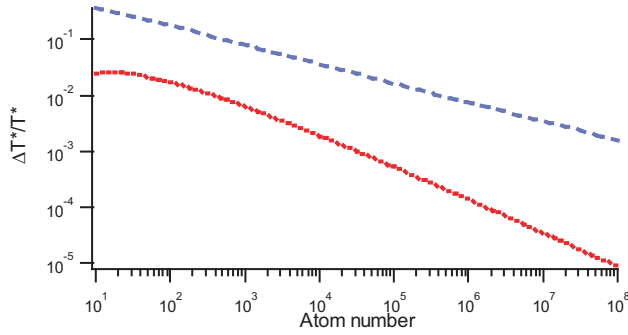


Fig. 1. Relative shift of the semi-classical transition temperatures T_c (dashed line) and T_{sc}^* (dotted line) to T_{ex}^* (see text) in function of the atom number. Both temperatures converge for high atom numbers. The critical temperature at thermodynamic limit, T_c , deviates by less than 1% for $N > 5 \cdot 10^5$. The semi-classical transition temperature defined for a finite atom number, T_{sc}^* , is much more accurate and deviates by less than 1% for $N > 400$.

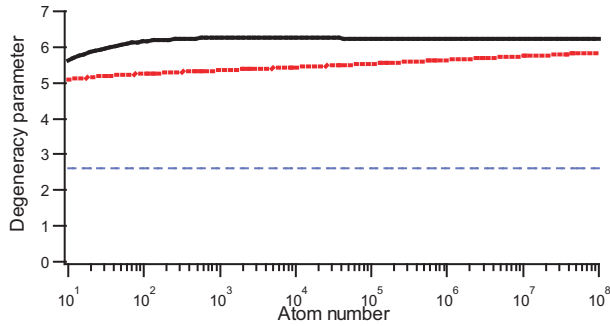


Fig. 2. The parameter $\rho(0)\lambda^3$ for the semi-classical model sc (dotted line) and for the exact calculation (solid line) is plotted in function of the atom number N for clouds at the transition temperature $T = T_{sc}^*$ and $T = T_{ex}^*$ respectively. Even if the degeneracy parameters are somewhat different, they both differ significantly to the usual value of 2.612 (dashed horizontal line). This deviation is due to an under-estimation of the ground-state density.

will be even more pronounced for anisotropic trap (see below).

Figure 2 shows the degeneracy parameter $\rho(0)\lambda^3$ in function of the atom number for clouds at $T = T^*$. We plot this number for the semi-classical approximation sc and for model ex . The two curves are higher than 2.612 and confirm the thermodynamic calculation presented above. The degeneracy parameter is astonishingly constant till 10^3 atoms and does not differ much even for smaller atom numbers. They both tend to the same asymptotic value but differ significantly for experimentally accessible atom numbers. This is because the term in $\frac{3}{2}\tau$ in model sc is not negligible. One finds $x_{sc}^* \approx \frac{(\tau_{sc}^*)^{\frac{3}{2}}}{\sqrt{\zeta(2)}} \left(1 + \frac{9}{8\zeta(2)} \tau_{sc}^* \ln \tau_{sc}^*\right)$ [11].

Figure 3 shows the evolution of the condensate fraction N_0/N and condensate peak density fraction in function of T for $N = 10^6$ atoms. What prevails in this figure is the

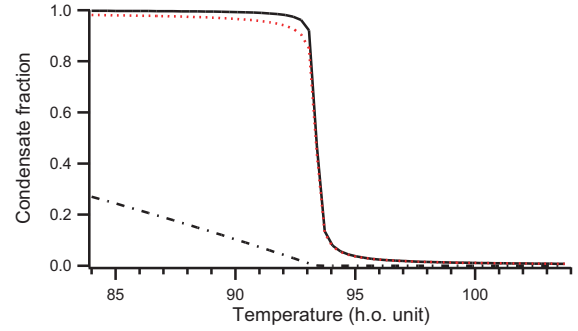


Fig. 3. Condensate atom number fraction N_0/N (dot-dash line) and peak density fraction $\rho_0(0)/\rho(0)$ (solid line) in function of the temperature in harmonic oscillator unit $\hbar\omega/k_B$. The cloud contains 10^6 atoms. The transition temperature is $T_{ex}^* = 93.37\hbar\omega/k_B$ and the asymptotic thermodynamic temperature is $T_c = 94.05\hbar\omega/k_B$. The ground-state peak density increases much more sharply than the ground-state population around the transition temperature. The former has also a significant value above T_{ex}^* . The model sc is indistinguishable for N_0/N , but is slightly different for $\rho_0(0)/\rho(0)$ (dotted line).

sharp increase of the condensate peak density compared to the condensate population. In this respect, the peak density is a much better marker of the Bose-Einstein condensation than the atom number. This feature is in fact used experimentally: the appearance of a small peak over a broad distribution is the usual criterion to distinguish clouds above or below the transition temperature. The increase of the density at threshold is very sharp and so the actual value of the density is very sensitive to the value of the temperature. This explains also the high sensitivity on the results shown in Fig.2. For this large atom number the temperature T_c and T_{ex}^* are already very close but can be distinguished in the small window around transition shown in the graph. One also notices that the ground-state peak density, even above transition, is significant. This will be even much more pronounced for smaller atom numbers.

