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Thermodynamics of a trapped Bose gas at low temperature: Departure from the Thomas-Fermi regime

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Abstract

We apply the finite temperature Thomas-Fermi (TF) approximation by using the Time dependent Hartree-Fock-Bogoliubov equations. The exploration of these equations at finite temperature leads to the fact that all the thermodynamics quantities deviate from the standard values in the TF regime

Keywords: Bose-Einstein condensation; variational equations; TDHFB; Thomas-Fermi .

1. Introduction

Our starting point is the Time Dependent Hartree-Fock-Bogoliubov (TDHFB) equations, which were derived in [1] using the Ballian-Vénéroni (BV) variational principle [2]. For a Hamiltonian H of the type:

$$H = \int_{\vec{r}} \psi^+(\vec{r}) \left[-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(r) - \mu \right] \psi(\vec{r})$$
$$+ \frac{g}{2}\int_{\vec{r}} \psi^+(\vec{r})\psi^+(\vec{r})\psi(\vec{r})\psi(\vec{r}) \qquad , (1.1)$$

and a Gaussian Ansatz for the density operator, they write:

$$i\hbar\dot{\Phi} = \left(H^{sp} + gn_c + 2g\tilde{n} \right)\Phi + g\tilde{m}\Phi^*,$$

$$i\hbar\dot{\tilde{m}} = 4\left(H^{sp} + 2gn + \frac{g}{4V}(2V\tilde{n}+1) \right)\tilde{m} + \frac{g}{V}(2V\tilde{n}+1)\Phi^2,$$

$$i\hbar\dot{\tilde{n}} = g\left(\tilde{m}*\Phi^2 - \tilde{m}\Phi*^2 \right)$$

$$(1.2)$$

where $H^{sp} = -\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(r) - \mu$ is the single particle Hamiltonian.

In equation (1.1), m is the atom mass, $\psi^+(\vec{r})$, $\psi(\vec{r})$ are the boson creation and annihilation operators respectively , $V_{\text{ext}}(r)$ is the external confining potential, μ the chemical potential and g is the coupling constant. Furthermore, in the Eqs. (1.2), Φ is the order parameter, $n_c = |\Phi|^2$ is the condensate density, $\tilde{n}$ the thermal cloud and $\tilde{m}$ is the anomalous density, $n = n_c + \tilde{n}$ is the total density. The volume V of the gas is introduced for dimensional reasons.

One may understand in few words how (1.2) have been derived simply by recalling that the BV variational principle provides dynamical equations for the variational parameters of the density operator. These parameters are directly related to the expectation values (with respect to the density operator) of the operators $\psi(\vec{r})$, $\psi^+(\vec{r})\psi(\vec{r})$ and $\psi(\vec{r})\psi(\vec{r})$, which determine the various densities. For

instance, $\Phi(\vec{r}) = \langle \psi(\vec{r}) \rangle$,

$\tilde{n}(\vec{r}) = \langle \psi^+(\vec{r})\psi(\vec{r}) \rangle - \langle \psi^+(\vec{r}) \rangle \langle \psi(\vec{r}) \rangle$ and

$\tilde{m}(\vec{r}) = \langle \psi(\vec{r})\psi(\vec{r}) \rangle - |\psi(\vec{r})|^2$. For further computational details, see Ref. [1].

The quantities $\tilde{n}$ and $\tilde{m}$ are related by the unitarity relation

$$I = (1 + 2V\tilde{n})^2 - (2V|\tilde{m}|)^2, \qquad (1.3)$$

where the Heisenberg parameter I is directly related to the temperature by $\sqrt{I} = Coth(\hbar\omega/2kT)$. For instance, $I=1$ at zero temperature.

The TDHFB equations possess a number of interesting properties such as the conservation of the energy and of the total number of particles. They are also characterized by a gapless excitation spectrum, which is compatible with the Hugenholtz-Pines theorem [3]. Furthermore, they provide a self-consistent dynamics of the order parameter, the thermal cloud and the anomalous density. They constitute in this sense a natural generalization of well known approximations such as the Gross-Pitaevskii, the Bogoliubov, the Popov, the Beliaev and the Hartree-Fock-Bogoliubov-De Gennes equations (HFB-BdG). See e.g. [4, 5, 6 and 7].

The HFB-de Gennes equations seem to derive from the linearization of the first equation in (1.2) around a static solution. Indeed, we easily get the equation

$$i\hbar\delta\dot{\Phi} = (H^{sp} + 2gn)\delta\Phi + g(\tilde{m} + \Phi^2)\delta\Phi^*, \quad (1.4)$$

which, upon setting $\delta\Phi = \sum_p (u_p e^{-i\varepsilon_p t} - v_p e^{i\varepsilon_p t})$

where u_p and v_p are real space function, turns out to be the HFB-De Gennes equations

$$\varepsilon_p u_p = (H^{sp} + 2gn)u_p - g(n_c + \tilde{m})v_p$$
$$-\varepsilon_p v_p = (H^{sp} + 2gn)v_p - g(n_c + \tilde{m})u_p \quad . \quad (1.5)$$

The properties of the Bose-Einstein condensation in the TF regime at finite temperature were explored by many experimental and theoretical groups. A recent experimental result shows a deviation of the condensate radius from the standard TF approximation [8]. Moreover, in Ref.[9], it was clearly demonstrated that the thermal cloud compresses the condensate. From these experiments and from the Ref. [10], one notes that the validity of the TF approximation depends not only on the number of atoms but also on the trap properties.

