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Dynamical Variational Approach for Trapped Gases at Finite Temperature

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Abstract

We analyze the static TDHFB equations in the Thomas-Fermi limit for a gas of bosons in a harmonic trap. These equations naturally generalize the Gross-Pitaevskii equation.
We first build a simple enough method that allows for the determination of the various density profiles. At zero temperature, we obtain familiar expressions for the chemical potential and the condensate radius. The standard Thomas-Fermi profile for the condensate density is also recovered. For finite temperatures and above the transition, we derive analytical expressions for the condensate radius, the chemical potential, the number of condensed atoms and the depletion as functions of the temperature. We observe that the condensate radius and the column density are surprisingly very slow functions of the temperature. Furthermore, the non-condensed density, although being quite uniform inside the trap, grows rapidly with the temperature. These facts imply therefore that the condensed atoms are very strongly attached and exhibit a certain robustness against "decondensation". Moreover, the transition to the non condensed phase seems to be much more controlled by the thermal cloud which rapidly grows from the borders toward the centre of the trap.

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

1. Introduction

Bose-Einstein condensation, although having been predicted theoretically almost a century ago, was not observed until the remarkable series of experiments of the JILA and the MIT groups in 1995, performed by trapping magnetically and then cooling atomic gases [1].
Since then, a great effort was devoted by researchers all around the world in order to understand and predict the condensate properties. The main tools, beside the Monte-Carlo calculations, were the Bogoliubov, the Popov, the Beliaev, the Hartree-Fock-Bogoliubov and the Bogoliubov-De Gennes approximations [2].
These approximations all adopt simplifying assumptions about the various quantities involved in the problem, such as the order parameter Φ, or the condensate density $n_c \equiv |\Phi|^2$, the non-condensed density or thermal cloud $\tilde{n}$ and the anomalous density $\tilde{m}$. A major well-known drawback of these methods is that they cannot be easily extended to situations where their main assumptions fail.
We therefore rely in this paper on a dynamical variational approach, which does not only retain the major properties of the preceding models, but seems to go beyond their regimes of applicability. Our main tool is a variational principle for the density operator. By adopting suitable choices for the trial classes, we derive a set of dynamical and non perturbative equations which couple the various atomic densities. This coupling, which is quite difficult to implement in the preceding approximations, is not only rather natural and consistent in our approach, but lies behind a great number of interesting results that we describe. We also discuss the static aspects and suggest a novel image for the condensation.

2. The TDHFB equations and their static solutions

The General TDHFB equations were derived in [3] using the Balian-Vénéroni (BV) variational principle. In a more appropriate notation for the BEC problem, one uses the boson field operator $\Psi(\vec{r})$ in the Schrödinger picture[2].

The gaussian density operator D(t), with variational parameters N(t), $\lambda(t)$ and $S(t)$ writes:

$$D(t) = N(t)\exp(\lambda\tau\alpha)\exp(\frac{1}{2}\alpha\tau S\alpha), \qquad (1)$$

where α is the vector field ($\Psi^+(\vec{r}), \Psi(\vec{r})$) and S and τ are symplectic numerical matrices. Introducing (1) in the BV variational action-like leads, beside the conservation of the partition function Z=Tr D(t), to what we may call the TDHFB equations:

$$\begin{aligned} i\eta\frac{d}{dt}<\alpha> &= \tau\frac{\partial < H >}{\partial <\alpha>}, \\ i\eta\frac{d}{dt}\rho &= -2\left[\rho, \frac{\partial < H >}{\partial \rho}\right], \end{aligned} \qquad (2)$$

in which $<H>$ is the mean-field energy ($<O>$ is the expectation value of the operator O with respect to D) and ρ is the single particle density matrix. Some interesting properties are discussed in [3,4].

In order to make connection with the BEC phenomenon, we introduce first the Hamiltonian for trapped bosons[5]:

$$\begin{aligned} H = &\int_{\vec{r}} \psi^+(\vec{r})\left[-\frac{\eta^2}{2m}\Delta + V_{ext}(\vec{r}) - \mu\right]\psi(\vec{r}) \\ &+ \frac{g}{2}\int_{\vec{r}} \psi^+(\vec{r})\psi^+(\vec{r})\psi(\vec{r})\psi(\vec{r}), \end{aligned} \qquad (3)$$

where $V_{ext}(\vec{r})$ is the trapping potential, μ is the chemical potential and g is the coupling constant. The energy E=$<H>$ is easily computed yielding:

