Effects of temperature upon the collapse of a Bose-Einstein condensate in a gas with attractive interactions

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We present a study of the effects of temperature upon the excitation frequencies of a Bose-Einstein condensate formed within a dilute gas with a weak attractive effective interaction between the atoms. We use the self-consistent Hartree-Fock Bogoliubov treatment within the Popov approximation and compare our results to previous zero temperature and Hartree-Fock calculations. The metastability of the condensate is monitored by means of the \( l = 0 \) excitation frequency. As the number of atoms in the condensate is increased, with \( T \) held constant, this frequency goes to zero, signalling a phase transition to a dense collapsed state. The critical number for collapse is found to decrease as a function of temperature, the rate of decrease being greater than that obtained in previous Hartree-Fock calculations.

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Mean field theories of the Bose-Einstein condensation of trapped alkali vapours have been extremely successful both qualitatively and quantitatively in determining the excitation frequencies of the condensates, especially at relatively low temperatures \((\leq 0.7 T_c)\) \cite{1}. These calculations have been based upon the Popov approximation to the Hartree-Fock Bogoliubov (HFB) treatment, where the anomalous average of the fluctuating field operator is neglected \cite{2}. In all cases the study has been of alkali vapours with positive s-wave scattering lengths (i.e., repulsive effective interactions). The case of attractive interactions (\(^7\)Li for example, as used in experiments at Rice University \cite{3}) has not been treated in this manner. Calculations have, rather, been based on the zero temperature Gross-Pitaevskii equation (GPE) \cite{4} or upon a Hartree-Fock variational calculation \cite{5}.

There are two main reasons why the HFB formalism was not used in the Hartree-Fock study referred to above. Firstly, in the case of negative scattering length, the HFB-Popov collective excitations of a homogeneous system are unstable at long wavelengths. Houbiers and Stoof \cite{5} therefore found it more appealing to use the Hartree-Fock method, which has stable excitations at long wavelengths. In the case of the trapped gas this does not present a problem, as one is saved from the infra-red limit by the finite zero-point energy of the trap. From an alternative viewpoint, the finite size of the condensate eliminates very long wavelength excitations. The HFB-Popov theory is hence quite applicable for trapped gases.

Secondly, there is the possibility that atoms with an attractive effective interaction can undergo a BCS-like pairing transition \cite{6}. This possibility is in fact included in the full theory that Houbiers and Stoof develop. However, in their numerical calculations, they ignore the possibility of pairing and the results presented are based on a Hartree-Fock treatment of Bose-Einstein condensation alone. If one is going to assume that there is no BCS transition, then a better description would appear to be that of the HFB-Popov formalism. This is the treatment adopted in this letter.

The purpose of the present investigation is to determine the stability of the condensate against mechanical collapse, and the effects thereon of thermal excitations. It has been shown \cite{7} in the homogeneous limit that the condensate is unstable at the densities required for BEC. In the trap, the additional kinetic energy can stabilise the condensate and a metastable state is possible. This state decays on a timescale which is long compared to the lifetime of the experiment, but only exists for condensates below a certain size. At some critical condensate number the condensate becomes unstable and collapses. This instability is characterised by the monopolar collective excitation going soft \cite{4} (viz., the excitation frequency goes to zero). Various predictions for the critical number, \( N_c \), have been made at zero temperature using the GPE and at finite temperatures using the Hartree-Fock treatment. Here we investigate the effects of temperature upon the collapse via the HFB-Popov approach as described briefly below.

We make the usual decomposition of the Bose field operator into condensate and noncondensate parts; \( \hat{\psi}(r) = \Phi(r) + \hat{\psi}(r) \). The condensate wavefunction \( \Phi(r) \) is then defined within the Popov approximation by the generalised Gross-Pitaevskii equation (GPE)

\[
-\frac{\nabla^2}{2m} + V_{\text{ext}}(r) + gn_0(r) + 2g\hat{n}(r) \Phi(r) = \mu \Phi(r).
\]

(1)
Here, \(n_0(r) = |\Phi(r)|^2\) and \(\tilde{n}(r) = \langle \tilde{\psi}(r) \tilde{\psi}(r) \rangle\) are the condensate and noncondensate densities respectively. The Popov approximation \([1, 2]\) consists of omitting the anomalous correlation \(\langle \psi(r) \tilde{\psi}(r) \rangle\), but keeping \(\tilde{n}(r)\). The condensate wavefunction in Eq.\([1]\) is normalised to \(N_0\), the total number of particles in the condensate. \(V_{\text{ext}}(r)\) is the external confining potential and \(g = 4\pi \hbar^2 a/m\) is the interaction strength determined by the s-wave scattering length \(a\). For \(^7\text{Li}\) the value of \(a\) used is -27.3 Bohr radii. The condensate eigenvalue is given by the chemical potential \(\mu\) \([1]\).