2. The Thomas-Fermi approximation at finite temperature

In this section, we would like to generalize the TF method worked out in Ref [11] to the finite temperature. To this end, the kinetic energy operator is replaced by its classical counterpart $p^2/2m$ in the equations (1.2). We simplify

our model by neglecting the anomalous density. The equations (1.2)-(1.3) take the form:

$$\left(\frac{p^2}{2m} + V_{ext}(r) + g(n_c + 2\tilde{n})\right)\Phi = \mu\Phi, \qquad (2.1)$$

$$\tilde{n} = \frac{\sqrt{I} - 1}{2V}. \qquad (2.2)$$

The equation (2.1) can also be written:

$$(\bar{\mu} - H_{cl})\Phi = 0, \qquad (2.3)$$

where $H_{cl} = \frac{p^2}{2m} + V_{ext}(r) + gn_c$ is the ''classical''

Hamiltonian of the system and $\bar{\mu} = \mu - \frac{g}{V}(\sqrt{I} - 1)$. The

solution of equation (2.1) for a repulsive case is given by

$$n_c(r) = Ag\left(\sqrt{1 + \frac{2}{Ag}\xi(r)} - 1\right), \qquad (2.4)$$

where

$A = \left(\frac{m\alpha}{2\pi^2\hbar^3}\right)^2 mN_c^2$, $\xi(r) = (\bar{\mu} - V_{est}(r))/g$ and

$\frac{1}{\alpha} = \int \frac{d\vec{r}d\vec{p}}{(2\pi\hbar)^3}\delta(\mu - H_{cl})$. In turn, the number of

condensed atoms N_c is computed via $N_c = \int d\vec{r}\, n_c(r)$. Further details are given in [11].

It is worth noticing that in the case of a repulsive interaction and for large values of N_c (that is very low temperatures), we can expand $n_c(r)$ around $\xi(r)$. The equation (2.4) becomes

$$n_c \approx \xi(r) + \frac{1}{KgN_c^2}\xi^2(r) + ... \qquad (2.5)$$

We see that the first order result

$$n_c = \frac{\mu - V_{ext}}{g} - \frac{\sqrt{I} - 1}{V}, \qquad (2.6)$$

which is the finite temperature correction to the TF condensate density is just a temperature dependent term.

3. Thermodynamic quantities

For later convenience let us write the temperature dependence of the chemical potential. Integrating equation (2.6) over the available space and substituting the number conservation $N = N_c + \tilde{N}$, where $\tilde{N}$ is the number of non-condensed atoms, we find

$$\frac{\mu}{kT_c^0} = \left[\left(1-t^3\right)^{2/5} + \frac{0.8t^3}{\left(1-t^3\right)^{3/5}} \right] \eta . \qquad (3.1)$$

Here, we have used the ideal gas result $N_c = N\left(1-t^3\right)$, where $t = T/T_c^0$ is the reduced temperature (T_c^0 is the ideal gas transition temperature). The scaling parameter

$$\eta = 1.57 \left(N^{1/6}\frac{a}{a_{H0}} \right)^{2/5} , \text{ where } N \text{ is the total number of}$$

atoms, a the s-wave scattering length and a_{H0} the oscillator length, describes the balance between interaction and thermal effects. Due to its relatively weak N dependence, η assumes values from 0.3 to 0.49 [10]. Equation (3.1) provides a useful correction of μ at finite temperature, which is expected to be valid in the range $T \le T_c$.

Let us first discuss the problem of the condensate fraction. Using the semi-classical picture for the thermal cloud[12], one may write

$$\tilde{N} = c\int_0^\infty d\varepsilon \frac{\varepsilon^2}{e^{(\varepsilon-\mu)/kT}} , \qquad (3.2)$$

were c is an integration constant. It is clear that at temperatures at and above T_c, the condensed and the anomalous densities can be neglected. The single particle energies are directly deducted from equation (1.5)

$$\varepsilon_p = \frac{p^2}{2M} + V_{ext}(r) + 2gn(r). \qquad (3.3)$$

Explicit integration of (3.2) provides a corrected expression for the condensate fraction

$$\frac{N_c}{N} = 1 - t^3 - 1.37t^2 \left[\left(1-t^3\right)^{2/5} + \frac{0.8t^3}{\left(1-t^3\right)^{3/5}} \right]\eta .$$
$$(3.4)$$

A similar calculation yields an approximate expression for the total energy of the system

$$\frac{E}{NkT_c^0} = 2.70t^4 + \frac{5+16t^3}{7}\left[\left(1-t^3\right)^{2/5} + \frac{0.80t^3}{\left(1-t^3\right)^{3/5}} \right]\eta$$
$$(3.5)$$

Notice that this expression can be obtained directly starting from the result (3.1), through the use of general thermodynamic properties.