$$E = \int_{\vec{r}} \begin{bmatrix} -\frac{\eta^2}{2m}\Phi^*\Delta\Phi - \frac{\eta^2}{2m}\Phi\Delta\Phi^* + \left(V_{ext}(\vec{r}) - \mu + 2g\tilde{n}\right)|\Phi|^2 \\ +\frac{g}{2}|\Phi|^4 - \frac{\eta^2}{2m}\tilde{n}\Delta + \left(V_{ext}(\vec{r}) - \mu\right)\tilde{n} + g\tilde{n}^2 \\ +\frac{g}{2}\left(|\tilde{m}|^2 + \tilde{m}^*\Phi^2 + \tilde{m}\Phi^{*2}\right) \end{bmatrix} \qquad (4)$$

where the condensate density n_c, the non-condensed density $\tilde{n}$ and the anomalous density $\tilde{m}$ are identified respectively with $|<\Psi>|^2$, $<\overline{\Psi}^+\overline{\Psi}>$ and $<\overline{\Psi\Psi}>$. The Eqs.(2) now take the form

$$\begin{aligned} i\eta\dot{\Phi} &= \frac{\partial E}{\partial \Phi^*}, \\ i\eta\dot{\tilde{n}} &= 2\left(\tilde{m}^*\frac{\partial E}{\partial \tilde{m}^*} - \tilde{m}\frac{\partial E}{\partial \tilde{m}}\right), \\ i\eta\dot{\tilde{m}} &= 2(2\tilde{n}+1)\frac{\partial E}{\partial \tilde{m}^*} + 4\frac{\partial E}{\partial \tilde{n}}\tilde{m}, \end{aligned} \qquad (5)$$

which constitutes a closed self-consistent system. The coupling between the order parameter, the non-condensed density and the anomalous density occurs via the derivatives of E which still contain $\tilde{n}$ and $\tilde{m}$. For further computational details see [3,4].

Beside the conservation of the energy, the equations (5) exhibit the unitary evolution of the density matrix (already visible in (2) by means of the conservation of the "Heisenberg parameter" I defined by the relation

$$I = (2\tilde{n}+1)^2 - 4|\tilde{m}|^2. \qquad (6)$$

We recall the reader that $I = \coth^2(\eta\omega/2kT)$ for a thermal distribution.

The expression (4) for the energy allows us to write down the Eqs.(5) more explicitly. They indeed read

$$\begin{aligned} i\eta\dot{\Phi} &= \left(-\frac{\eta^2}{2m}\Delta + V_{ext} - \mu + gn_c + 2g\tilde{n}\right)\Phi + g\tilde{m}\Phi^*, \\ i\eta\dot{\tilde{n}} &= g\left(\tilde{m}^*\Phi^2 - \tilde{m}\Phi^{*2}\right), \\ i\eta\dot{\tilde{m}} &= 4\left(-\frac{\eta^2}{2m}\Delta + V_{ext} - \mu + 2gn\right)\tilde{m} + g(2\tilde{n}+1)(\tilde{m}+\Phi^2). \end{aligned} \qquad (7)$$

The consistency of our derivation mentioned in the introduction is now clear. Indeed, we obtain in Eqs.(7) a self-consistent dynamics of the order parameter, the thermal cloud and the anomalous density. The equation governing the evolution of Φ has been obtained elsewhere [2,5,6] as an extension of the Gross-Pitaevskii equation, but to our knowledge, the two last equations in (7), governing the evolution of $\tilde{n}$ and $\tilde{m}$, were never written down before at finite temperature. It is worth noticing that this dynamics is also number conserving since the total density n=n_c+ $\tilde{n}$ is preserved during the evolution.

Let us now turn to the analysis of the static solutions. In the standard Thomas-Fermi (TF) limit, the kinetic terms are often neglected. This is particularly satisfied for trapped bosons since they are slowed down in order to obtain condensation. It is important to notice at this level that the neglect of the kinetic energy is a somewhat hazardous hypothesis for the thermal cloud[7]. However, a more detailed analysis, carried out in [8,9] shows that lifting out this approximation does not alter significantly the main results depicted along this work except perhaps near the transition, where the kinetic terms come out to play a major role.

