The condensate fraction and critical temperature for ultra cold Bose-Einstein condensates

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Abstract— We present numerical results of the condensate fraction and the critical temperature of a harmonically confined Bose gas in the Hartree-Fock-Bogoluibov-Popov (HFB-Popov) and generalized Hartree-Fock-Bogoluibov (GHFB) approximations. We determine the power law dependence of the condensate fraction on the reduced temperature and the shift in the critical temperature T_c. We find a good agreement with literature and experimental data.

Keywords— HFB-Popov approximation**;** GHFB approximation; Bose Einstein condensation

1. Introduction

In the last few years an increasing interest has been directed toward the study of gaseous Bose-Einstein condensates (BEC) trapped by harmonic potentials at zero and finite temperature. Many experiments, such as those of JILA and MIT [1-3] are performed in order to study the properties of a wide variety of condensed gases. The results have opened the door to several theoretical works which focus not only on the low temperature regime but also the near T_c one [4-5].

Most of the models are based on the mean field approach. In particular, the fundamental state of the system which describes the condensate is determined from a variational method that endows an independent evolution of each atom of the gas in the mean field created by the other atoms. In particular, no correlation is present in this formalism.

This approach is however incompatible with the Goldstone theorem [6]. The Bogoluibov approach is in this respect more appropriate since it yields not only the true fundamental state but also the first excited states [7-10].

The GHFB approach is much more promising since it not only generalizes the Gross-Pitaevkii equation to finite temperature, but it also accounts for the Bogoluibov excitations.

In this work, we solve the full GHFB equations for large atom numbers in order to determine the condensate fraction and the critical temperature. We observe a clear deviation from the ideal gas behavior and determine the parameter that describes this deviation. We also compare with experiments and conclude that the GHFB approximation correctly reproduces well known data.

2. Formalism

We start our study by using the Generalized Gross-Pitaevskii equation for the condensate wave function $\varphi_0(r)$ for a system of bosonic atoms in a harmonic trap with potential $V_{trap}(r)=\frac{1}{2}m\omega^2 r^2$ [4]:

$$\left(-\frac{1}{2}\Delta+V_{\text{trap}}(r)+g[n_c(r)+2\tilde{n}(r)+\tilde{m}(r)]\right)\varphi_0(r)=\mu\varphi_0(r), \tag{2.1}$$

which is derived by inserting the standard separation of the field operator into a condensate wave function $\varphi_0(r)$ and a fluctuating field operator $\tilde{\Psi}(r)$ in the Hamiltonian of system [4,11]. In the equation (2.1), $n_c(r)\equiv N_c\langle\varphi_0(r)\rangle^2$ is the condensate density and $\tilde{n}(r)\equiv\langle\tilde{\Psi}^+(r)\tilde{\Psi}(r)\rangle$ is the non condensate density (or thermal cloud). The quantities $\tilde{n}(r)$ and $\tilde{m}(r)$ are determined by the quasi-particle amplitudes $(u_i(r),v_i(r))$ and energies E_i by means of the following expressions:

$$\tilde{n}(r)=\sum_i\left\{\left(|u_i(r)|^2+|v_i(r)|^2\right)f_B(E_i)+|v_i(r)|^2\right\}, \tag{2.2}$$

$$\tilde{m}(r)=-\sum_i u_i(r)v_i^*(r)(1+2f_B(E_i)), \tag{2.3}$$

Where $f_B(E_i)$ is the Bose-Einstein function:

$$f_B(E_i)=\frac{1}{z^{-1}\exp\beta E_i-1} \tag{2.4}$$

and $\beta=\frac{1}{k_BT}$ is the inverse temperature. The fugacity z is given by $z^{-1}=1+N_c^{-1}$ (where N_c is the number of particles in the condensate). The quantities $u_i(r), v_i(r)$ and E_i satisfy the coupled Bogoluibov-de Gennes (BdG) equations [4]:

$$\begin{cases}Lu_i(r)-g(n_c(r)+\tilde{m}(r))v_i(r)=E_iu_i(r),\\ Lv_i(r)-g(n_c(r)+\tilde{m}(r))u_i(r)=-E_iv_i(r),\end{cases} \tag{2.5a-2.5b}$$

in which

$$L=-\frac{1}{2}\Delta+V_{\text{trap}}(r)-\mu+2g[n_c(r)+\tilde{n}(r)] \tag{2.6}$$

