Gapless finite-$T$ theory of collective modes of a trapped gas

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We present predictions for the frequencies of collective modes of trapped Bose-condensed $^{87}\text{Rb}$ atoms at finite temperature. Our treatment includes a self-consistent treatment of the effects upon the mean-field from finite-$T$ excitations and the anomalous average. This is the first gapless calculation of this type for a trapped Bose-Einstein condensed gas. The corrections quantitatively account for the downward shift in the $m = 2$ excitation frequencies observed in recent experiments as the critical temperature is approached.

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Measurements of the collective excitation frequencies of trapped, Bose-Einstein condensed alkali vapours are providing the most stringent tests of the theoretical understanding of these newly produced systems. Mean-field theories have been used, with great success, both qualitatively and quantitatively in determining the excitation frequencies of the condensates, especially at relatively low temperatures ($\leq 0.7 T_{c}$) \cite{PC}. These calculations have been based upon the Popov approximation to Hartree-Fock Bogoliubov (HFB) theory, where the anomalous average of the fluctuating field operator is neglected, or upon simpler versions of (finite-$T$) mean-field theory \cite{goebel}. However, recent experimental results from JILA \cite{JILA} indicate a discrepancy with these theoretical results as one approaches the critical temperature. This has raised questions about the validity of the HFB-Popov approach and mean field theories in general, when the condensate is strongly depleted and lead to debate as to how one can consistently improve upon this theory. In particular, if one retains a contact ($\delta$-function) interaction potential and simply includes the self-consistent anomalous average, a gap is found in the excitation spectrum \cite{PC}. In addition, the most naive treatment of the anomalous average results in a (ultra-violet) divergent quantity if one retains a simple contact interaction. The validity of replacing the true interaction with a contact interaction must be addressed at the same time as the divergence if one is to go beyond the Popov approximation in a consistent manner.

In this letter we address these questions, with a consistent, gapless theory that goes beyond the Popov approximation. We show how the anomalous average should be renormalised in a full computation to remove the resulting ultra-violet divergence, in a manner that is closely related to those developed using a many-body T-matrix approach for homogeneous systems \cite{Wu}. We then examine what changes these extensions make to the predictions of the theory in both an isotropic geometry and for a trap corresponding to the JILA experiments. Our results are then compared in detail to those obtained experimentally.

We start with a brief review of the HFB theory. The treatment presented here follows closely that previously discussed by Griffin \cite{Griffin} and yields the collective excitations of the condensate in the presence of a static thermal cloud as in previous studies. The condensate wavefunction, $\Phi(\mathbf{r})$, is obtained from the generalised Gross-Pitaevskii equation \cite{Wu}

$$\left\{-\frac{\nabla^2}{2M} + V_{\text{ext}}(\mathbf{r}) + g[n_c(\mathbf{r}) + \tilde{m}(\mathbf{r}) + 2\tilde{n}(\mathbf{r})]\right\}\Phi(\mathbf{r}) = \mu\Phi(\mathbf{r}). \tag{1}$$

Here we have made the usual decomposition of the Bose field operator, $\hat{\psi}(\mathbf{r})$, into condensate and noncondensate parts, i.e., $\hat{\psi}(\mathbf{r}) = \Phi(\mathbf{r}) + \hat{\psi}(\mathbf{r})$. The terms involving the interaction strength, $g = 4\pi\hbar^2a/\hbar M$, arise from the use of a contact interaction, $g\delta(\mathbf{r})$, where $a$ is the scattering length measured for binary scattering in vacuo.

The collective excitations are then given by the coupled HFB equations \cite{Wu}

$$\hat{\mathcal{L}}u_i(\mathbf{r}) - g[n_c(\mathbf{r}) + \tilde{m}(\mathbf{r})]v_i(\mathbf{r}) = E_iu_i(\mathbf{r}) \tag{2}$$

$$\hat{\mathcal{L}}v_i(\mathbf{r}) - g[n_c(\mathbf{r}) + \tilde{m}(\mathbf{r})]u_i(\mathbf{r}) = -E_iv_i(\mathbf{r}), \tag{3}$$

with

$$\hat{\mathcal{L}} \equiv -\frac{\nabla^2}{2M} + V_{\text{ext}}(\mathbf{r}) + 2gn(\mathbf{r}) - \mu \equiv \hat{h}_0 + g[n_c(\mathbf{r}) - \tilde{m}(\mathbf{r})], \tag{4}$$

$$\mu \equiv \frac{\hbar^2}{2M}a.$$
defining the quasiparticle excitation energies \( E_i \) and amplitudes \( u_i \) and \( v_i \). Here \( n_c(r) \equiv |\Phi(r)|^2 \) is the density of condensed atoms, \( \tilde{n}(r) \equiv \langle \psi(r^{\dagger}) \psi(r) \rangle \) gives the excited state population density and \( \tilde{m}(r) \equiv \langle \psi(r^{\dagger}) \psi(r) \rangle \) is the anomalous average.

