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A Hartree–Fock study of a Bose condensed gas

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Abstract. We present a numerical study of an inhomogeneous condensed Bose gas by solving the Hartree–Fock equations. The density profile of the Bose gas is solved with several different harmonic trapping potentials in one, two and three dimensions. We also present an investigation of the critical temperature given by the Hartree–Fock theory and discuss possible shortcomings of the theory to describe the transition region between an ordinary gas and a Bose condensed gas.

1. Introduction

The recent realization of Bose–Einstein condensation (BEC) in dilute gases of trapped alkali atoms has provided the opportunity to investigate macroscopic quantum effects in a novel system [1–3]. The second generation of experiments in Rb and Na vapours [4–8] give detailed information about the condensate coherence which distinguishes it from ordinary thermal samples. These atoms are known to have a positive scattering length (repulsive interaction) but recent experiments on Li [9] show that for limited ranges of particle density even attractively interacting particles can form a condensate. In this paper we concentrate on the more stable situation of a repulsive interaction.

Much work on the shape of the condensate and the elementary excitation modes of the macroscopic wavefunction has been carried out starting from the Gross–Pitaevskii (GP) equation [10–13]. This is, however, assumed to be valid only at zero temperature, \( T = 0 \). At present intense numerical and analytic work is being carried out to determine the excitation spectrum in the Hartree–Fock–Bogoliubov (HFB) equations with the Popov approximation providing results for all temperatures [14, 15].

The temperature dependence of the condensation phenomenon has been described by the Hartree–Fock (HF) approximation [16, 17], which is considerably simpler than the more complete description given by the full HFB equations. The HF approach cannot give the correct elementary excitations, its effective single-particle spectrum always displays a gap. Thus the low-temperature properties are not reproduced correctly. The phase transition at the onset of condensation emerges from the HF approach, but being an effective field theory the HF approach excludes all critical fluctuations. Thus it tends to display a phase transition in all dimensions, which for the Bose systems may not be correct in one and two dimensions. In two dimensions we expect to find a Kosterlitz–Thouless transition [18], but this is not the one emerging from HF.

In this paper we solve the HF equations numerically and investigate the condensation phenomenon as a function of the parameters. Even this simple theory offers a tremendous numerical challenge, and consequently the calculations cannot be carried out for realistic
parameters. We do, however, expect that the qualitative features of the phase transition can be investigated and the gross behaviour of the physics will emerge correctly. Here the insensitivity of the theory to dimensionality can be made into a virtue. The transition in two dimensions is much simpler to investigate, but it may, in fact, not differ very much from the way a three-dimensional system behaves. The parameter values are, of course, quite different.

We calculate the density profile of the condensate and the thermally excited parts as functions of temperature, particle number and interaction strength. The numerics set definite limits to the possible ranges of all these. However, we are able to follow the behaviour of the system through the transition temperature $T_c$ and with various potentials in one, two and even three dimensions.

The organization of the paper is as follows. Section 2 reviews the HF equations to be used following the presentation of [16]. For completeness we also briefly remind the reader of the main steps in their derivation. Of particular physical importance is the difference in the equations above and below the critical temperature. In section 3 we report the numerical methods used and discuss their advantages and limitations. The results of the calculations are presented in section 4, where their main features are brought forward and various situations are compared. Finally section 5 comments on the calculations and their results.

2. The HF equations

The Hamiltonian for an interacting Bose gas in second quantization can be written in the form

$$\hat{H} = \int \! dr \, \psi^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right] \psi(r) + \frac{1}{2} \int \! dr \int \! dr' \, \psi^\dagger(r') \psi^\dagger(r) V(r-r') \psi(r) \psi(r')$$  \hspace{1cm} (1)

where $\psi(r)$ and $\psi^\dagger(r)$ are the Bose field operators which obey the commutation rule

$$[\psi(r), \psi^\dagger(r')] = \delta(r' - r)$$  \hspace{1cm} (2)

and $U(r)$ is the external trap that confines the atoms. Using the short-range approximation for the interaction between the atoms we get

$$V(r-r') = v \delta(r-r')$$  \hspace{1cm} (3)

where $v$ is the interaction strength

$$v = \frac{4\pi\hbar^2a}{m}$$  \hspace{1cm} (4)

with the s-wave scattering length $a$. We now introduce the thermodynamic free energy $\Omega(T, \mu)$, which is defined by