The usual Bogoliubov transformation, \(\psi(r) = \sum_i [u_i(r) \hat{\alpha}_i - v_i(r) \hat{\alpha}_i^\dagger]\), to the new Bose operators \(\hat{\alpha}_i\) and \(\hat{\alpha}_i^\dagger\) leads to the coupled HFB-Popov equations \([\tilde{L}\] \(\tilde{u}_i(r) - gn_0(r)v_i(r) = E_i u_i(r)\)
\[\tilde{L} v_i(r) - gn_0(r)u_i(r) = -E_i v_i(r),\]
with \(\tilde{L} = -\nabla^2/2m + V_{\text{ext}}(r) + 2gn(r) - \mu = \hat{h}_0 + gn_0(r)\). These equations define the quasiparticle excitation energies \(E_i\) and the quasiparticle amplitudes \(u_i\) and \(v_i\). Once these quantities have been determined, the noncondensate density is obtained from the expression \([\tilde{L}\]
\[\tilde{n}(r) = \sum_i \{ |v_i(r)|^2 + |u_i(r)|^2 + |v_i(r)|^2 \} N_0(E_i) \]
\[= \tilde{n}_1(r) + \tilde{n}_2(r),\]
where \(\tilde{n}_1(r)\) is that part of the density which reduces to the quantum depletion of the condensate as \(T \to 0\). The component \(\tilde{n}_2(r)\) depends upon the Bose distribution, \(N_0(E) = (e^{\beta E} - 1)^{-1}\), and vanishes in the \(T \to 0\) limit.

Rather than solving the coupled equations in Eq.\([\tilde{L}\]) directly, we introduce the auxiliary functions \(\psi_1(\pm)(r) \equiv u_i(r) \pm v_i(r)\) which are solutions of a pair of uncoupled equations (a more detailed discussion of the method is presented in Hutchinson et al. of Ref.[1]). The two functions are related to each other by \(\hat{h}_0 \psi_1(+) = E_i \psi_1(-)\). We note that the collective modes of the condensate can be shown to have an associated density fluctuation given by \(\delta n_i(r) \propto \Phi(r) \psi_1(-)^1\).

To solve these equations we introduce the normalised eigenfunction basis defined as the solutions of \(\hat{h}_0 \phi_0(r) = \varepsilon_0 \phi_0(r)\) and diagonalize the resulting matrix problem. The lowest energy solution gives the condensate wavefunction \(\Phi(r) = \sqrt{N_0} \phi_0(r)\) with eigenvalue \(\varepsilon_0 = 0\).

The calculational procedure can be summarised for an arbitrary confining potential as follows: Eq.\([\tilde{L}\]) is first solved self-consistently for \(\Phi(r)\), with \(\tilde{n}(r)\) set to zero. Once \(\Phi(r)\) is known, the eigenfunctions of \(\hat{h}_0\) required in the expansion of the excited state amplitudes are generated numerically. The matrix problem is then set up to obtain the eigenvalues \(E_i\), and the corresponding eigenvectors \(\psi_i^{(0)}\) are used to evaluate the noncondensate density. This result is inserted into Eq.\([\tilde{L}\]) and the process is iterated, keeping the condensate number \(N_0\) and temperature \(T\) fixed. The level of convergence is monitored by means of the noncondensate number, \(\bar{N}\) and the iterations are terminated once \(\bar{N}\) is within one part in \(10^7\) of its value on the previous iteration \([\tilde{L}\]). In this way, we generate the self-consistent densities, \(n_0\) and \(\tilde{n}\), as a function of \(N_0\) and \(T\).

We consider first the case of \(T = 0\) for an isotropic harmonic trap with a frequency equal to the geometric average of the frequencies corresponding to the Rice trap \([1, 2]\), \(\nu = 144.6\) Hz. This is the geometry considered previously by Houbiers and Stoof \([3]\) and with whom we find qualitatively agreement. There are several signatures of a collapse of the condensate with increasing condensate number \(N_0\). First, we can look at the behaviour of the convergence parameter (the total number of particles in the noncondensate for a given condensate number and temperature) used to monitor the convergence of the solution to the HFB-Popov equations. In Fig. 1 we show \(\bar{N}\) as a function of iteration number for the three values \(N_0 = 1243, 1244\), and 1245. The convergence is clear in the first two cases, whereas in the final case the algorithm diverges catastrophically and no stable solution can be found. We therefore identify the critical number, \(N_c\), of atoms in the condensate as 1244, beyond which the condensate is no longer metastable, but unstable to the formation of a dense solid phase. This value of \(N_c\) is slightly greater than the value of 1241 obtain by Houbiers and Stoof using the Hartree-Fock approximation. A second, more physical indicator of the collapse is the observed strong dependence of the excitation frequencies on the number of condensate atoms. In particular, we find that the \(l = 0\) mode goes soft as \(N_0\) approaches the critical number found above. We shall focus on this criterion for the instability in the following.