The equations (2.1-2.5a-2.5b) form a closed set to be solved self-consistently. The point is that the anomalous density is UV-divergent and requires regularization. To this end, one may use the prescription of Morgan [9] which states that it is sufficient to remove the 1 from the $1+2f_B(E_i)$ term in the equation (2.3). We use the algorithm described in ref. [12] in order to determine the non condensate density and the anomalous density. We determine the condensate population by using the relation:

$$N_c=N-\int\tilde{n}(r)d^3r \tag{2.7}$$

In order to determine the critical temperature, we will examine the interaction effects between atoms. These interactions which present a repulsive character in our case are described by the term $2g(n_c(r)+\tilde{n}(r))\equiv 2gn(r)$ contained in the equation (2.6). These interactions are treated in the mean field approximation based on the Hartree-Fock theory, which consists in assuming the atoms to behave as non interacting bosons moving in a self-consistent mean-field produced by the other atoms.

The Hartree-Fock Hamiltonian coincides with the single particle Hamiltonian, which describes the excitations of the time dependent Gross-Pitaevskii equation after neglecting the quasi particle amplitude $v_i(r)$ in the equations of (2.5a and can be written as:

$$(-\frac{\hbar^2}{2m}\Delta + V_{trap}(r) + 2gn(r))u_i(r) = \hbar\omega_i u_i(r) \tag{2.8}$$

$V_{trap}(r) + 2gn(r)$ is the effective potential and $2gn(r)$ is the mean field created by the other atoms. We use the semi-classical approximation, which allows for an easier computation of the thermal average using the eigenvalues of the first term in equation (2.8). The total number of atoms is:

$$N = \int drn\ (r, T_c, \mu_c) \tag{2.9}$$

where μ_c takes the minimal value of the chemical potential, the eigenvalue of Hamiltonian of Hartree Fock that is equal for a large number of particle to $2gn(0)$.

By expanding the right hand of equation (2.9) around $\mu_c = 0$ and $T_c = T_c^{ideal}$ one obtains the following result for the shift of the critical temperature [13]:

$$T_c(N) = T_c^{ideal}\left(1 - 1.3\frac{a}{d}N^{1/6}\right) \tag{2.10}$$

With $T_c^{ideal} = \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}$ is the critical temperature of the ideal gas.

3. Results and discussion

In this section, we present the numerical results. In particular, we explore how the condensate fraction depends on T_c by using a gas of Rb(87) in a spherically symmetric trap with frequency equal to 200 Hz [14]. We plot in figure 1 N_c / N as a function of the reduced temperature T / T_c for $N = 2\times10^3$, 4×10^4 and 5×10^4. For the sake of comparison, we report also the results of [15] and [16-17].