$$e^{-\beta\Omega} = \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}]$$  \hspace{1cm} (5)

where $\mu$ is the chemical potential, $N$ is the particle number and $\beta$ is the inverse temperature. In order to achieve temperature-dependent equations we are going to use a thermodynamic variational principle [16]

$$\Omega(\hat{H}) \leq \Omega(\hat{H}_t) + \langle (\hat{H} - \hat{H}_t) \rangle_t$$  \hspace{1cm} (6)
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where

$$\langle \hat{A} \rangle_t \equiv \frac{\text{Tr}[e^{\hat{H}_t - \mu \hat{N}} \hat{A}]}{\text{Tr}[e^{\hat{H}_t - \mu \hat{N}}]}$$  \quad (7)$$

and \( \hat{H}_t \) is here chosen to be a single-particle Hamiltonian

$$\hat{H}_t = \sum \alpha E_{\alpha} a_{\alpha}^\dagger a_{\alpha} = \int dr \sum \alpha E_{\alpha} |\psi_{\alpha}(r)|^2 a_{\alpha}^\dagger a_{\alpha}. \quad (8)$$

The single-particle states \( \psi_{\alpha}(r) \) are to be determined such that they minimize the thermodynamic free energy \( \Omega_1 \). The next step is to expand our field operators

$$\psi(r) = \sum \alpha \psi_{\alpha}(r) a_{\alpha}$$  \quad (9)$$

$$\psi^\dagger(r) = \sum \alpha \psi^*_{\alpha}(r) a_{\alpha}^\dagger.$$  \quad (10)

Inserting this expansion into equation (1) gives the Hamiltonian

$$\hat{H} = \int dr \sum \alpha \psi^*_{\alpha}(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right] \psi_{\alpha}(r) a_{\alpha}^\dagger a_{\alpha}$$

$$+ \frac{1}{2} v \int dr \sum \alpha \psi^*_{\alpha}(r) \psi^*_{\beta}(r) \psi_{\gamma}(r) \psi_{\delta}(r) a_{\alpha}^\dagger a_{\beta}^\dagger a_{\gamma} a_{\delta}. \quad (11)$$

With the single-particle Hamiltonian \( \hat{H}_t \), we can then write the thermodynamic free energy as

$$\Omega = \Omega_t + \int dr \tilde{\Omega}(r) \quad (12)$$

where

$$\Omega_t = -\frac{1}{\beta} \sum \alpha \ln[1 - e^{-\beta(E_{\alpha} - \mu)}] \quad (13)$$

and

$$\tilde{\Omega}(r) = \sum \alpha \psi^*_{\alpha}(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) - E_{\alpha} \right] \psi_{\alpha}(r) (N_{\alpha})_t$$

$$+ \frac{v}{2} \sum \alpha |\psi_{\alpha}(r)|^4 (N_{\alpha}(N_{\alpha} - 1))_t + v \sum_{\alpha \neq \beta} |\psi_{\alpha}(r)|^2 |\psi_{\beta}(r)|^2 (N_{\alpha} N_{\beta})_t. \quad (14)$$

Here we have used the independent particle properties of \( \hat{H}_t \) and set

$$N_{\alpha} = a_{\alpha}^\dagger a_{\alpha},$$

$$\langle a_{\alpha}^\dagger a_{\alpha} a_{\beta} a_{\alpha}^\dagger \rangle_t = (N_{\alpha}(N_{\alpha} - 1))_t \quad (15)$$

$$\langle a_{\alpha} N_{\beta} \rangle_t = \langle N_{\alpha} \rangle_t \langle N_{\beta} \rangle_t.$$  \quad (16)

We will now minimize the thermodynamical free energy \( \Omega \) with respect to \( \psi^*_{\alpha}(r) \). This means we have to calculate the functional derivative

$$\frac{\delta F[\psi^*_{\alpha}(r)]}{\delta \psi^*_{\alpha}(r)} = 0 \quad (16)$$