The equations (3.4)-(3.5) show that the effects of the interaction depend linearly on η and are consequently expected to deviate from the predictions Ref. [10] and [12].

4. Results and discussions

Let us consider a system of ^{87}Rb atoms trapped by an isotropic harmonic potential. We use the following parameters $a/a_{H0} = 7.64\,10^{-3}$ and a total number of atoms $N = 2000$. Distances are measured in units of $a_{HO} = \sqrt{\hbar/m\omega_0}$ and densities in units of a_{HO}^{-3}. We begin by studying the chemical potential as a function of the scaling parameter for various temperatures.
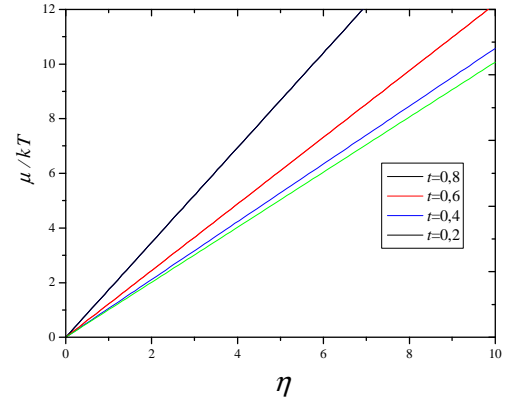

Fig 1: Chemical potential as function of the scaling parameter

The figure 1 shows that the chemical potential depends linearly on the scaling parameter and increases with temperature.
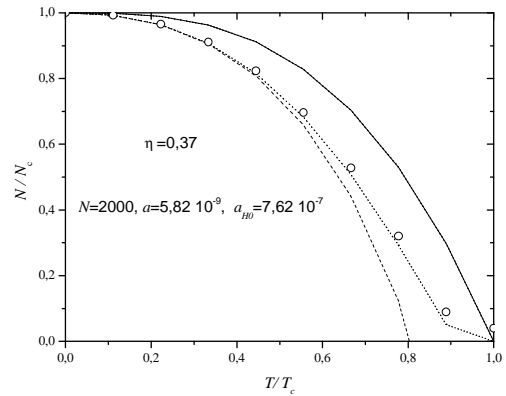

Fig 2: Condensate fraction as a function of the reduced temperature. The circles are the results of Ref.[13] for $\eta = 0.37$, obtained without using the semi classical approximation. The dotted line is the result of ref [12] for the same configuration. The dashed line is our calculation for the same configuration. The solid line is the ideal gas result in the large N limit.

Figure 2 shows that our prediction for the condensate fraction is much likely close to HFB-De Gennes calculation
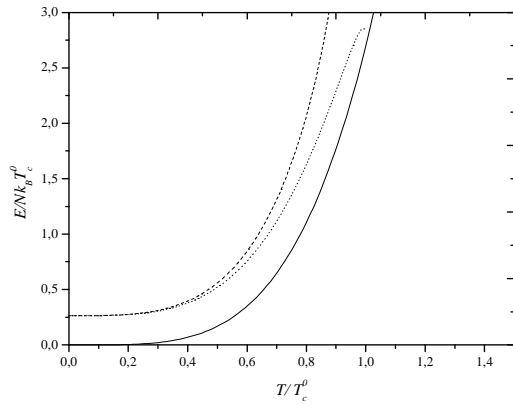
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Fig 3: Total energy of the system as function of the reduced temperature for η =0.37. The dotted line is from Ref.[12]. The dashed line is our calculation for the same configuration. The solid line is the ideal gas result in the large N limit.

Figure 3 represents the total energy of the system and it is predicted to be larger than the one predicted by the non interacting gas. It coincides with the result of [12] for

$$T\big/T_c^0 \leq 0.5 \,.$$

5. Conclusion

In this work, we have studied the Thomas-Fermi approximation for trapped Bose gases at finite temperature. We have extended a semi classical method developed for the T=0 case.

Our calculations allow us first to establish original analytical expressions for the condensate density and some other thermodynamic quantities such as the chemical potential, the condensate fraction and the total energy of the system. These expressions are natural extensions of those obtained in Refs [11, 12].

Moreover, our numerical results show a linear dependence of the chemical potential with the scaling parameter and with the temperature. The total energy of the system is also shown to be larger than what has been predicted by semi classical methods.

Finally, we may conclude that the finite temperature extension of the Thomas-Fermi approximation, together with the full TDHFB equations can offer a powerful tool for the study of trapped self-interacting Bose quantum gases.

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