Figure 4 shows the density profile of clouds at the same temperature for atom numbers around N_{ex}^* , the number of atoms for which $T = T_{ex}^*$ ($N = N_{ex}^*$ corresponds to the dotted line). Only the central part is sensitive to the atom number indicating that the excited states are already saturated. Moreover, by looking at the graph, one would rather think that the Bose-Einstein transition occurs for a smaller atom number. This points out that the definition on the transition temperature on an atom number criterion does not fully correspond to a criterion based on the atomic density which would be more connected to experiments. The inset shows the excited states and ground state density profile at threshold. The excited states density exhibits a dip in the center of the cloud, obviously not present in semi-classical models (monotonic functions). We check that the height of the dip is proportional to $1/\tau$ for various atom number and can almost be totally attributed to the first excited state occupation.

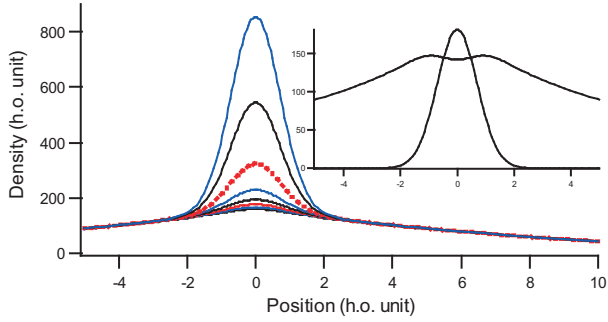


Fig. 4. Atomic density in function of r/σ where σ is the size of the harmonic oscillator ground-state. The temperature is $T = 93.37\hbar\omega/k_B$ and the atom number N spans from $0.990 \cdot 10^6$ to $1.004 \cdot 10^6$ by step of 2000 atoms. The curve at threshold is in dotted line. The inset shows the excited states and ground state density profile at threshold. The dip around $r = 0$ is mainly due to the first excited state population.

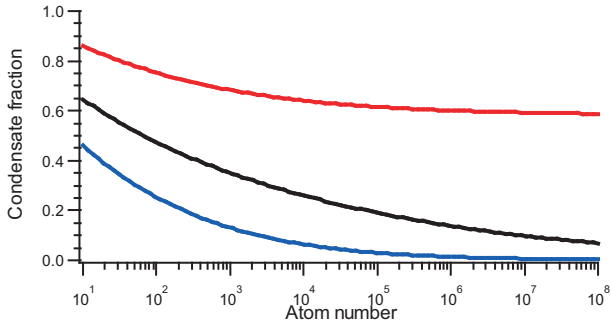


Fig. 5. Contribution of the ground-state on the peak density for, from bottom to top, 1D, 2D and 3D images in function of the number of trapped atoms. The clouds are at the transition temperature T_{ex}^* . A 3D image would give the density in all three dimensions of space [16] whereas 2D (resp. 1D) image corresponds to the density integrated over one (resp. 2) dimension. For $N = 10^4$ atoms the ground-state contributes to $\sim 26\%$ in 2D images and $\sim 6\%$ in 1D images. In contrast to 3D image, the ground-state contribution is very small for large atom number; it is not for typical atom numbers accessible in experiments.

We have shown results on the atomic density at the vicinity of the transition temperature. Detection techniques use rather 1D-integrated density (absorption images) or 2D-integrated density (see [15] for instance). One can show that, at threshold, the 1D and 2D-integrated peak density of the ground-state is vanishingly small at the thermodynamic limit. The peak 1D-integrated density fraction behaves at threshold as $\sqrt{\tau}$ and the 2D-integrated peak density as τ . For typical atom number this is nevertheless not negligible, as can be seen in Fig.5. We have also added, for comparison, the result for the full 3D density. At the transition temperature T_{ex}^* , the ground-state contributes to more than 10% for $N < 2500$ atoms in 1D images and for $N < 8 \cdot 10^6$ atoms for 2D images.

In conclusion, we have shown that the peak density of an ideal atomic gas is higher than expected near the transition temperature. Apart from the atomic density, two- and three-body inelastic loss rates will also be affected and could be 20 to 30% higher than expected around the transition temperature for typical atom numbers.

For anisotropic traps the term $\frac{3}{2}\tau$ in eq 2 becomes $\frac{3}{2}\tau\frac{\tilde{\omega}}{\bar{\omega}}$, with $\bar{\omega} = (\prod_i \omega_i)^{1/3}$ the geometric mean and $\tilde{\omega} = \frac{1}{3} \sum_i \omega_i$ the arithmetic mean [2]. Thus the effect will be even more pronounced for anisotropic traps because $\tilde{\omega} \gg \bar{\omega}$. Besides, the interatomic interactions have been neglected in our analysis and will modify our conclusions. Previous calculations treated separately finite size and interactions effects, both corrections being finally added. The main result presented here, the ground-state contribution on the density, tends to prove that both effects have to be investigated together. A full three-dimensional density measurement would be valuable to this respect; this type of measurement is at the edge to be available in our experiment on metastable helium in Orsay [16].

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