where

$$F[\psi^*_{\alpha}(r)] = \int dr \tilde{\Omega}(r). \quad (17)$$
We now have to distinguish between two situations. If we assume we are above the critical temperature \( T_c \) there is no condensate and thus
\[
\langle N_\alpha N_\beta \rangle_t = \langle N_\alpha \rangle_t \langle N_\beta \rangle_t \quad \alpha \neq \alpha_0
\]
(18)
\[
\langle N_\alpha (N_\alpha - 1) \rangle_t = \langle a_\alpha^\dagger a_\alpha^\dagger a_\alpha a_\alpha \rangle_t = 2 \langle N_\alpha \rangle_t^2
\]
(19)
where we have assumed Gaussian-like occupation. Equation (16) then gives us the equation for the single-particle states
\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + 2v_n(r) \right] \varphi_\alpha(r) = E_\alpha \varphi_\alpha(r)
\]
(20)
with
\[
n(r) = \sum_\alpha \langle N_\alpha \rangle_t |\varphi_\alpha(r)|^2
\]
(21)
and
\[
\langle N_\alpha \rangle_t = \frac{1}{e^{\beta(E_\alpha - \mu)} - 1}.
\]
(22)
If we assume we are below the critical temperature \( T < T_c \) we have to treat the ground-state part \( \alpha = \alpha_0 \) differently. Now we have
\[
\langle N_{\alpha_0} (N_{\alpha_0} - 1) \rangle_t = N_{\alpha_0}^2 - N_{\alpha_0}.
\]
(23)
This gives the equations
\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + 2v_n(r) + v n_0(r) \right] \varphi_{\alpha_0}(r) = E_{\alpha_0} \varphi_{\alpha_0}(r)
\]
(24)
\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + 2v(n'(r) + n_0(r)) \right] \varphi_\alpha(r) = E_\alpha \varphi_\alpha(r)
\]
(25)
with
\[
n_0(r) = N_{\alpha_0} |\varphi_{\alpha_0}(r)|^2 \quad n'(r) = \sum_{\alpha \neq \alpha_0} \langle N_\alpha \rangle_t |\varphi_\alpha(r)|^2
\]
(26)
and \( \alpha \neq \alpha_0 \) in equation (25). Equations (20), (24) and (25) are highly nonlinear and have to be solved self-consistently.

3. Numerical methods

Because of the nonlinear character of equations (20), (24) and (25) we have to solve them using an iterative approach (see figure 1). We first assume a set of eigenfunctions which will give us the densities and an effective potential. The equation is then solved with this potential and the resulting eigenfunctions and eigenvalues are then used to calculate a new density. The procedure is iterated until we find a self-consistent solution for the density and the eigenfunctions. Throughout these calculations we have checked the convergence by looking at the ground-state eigenvalue. The same iterative method is used both for \( T > T_c \) and \( T < T_c \). The only difference is that at \( T < T_c \) the two equations (24) and (25) have to be solved simultaneously.

The chemical potential \( \mu \) plays a central role in the calculations because the density is a function of \( \mu \). In the case \( T > T_c \) we have to make sure that we have the correct \( \mu \) after
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Figure 1. The nonlinear HF equations are solved iteratively. The procedure is here illustrated for the case $T > T_c$. For $T < T_c$, the procedure is similar with two equations to be solved simultaneously.

Each iteration. This is equivalent to having the right number of particles. Because we have a fixed number of particles $N$ in the Bose gas we use the relation

$$N = \sum_{\alpha} \frac{1}{e^{\beta (E_{\alpha} - \mu)} - 1}$$

(27)

to calculate $\mu$. This is carried out in the same self-consistent manner as the rest of the method. When we solve the case ($T < T_c$) we do not have to worry about the chemical potential because if there is a condensate present, $\mu$ is put equal to the ground-state energy ($\mu = E_{\alpha_0}$). For a fixed number of particles we can then solve equations (24) and (25) at arbitrary temperatures as long as we stay below the critical temperature. When we approach the critical temperature all the particles are drained out of the condensate and eventually the solution becomes inconsistent with the assumption $T < T_c$, i.e. it cannot support the number of particles in the Bose gas any more and the assumption breaks down.