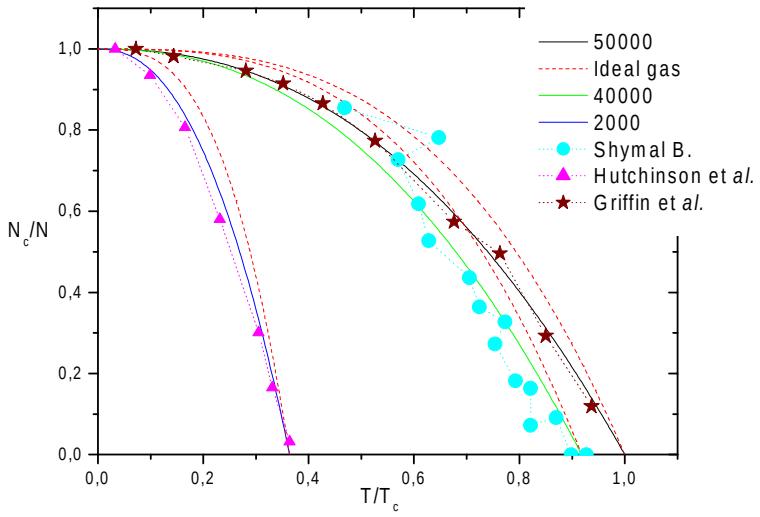

Figure 1: Condensate fraction vs. the critical temperature for different values of the total atom number *N*. The continuous curve is the GHFB results, while the dashed (red) curve is the ideal gas result. The triangles (magenta), circles (cyan) and stars (wine) are respectively the results of [15], [16] and [17].

It is evident on this figure that the interactions yield a deviation of the condensate fraction from the ideal gas given by the relation:

$$\frac{N_c}{N} = \left(1 - \left[\frac{T}{T_c}\right]^3\right). \tag{3.1}$$

Upon writing

$$\frac{N_c}{N} = \left(1 - \left[\frac{T}{T_c}\right]^{\alpha}\right), \tag{3.2}$$

and treating α as a fitting parameter, we find α=2.3 (instead of 3) for the whole set of curves. Let us now examine how the critical temperature is influenced by the interactions. This last quantity is determined numerically by the following condition: we calculated the temperature T which vanish the condensate fraction N_c. At each step we determine the critical temperature relative to the total number of atom in trap N. We plotted in figure 2 the critical temperature as function as the total number of atom N. We showed a deviation from the ideal gas result for large atom numbers. This deviation is negative for repulsive interactions, which has been already predicted by [18-21].

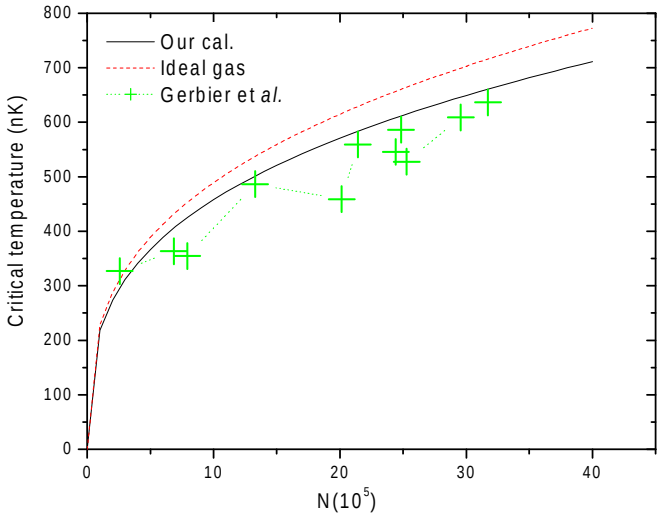

Figure 2: Critical temperature vs. the total atom number *N*. The continuous curve is the outcome of expression (2.10), while the dashed (red) curve is the ideal gas result. The experimental data [22] are labelled by + .

Finally, we conclude that our numerically results are compatible with the experimental results and provides the same predictions as other theoretical works [18-21]. We can stay here that our objective is confirmed by the available GHFB approximations.

4. Conclusion

In the present work, we have used a more elaborate algorithm to determine various quantities such as the condensate fraction and the critical temperature for large number of particles in isotropic traps. We have deduced the power law dependence of the first quantity, condensate fraction, as function of the temperature from equation (3.1) relative to the ideal gas and by using the analysis curve. For the second quantity, shift in the critical temperature T_c, we observed a linearly dependence of the scattering length and a negative relative variation who is compatible with the theoretical study [13]. As consequence, we conclude that the interactions between atoms are responsible to describe this system of gas. Finally, we have compared our results with others groups, we find a good agreement [15, 16, 17, 22] and consequently the validity of the model used is confirmed.

One of us (S.K) would like to thank N. Van Giai for his helpful comments on the numerical algorithm and for his warm hospitality at the Theoretical Division of the Nuclear Physics Institute -Orsay France.

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