We next consider a trap with confining frequency 150 Hz. The excitation frequencies are again calculated as a function of the number of particles in the condensate, both at \(T = 0\) and at finite temperature. The lowest lying modes at temperatures of 0, 200, and 400 nK are shown in Fig. 2. The lowest mode is the \(l = 1\) Kohn mode, which corresponds to a rigid centre of mass motion. For a harmonic trap the excitation frequency of this mode should be identically equal to the trap frequency. However, the dynamics of the noncondensate are neglected in this
treatment and the calculated excitations are those of the condensate alone, moving in the effective static potential
\[ V_{\text{eff}} = V_{\text{ext}} + 2g \tilde{n}(r). \]
Due to the presence of the noncondensate, the effective potential is not parabolic and hence the generalised Kohn theorem does not apply. The Kohn theorem is approximately obeyed for low temperatures and low particle numbers since the noncondensate is either small, or relatively uniform over the extent of the condensate and hence does not introduce a significant anharmonicity. It is only for higher temperatures near \( N_c \) where the noncondensate density is both large and sharply peaked around the centre of the trap that there is a marked deviation from the trap frequency.

As mentioned above, the softening of the \( l=0 \) breathing mode is a signature of the instability from a metastable condensate to a completely collapsed state. For \( T=0 \) the critical number, \( N_c \), is found to be 1227, which is slightly lower than that obtained in the previous case with a stronger confining potential. This is the change in the critical number expected \( \dagger \) on the basis of the dependence \( N_c \propto 1/\sqrt{\alpha_0} \), which shows that the critical number increases as the trap confinement is relaxed. With increasing temperature, the frequency of the \( l=0 \) mode is found to go to zero at lower condensate numbers. This is because the attractive nature of the interactions with the thermal cloud creates an effective potential for the condensate which is stiffer than the applied external potential. \( \dagger \). The peak density of the condensate hence increases with temperature (for fixed \( N_0 \)) and the critical condensate number is reduced. The critical number for 200 nK, as obtained from the failure to find a converged solution at larger \( N_0 \), is \( N_c = 1093 \). That for \( T = 400 \) nK is \( N_c = 1016 \). The temperature dependence of the critical condensate number as a function of temperature is shown in the inset of Fig. 2.

It should be noted that the total number of trapped atoms, \( N \), varies for each point in the figure. Alternatively one could vary \( T \) (and hence \( N_0 \)) keeping \( N \) fixed, which would give a critical temperature for collapse. Experimentally evaporative cooling removes atoms. A certain total number, corresponding to the transition temperature, is reached at which condensation occurs. Further cooling (removal of atoms) then proceeds to a point where a second critical temperature (or total number) is reached, at which point the second phase transition (i.e. collapse) is observed. However for the experiments on \(^7\)Li the different excitation spectra calculated in the two formalisms. In our treatment we calculate (and populate) the collective excitations, which include the low lying \( l = 0 \) mode. Near collapse this mode has a much lower frequency than the lowest single particle excitation of the Hartree-Fock spectrum. The population of excited states is therefore underestimated in the Hartree-Fock treatment, and as a result, the thermal population of the state is lower than it is with the HFB-Popov spectrum. The noncondensate population, and hence peak density, increases more rapidly as a function of temperature in our calculation (c.f. inset to Fig. 3 and Fig. 7 of Ref. 5). This is what gives rise to the more rapid reduction in the critical number as the temperature is increased.

In conclusion, we have presented the first self-consistent HFB-Popov calculations for a dilute gas of atoms with attractive effective interactions. We have studied the collective mode frequencies of such a gas and using these frequencies, investigated the phase transition from metastable Bose-Einstein condensate to a collapsed dense phase. The results from these calculations are in general agreement with previous Hartree-Fock results, but we feel that the HFB-Popov approach is the more appropriate one to use if only a BEC transition is assumed to take place. We find a significantly greater dependence of the critical number upon temperature in the HFB-Popov treatment.

If one includes the possibility of a BCS-like pairing transition then this is not the appropriate approach as the omitted pair correlations (the so called anomalous average) are very important. Indeed the pair correlation term, \( \langle \psi(r)\psi(r) \rangle \), becomes the order parameter for the BCS-like transition. The possibility of such a transition, or the existence of mixed phases containing both BEC and BCS macroscopic quantum states is currently under investigation.

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FIG. 1. Noncondensate number as a function of the numerical iteration number for a trap corresponding to the Rice experiment. For $N_0 = 1243$ and $N_0 = 1244$, where $N_0$ is the number of atoms in the condensate, a converged solution is obtained with a self-consistent value for $\tilde{N}$ which varies by less than one part in $10^8$ between iterations. For $N_0 = 1245$ no stable solution can be found. The critical number is identified as $N_c = 1244$ which is the condensate number for which the $l = 0$ mode frequency goes to zero.

FIG. 2. Low lying mode frequencies as a function of condensate number for $T = 0$ (solid), $T = 200$ nK (dashed), and $T = 400$ nK (dotted) for a trap with a confining frequency of 150 Hz. Note the softening of the $l = 0$ mode for large $N_0$ and the decrease in the critical number at which the mode goes soft as the temperature is increased. The variation of the critical number as a function of temperature is shown in the inset.

FIG. 3. Noncondensate density for a range of $N_0$ at a temperature of 100 nK in a spherical harmonic trap of frequency 150 Hz. The curves, in increasing order of peak density, are for $N_0 = 50, 1000, 1100, 1130$, and 1146. The final figure is the critical number. The inset shows the peak noncondensate density as a function of temperature at the critical number.