In the experiments with Bose condensed gases the trapping potential has usually been approximately harmonic. We therefore choose our external potential to be

$$U(x, y, z) = \frac{1}{2}m(\Omega_x^2 x^2 + \Omega_y^2 y^2 + \Omega_z^2 z^2).$$

(28)

The iterative method of treating equations (20), (24) and (25) is by just solving an ordinary linear differential equation until we have a self-consistent solution. Because of the harmonic external potential we can expand our solution in the harmonic oscillator eigenfunctions $\Phi_i(r)$ as

$$\psi(r) = \sum_i a_i \Phi_i(r)$$

(29)
which gives us the eigenvalue problem at $T > T_c$

$$(E_i^{HO} - E)a_i + \sum_{i'} W_{i,i'} a_{i'} = 0$$  (30)

with the matrix element

$$W_{i,i'} = 2v \int d r \Phi_i^*(r)n(r)\Phi_{i'}(r).$$  (31)

For $T < T_c$ the procedure is similar with two eigenvalue problems to be solved simultaneously. One can also use a more direct method where one discretizes the solutions and the derivatives on a grid, $\varphi(r) \rightarrow \varphi_i$. This gives us an eigenvalue problem with a tridiagonal matrix whose eigensolutions and eigenvalues directly correspond to our solutions. Here we have used both methods depending on the speed of the convergence and the amount of memory needed.

4. Results

The results presented here are calculated for both symmetric and asymmetric external potentials which have been used in recent experiments. We have also solved the HF equations in all three dimensions and compared the behaviour of the condensate. The results are calculated using $^{87}$Rb atoms with the mass $1.4 \times 10^{-25}$ kg and with a trap frequency $\Omega = 10$ Hz. The corresponding harmonic oscillator length is $r_{HO} = 8.68 \times 10^{-6}$ m. All energy terms are put into dimensionless form scaled to $\frac{1}{2}\hbar \Omega$.

4.1. The spherically symmetric trap

The simplest case to consider is when the condensate is located in a spherically symmetric trap. Then equations (20), (24) and (25) become one-dimensional equations with respect to the radial coordinate. In figures 2(a) and (b) we show the density of the condensed gas in the external trap

$$U(r) = \frac{1}{2}m\Omega^2 r^2$$  (32)

with $N = 1000$ and $v = 0.02$ at the inverse temperature $\beta = 0.058$ and $\beta = 0.06$. In figure 2(a), $\beta = 0.058$, we are close to the critical temperature which can be seen by the condensate just starting to develop in the centre of the trap. In figure 2(b) the spherically symmetric density is plotted for $\beta = 0.06$. The shape of the density curve is not very sensitive to changes in the interaction strength $v$ as soon as $T < T_c$. The interaction strength can take values between 0.0002 and 0.02 without any qualitative effects on the density profiles.

The width of the condensate is, however, a function of the interaction strength $v$. With a very low number of particles like $N \sim O(100)$ we are not in the Thomas–Fermi (TF) regime where we can neglect the kinetic term and consequently use

$$n_{TF}^v(r) = \frac{1}{v}(\mu - r^2)$$  (33)

but the profile must be obtained numerically. In figure 3(a) we show the computed condensate half width as a function of $v$. In figure 3(b) we vary the total number of particles from 100 to 2000 and plot the width of the condensate scaled to the width $\sigma_0$ of the noninteracting ($v = 0$) case. The result here is compared with the result obtained by the TF approximation. The width is slightly nonlinear both as a function of $v$ and $N$. In figure 3(c) we compare the chemical potential from the TF approximation, $\mu^{TF} = (N^{TF}v/8\pi)^{2/5}$, with
Figure 2. The spherically symmetric density plotted with the interaction strength $\nu = 0.02$ and $N = 1000$. (a) The density close to the critical temperature $\beta = 0.058$. The condensate part has just started to develop in the centre of the trap. (b) The inverse temperature is $\beta = 0.06$ with a dominating condensate part.

Figure 3. (a) Plot of the HWHM of the condensate as a function of the interaction $\nu$ with $N = 1000$. The width is scaled by the width $\sigma_0$ of the ground state at $\nu = 0$, which is a Gaussian. (b) Plot of the width of the condensate from the HF calculations and the TF result as a function of the particle number. The width is slightly nonlinear as a function of $\nu$ and $N$. (c) The comparison of the chemical potential calculated from the TF approximation with the HF results. The TF result clearly fails at a small number of particles. These calculations were performed at $\beta = 0.3$. 
The density calculated from the GP equation (equation (34)) is compared with the HF calculation at the temperature $\beta = 0.1$ and $N^{HF} = 1000$. The GP equation is solved with $N = N_0^{HF}$ where $N_0^{HF}$ is the number of particles in the condensate calculated from the HF equations. With $\beta = 0.1$ we get $N_0^{HF}/N = 0.73$. The difference between the two densities is of the order 0.001 compared with the density itself whose shape is indicated in the inset.