The static equations corresponding to (7) in the TF limit now write

$$\begin{aligned} &\left(V_{ext} - \mu + gn_c + 2g\tilde{n}\right)\Phi + g\tilde{m}\Phi^* = 0, \\ &\tilde{m}^*\Phi^2 - \tilde{m}\Phi^{*2} = 0, \\ &\frac{g}{4V}(2V\tilde{n}+1)(\tilde{m}+\Phi^2) + \left(V_{ext} - \mu + 2gn\right)\tilde{m} = 0. \end{aligned} \qquad (8)$$

It is easily shown that they are naturally gapless and satisfy the Hugenholtz-Pines theorem[10]. Indeed, owing to the second equation in (8), one may verify that at zero momentum, the relation $\mu = g(n + \tilde{n} - |\tilde{m}|)$ is satisfied

without adding further assumptions, as is usually performed[10,11].

In order to solve these equations, we may distinguish two rather different situations. The first one is for T=0. When all the atoms are condensed $\tilde{n} = \tilde{m} = 0$, and n_c equals the total density of the gas. The last two equations in (8) become therefore meaningless, and we are left with a simple expression for the condensate density

$$n_c(r) = \frac{\mu - V_{ext}(r)}{g}. \qquad (9)$$

For a spherical trapping potential $V_{ext}(r) = \frac{1}{2} m\omega^2 r^2$ and upon defining the "size" of the fundamental state $a_0 = \sqrt{\eta / m\omega}$ and the s-wave scattering length $a = mg / 4\pi\eta^2$, we obtain the condensate radius R_c and the reduced chemical potential $\nu_0 = 2\mu / \eta\omega$ for a gas of N bosons as

$$R_c = a_0 \left(15N \frac{a}{a_0}\right)^{1/5}, \qquad \nu_0 = \left(15N \frac{a}{a_0}\right)^{2/5}. \qquad (10)$$

When $0 \le T < T_{BEC}$, a judicious combination of the equations (8) leads us to the remarkable expressions:

$$Vn_c = \sqrt{\boldsymbol{I}} \left(b + \frac{1}{4}(3Y(b) + 1/Y(b)) \right),$$
$$1 + 2V\tilde{n} = -\frac{\sqrt{\boldsymbol{I}}}{2}\left(Y(b) + 1/Y(b)\right), \qquad (11)$$
$$V|\tilde{m}| = \frac{\sqrt{\boldsymbol{I}}}{4}\left(Y(b) - 1/Y(b)\right).$$

In Eqs.(11), we have introduced the quantities b and Y defined as

$$b = \frac{1}{\sqrt{\boldsymbol{I}}}\left(1 - \frac{V}{g}(V_{ext}(r) - \mu)\right),$$
$$Y = \frac{1}{\sqrt{\boldsymbol{I}}}\left(\frac{2V}{g}(V_{ext}(r) - \mu + gn) - 1\right). \qquad (12)$$

It turns out that Y is a solution of the simple equation: $5Y^4 + 6bY^3 - 2Y^2 - 2bY + 1 = 0.$ This solution exists only for $b \ge 1$. For the sake of convenience only, we report here the best fit:

$$Y = -\frac{1}{\sqrt{3}}\left(\frac{b^{3/2} + 2/3}{b^{3/2} + 5/3\sqrt{3} - 1}\right). \qquad (13)$$

One may also work with the numerical values obtained from the resolution of the quartic equation above but this does not alter the results given below.

From the very definition (12) of b, we see that the condition of existence of this solution provides an upper bound for the radial distance r from the centre of the trap. This limiting value may be understood as the extension of the gas. In fact, we will see that it is just the size of the condensate, and it is given by

$$R_g = R_c \left(1 + \frac{1 - 2\sqrt{\boldsymbol{I}}(1+J)}{2N}\right)^{1/5}, \qquad (14)$$

where R_c is defined by (10). Furthermore, one may also compute in the same way the reduced chemical potential:

$$\nu = \nu_0 \left(1 + \frac{1 - 2\sqrt{\boldsymbol{I}}(1+J)}{2N}\right)^{2/5} \left(1 + \frac{2}{5N} \frac{\sqrt{\boldsymbol{I}} - 1}{1 + \frac{1 - 2\sqrt{\boldsymbol{I}}(1+J)}{2N}}\right). \qquad (15)$$

One can notice the similarities with (10). The Eqs.(14-15) appear therefore as a finite temperature generalization of (10). The quantity J which appears in (14-15) is the integral:

$$J = \frac{3}{2}\int_0^1 dx\, x^2 Y(b(x)) \quad x = r / R_g. \qquad (16)$$

We can now go further by computing some other interesting properties of the condensate such as, the number N_c of condensed atoms

$$N_c = N + \frac{1}{2}\left(1 + \sqrt{\boldsymbol{I}}(J + K)\right), \qquad (17)$$

and the number $\tilde{N}$ of non-condensed atoms

$$\tilde{N} = -\frac{1}{2}\left(1 + \sqrt{\boldsymbol{I}}(J + K)\right). \qquad (18)$$

In Eqs.(17-18), K is an integral defined in the same way as J in (16), but with Y replaced by Y^{-1}. In fact, owing to the form (13) of Y, the properties (as well as the numerical values) of J and K can obviously be deduced from each other.