The limit $T \to 0$ gives from equation (24) the GP equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + U(r) + N \nu |\Psi_0(r)|^2 \right] \Psi_0(r) = \mu \Psi_0(r)$$

(34)

which has been solved in the same iterative manner as the HF equations (20), (24) and (25). The validity of the GP solution usually assumes that all $N$ particles are in the condensate. However, if we renormalize the GP solution so that we get the same number of particles as in the solution for the condensate part from the HF equations at some temperature $T < T_c$, we can compare the shapes of the densities. It turns out that the renormalized GP solution is almost identical with the condensate density from the HF equations. The two solutions are shown in figure 4, with the total number of particles $N = 1000$ and the inverse temperature $\beta = 0.1$.

4.2. The critical temperature

The HF equations do not describe well the transition region between an ordinary gas and a Bose condensed one, but they do give a general view of what is going on. If we define the critical temperature as the temperature where the number of particles in the condensate goes to zero, we can calculate this number of particles with the equations for $(T < T_c)$ at different temperatures until we reach the point where all particles in the condensate have been excited. The results are reported in figure 5. We know that there is no phase transition present in one and two dimensions even if there can be a macroscopic occupation of the ground state. The HF equations are expected to give a critical temperature in all dimensions. In three and two dimensions the critical temperature decreases with increasing interaction strength, whereas in one dimension the HF critical temperature increases with increasing interaction. The critical temperature can also be deduced from the chemical potential by
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Figure 5. The fraction of particles in the condensate is calculated as a function of temperature. In one dimension the critical temperature is increasing with increasing interaction strength $v$. The critical temperature is $T_{c}^{1D} = 52.10$ whereas in the ideal gas case it is $T_{c}^{1D} = 52.06$. In two and three dimensions the critical temperature is decreasing as a function of $v$ with $T_{c}^{2D} = 14.34$ ($T_{c}^{2D} = 14.38$) and $T_{c}^{3D} = 7.41$ ($T_{c}^{3D} = 7.43$).

Figure 6. The chemical potential $\mu$ is plotted as a function of the temperature in a three-dimensional spherical trap with $N = 100$ and $N = 1000$. Below $T_{c}$ the chemical potential equals the ground-state energy, whereas it is determined by the particle number above $T_{c}$. The crossing of the two curves should correspond to the critical temperature. The two curves cross approximately at $1/\beta = 4.93$ ($N = 100$) and $1/\beta = 16.4$ ($N = 1000$). The arrows indicate the temperatures for the crossings and the $(N_{0} = 0)$ temperatures $1/\beta = 7.41$ and $1/\beta = 17.3$ looking at the crossing between the ground-state energy for $T < T_{c}$ and $\mu$ for $T > T_{c}$, see figure 6. For $N = 100$ the crossing and the $N_{0} = 0$ temperatures do not coincide. The situation is improved with more particles as seen in the figure.
Condensate part | Excited part
---|---

Figure 7. The density of the condensate part and the excited part situated in an asymmetric two-dimensional harmonic trap. The ratio between the two frequencies in the \(x\) and \(y\) directions is \(\Omega_1/\Omega_0 = 0.8\). Because of the very low temperature \((\beta = 0.25)\) almost all particles are in the ground state.

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Condensate part | Excited part
---|---

Figure 8. The density of the condensate part and the excited part in the asymmetric three-dimensional trap \(U_{\text{ext}}(r,z) = \frac{1}{2}m(\Omega_0^2 r^2 + \Omega_z^2 z^2)\) with \(\Omega_1/\Omega_0 = 0.8\) and \(\beta = 0.25\). The condensate has got rotational symmetry around the \(z\)-axis. The figure shows the \(r\) coordinate along an arbitrary diameter of the condensate.

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4.3. The asymmetric trap in two and three dimensions

A more realistic external potential is the asymmetric one, which has been used in several experiments. We have here calculated the density profiles in two and three dimensions with the potentials

\[
U^{2D}(x, y) = \frac{1}{2}m(\Omega_x^2 x^2 + \Omega_y^2 y^2)
\]

\[
U^{3D}(r, z) = \frac{1}{2}m(\Omega_r^2 r^2 + \Omega_z^2 z^2).
\]

The two-dimensional system has recently received new relevance because of the experimental effort to build an atom laser [19]. It is very time and memory consuming to calculate the density profiles with totally asymmetric potentials. Because of the cylindrical symmetry in the \(xy\) plane for \(U^{3D}(r, z)\) it is possible to calculate the three-dimensional case without any extreme amount of memory. In figures 7 and 8 we show the density with \(N = 100\) and \(\Omega_{z,c}/\Omega_{x,r} = 0.8\). Here the inverse temperature \(\beta = 0.25\). One can clearly see the elliptic shape of the condensate part and the dip in the centre of the excited part.
With increasing ratio $\Omega_{y,z}/\Omega_{x,e}$ the two peaks of the excited part become more pronounced. Because of the very low temperature the density is here clearly dominated by the condensate part.

5. Conclusions

In this paper we present calculations of the properties of a Bose-condensed gas using HF theory. The main result that we obtain is the density of the gas as a function of the temperature. It is clear that the HF equations do not describe the Bose gas well for all temperatures. Close to the critical temperature the theory breaks down because we have neglected all fluctuations which become important near $T_c$. The temperature must also fulfil the criterion $1/\beta \gg v n_0$ which prevents us from using solutions to the HF equations at too low a temperature. The equations are inadequate in this region because they predict a gap in the spectrum of the excitations of the order of $v n_0$ (see [16]). In our calculations we present the density of the gas for several different geometries. It is, however, clear that the calculated density in the asymmetric traps is far from any experimental situation where the number of particles can be of the order $10^4$–$10^5$ compared with our few thousand particles.

Even if the HF equations do not describe well the transition region between an ordinary gas and a Bose condensed gas, we can get a feeling for what is going on by looking at the $(T < T_c)$ equations when we approach the critical temperature. With a very small number of particles ($N = 100$) we can easily follow the temperature dependence of the condensate until the $(T < T_c)$ solutions break down at the predicted critical temperature. With such a small number of particles as $N = 100$ we get, close to the critical temperature, a slightly unphysical density which has got a dip in the centre of the trap. The excited part of the density gives rise to this effect because it does not become Gaussian shaped at the same time as the condensate part is drained away and the particles go into the excited states. With increasing density the situation is considerably improved. At $N = 1000$ the dip in the centre is much smaller and goes from the characteristic ‘condensate peak’ to a broad Gaussian-shaped density when we cross the transition point. It is also evident that the transition region causes problems in the HF theory when we look at the chemical potential for $T > T_c$ and the ground state energy for $T < T_c$. Below $T_c$ we have $\mu = E_0$ and we should have the critical temperature at the crossing of $\mu$ calculated from the two situations. Again at the very low density $N = 100$, the $\mu$-crossing and the $N_0 = 0$ temperatures do not coincide. If we go to higher densities we can use the TF approximation where the crossing coincides with the $N_0 = 0$ temperature (see [17]).

If we let $T \to 0$ in the HF equations we get as a limit the GP equation. The GP equation has been studied extensively in [10]. We have solved the GP equation in the same manner as the HF equations which turned out to be a reasonably efficient method with our parameters. The relative difference of the GP solution and the HF solution is of the order $10^{-3}$ which gives an indication that the GP solution is a good approximation for the condensate part at temperatures below $T_c$ when the appropriate number of particles is used.

In these numerical calculations we have used both the basis-set method and the grid method depending on the nature of the problem. The grid method works best in the spherically symmetric situation. The GP equation was also solved with the grid method. The grid method was especially good at $T > T_c$ where $\mu$ has to be calculated after each iteration. This fact caused some problems with the basis-set method. The basis-set method turned out to be more reliable and less memory and time consuming in the asymmetric calculations. With both methods a typical run needed five iterations to get an accuracy within four digits for the eigenvalues. The GP equation and the high-density calculations
needed up to 10 iterations to obtain the same accuracy. The limitations of these numerical calculations are primarily set by the particle number. The more particles we want to use, the higher temperatures we need in order to reach the transition region. The high temperatures on the other hand demand a lot of states when we want to calculate the density from equation (26). In practice this meant that we were able to calculate the density of the condensate up to the critical temperature with 1000 particles using the basis-set method. In the corresponding eigenvalue problem we had to diagonalize a $1681 \times 1681$ matrix with the $l$ quantum numbers included in the matrix. For temperatures well below the critical temperature we could increase the particle number up to 2000 particles before the solution started to oscillate and did not converge properly. For most cases the basis-set method and the grid method were found to have approximately the same limit for the break down of the convergence. These calculations were performed on a DEC AlphaStation 600 5/333 computer.

References