Before ending this section, let us return briefly to the T=0 case in order to determine the non-trivial static solution with a quantum depletion. We notice that the previous equations remain unchanged except that now, $\sqrt{\boldsymbol{I}} = 1$. It is then obvious that, since $N \approx 10^4 - 10^5$ in typical situations, the equations (14-15) reduce to (10). The condensed density is almost the same as the one given in (9). But now, the "cloud", even if it is very small (and largely homogeneous) compared to n_c, is non-zero except at the boundaries where it vanishes *exactly*. Thus, in practice, the approximation of a null quantum depletion at zero temperature is largely justified.

3. Results and discussions

We see at first that the equation for Y has a doubly degenerate real solution Y=-1 when b=1. Hence, for r=R_g,

the condensate density vanishes and the non-condensed density equals the total density

$$\tilde{n}(R_g) = n(R_g) = \frac{\sqrt{I} - 1}{2V}, \qquad (19)$$

where we recover in particular, the vanishing of the zero temperature quantum depletion at the boundaries.

The general result (19) deserves several comments. First of all, since $n_c(R_g)$ vanishes, the quantity R_g, which we have at first glance considered as the spatial extension of the gas, is the size of the condensate itself and this in turn gives all its significance to a formula like (14).

The expression (14) shows that R_g is a slowly varying function of the temperature since N is generally large and the integral J is a bounded function. For R_g to vary sensibly with the temperature, $\sqrt{I}$ must be of the order N, which means a relatively high transition temperature. This in turn provides a column density quite insensible to the temperature. That means in particular that, upon rising the temperature, the condensate does not collapse *abruptly*. Secondly, the fact that the thermal cloud does not disappear at the boundaries brings up an interesting image of the way the two phases (condensed and non-condensed) mix up in the gas. The condensed atoms appear in this image as an "iceberg" surrounded by a (homogeneous) sea of excited atoms. The transition to the normal phase is therefore much more due to the invasion of excited atoms from the borders to the centre of the trap, than to the collapse of the condensate itself. On the other hand, the expression (15) for the reduced chemical potential shows that it is also a slowly varying function of the temperature.

The previous image of the way the condensate disappears, exhibiting a certain robustness against the variations of the temperature, is nonetheless plagued with a number of drawbacks. The first one, lying in the borders of the trap, is the non vanishing of the thermal cloud there. The second is the quite uniform thermal cloud. Last but not least, is the relatively high transition temperature that we have inferred from the above considerations. In fact, we can evaluate it to be of the order of a hundred of μK. We strongly believe that all these drawbacks are just artifacts of the TF approximation. Indeed, we have already performed a more elaborate calculation going beyond the TF approximation, that is, taking explicitly into account the kinetic terms present in (7) in their differential form. The results show effectively that the thermal cloud does indeed vanish at the boundaries and that the transition temperature is seriously lowered (being of the order of a few nK) [9]. The thermal cloud remains however quite uniform inside the trap. Most importantly, the robustness of the condensate against variations of the temperature remains unchanged, therefore confirming the interesting image that has emerged from our calculations.

4. Concluding remarks

We present in this paper a finite temperature analysis of the static TDHFB equations (derived in a previous paper) in the Thomas-Fermi limit for a gas of bosons in a harmonic trap. These equations generalize consistently the Gross-Pitaevskii equation and are naturally gapless since they satisfy the Hugenholtz-Pines theorem.

We first build a simple enough method that allows for the determination of the various density profiles. At zero temperature, we obtain familiar expressions for the chemical potential and the condensate radius. The standard Thomas-Fermi profile for the condensate density is also recovered. For finite temperatures and above the transition, we derive analytical expressions for the condensate radius, the chemical potential, the number of condensed atoms and the depletion as functions of the temperature. We observe that the condensate radius and the column density are surprisingly very slow functions of the temperature. Furthermore, the non-condensed density, although being quite uniform inside the trap, grows rapidly with the temperature. These facts imply therefore that the condensed atoms are very strongly attached and exhibit a certain robustness against "decondensation". Moreover, the transition to the normal phase seems to be much more controlled by the thermal cloud which rapidly grows from the borders toward the centre of the trap.

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