The expressions for \( \tilde{n}(r) \) and \( \tilde{m}(r) \) in terms of the quasiparticle spectrum are;

\[
\tilde{n}(r) = \sum_i \left\{ |u_i(r)|^2 + |v_i(r)|^2 \right\} N(E_i),
\]

and

\[
\tilde{m}(r) = -\sum_i u_i^*(r)v_i(r) \left\{ 2N(E_i) + 1 \right\},
\]

where the Bose factor is given by

\[
N(E_i) = \frac{1}{e^{\beta E_i} - 1}.
\]

The HFB equations provide a variationally lowest free-energy for the system and could, in principle, be used as they stand. They cannot however guarantee to give the best excitation frequencies. Indeed it is well known that the inclusion of the anomalous average leads to a theory with a (unphysical) gap in the excitation spectrum. This can be seen to arise from the fact that the effective interaction between a pair of particles depends upon whether both come from the condensate or one is excited. The standard treatment in calculations for trapped gases has been to neglect \( \tilde{m}(r) \) in the above equations, which restores the symmetry and hence leads to a gapless theory. This is the Popov approximation.

In addition, one finds that the anomalous average is divergent if one uses an bare contact interaction. To go beyond Popov one has to renormalise the anomalous average to remove this ultra-violet divergence. This is done by noting that \( \tilde{m} \) effectively alters the interaction strength of the particles due to the presence of the condensate. The interaction strength used is based upon measurements of the scattering length in vacuo. One should, therefore, subtract off the vacuum perturbative limit of \( \tilde{m} \) as these effects are already included in the measured scattering length. At high energies the perturbative and HFB values for \( \tilde{m} \) are equivalent, hence the ultra-violet divergence is removed by the subtraction. A second, simpler, renormalisation involves subtracting the “zero-T” component of \( \tilde{m}(r) \) from itself (i.e. dropping the 1 in the \( \{ 2N(E_i) + 1 \} \) term). This can be seen, in a homogeneous system, to be equivalent to the correct renormalisation, e.g.,

\[
\lim_{k \to \infty} \tilde{m}(T) = \lim_{k \to \infty} \int d\mathbf{k} u_k v_k \left\{ 2N(E_k) + 1 \right\} \sim \lim_{k \to \infty} \int d\mathbf{k} u_k v_k \{1\}. \tag{8}
\]

Relaxing the requirement of taking the limit makes this renormalisation equivalent to dropping the 1 in the \( \{ 2N(E_i) + 1 \} \) term.

This procedure renders the HFB theory non-divergent, but leaves it with a gap in the excitation spectrum. This gap is due, as we remarked above, to the inconsistent treatment of interactions between particles. One would expect the effective interactions between any pair of particles, whether both come from the condensate or otherwise, to be the same. In HFB this is not the case. To be precise, one should expect there to be a dependence on the relative momentum of the pair, but this will be weak and we shall ignore it (as discussed in \([5]\) and \([9]\)).

To go beyond Popov consistently one has to treat the inter-particle interactions in a different manner. One can retain the gapless nature of the HFB-Popov equations which neglect \( \tilde{m} \) in both the generalised Gross-Pitaevskii equation and in the HFB equations by simply modifying the interaction strength \( g \) by making the substitution

\[
g \longrightarrow g \left\{ 1 + \frac{\tilde{m}(r)}{n_c(r)} \right\}. \tag{9}
\]

The form of this equation is motivated by the formal discussions given by Stoof \([5]\) and Proukakis \([11]\) and is equivalent to the low momentum limit of the many body T-matrix for a homogeneous system \([12]\).

These two steps generate a self-consistent, gapless, non-divergent theory which goes beyond the Popov approximation. Indeed this is the first consistent step, in terms of the treatment of the inter-particle interactions, that one can take beyond the Popov approximation to the HFB theory. In the homogeneous limit this treatment is related to the Beliaev formalism if the thermal cloud is taken to be static and any damping effects are ignored.
We now present results from three different formalisms; Hartree-Fock-Bogoliubov with Popov approximation (Popov), Hartree-Fock-Bogoliubov (HFB) and the gapless Hartree-Fock-Bogoliubov (GHFB). Each theory represents a closed set of equations which can be self-consistently solved numerically. First we present results from each of the calculations for an isotropic trap of frequency 200 Hz containing 2000 rubidium atoms and for an anisotropic trap corresponding to the recent JILA experiments.

In the case of the isotropic trap with relatively small numbers of atoms the differences between the different treatments are virtually unobservable, see Fig. 1. Indeed even when the number of particles is increased in the isotropic trap, the shifts in the excitation frequencies are only of the order of 1%.

For the anisotropic trap, here chosen to correspond to the JILA experiment, there is small but significant change from the Popov results, cf. Fig. 2. Even here the shift is only of the order of 2-3% and is downward in frequency for both the $m = 2$ and $m = 0$ modes. This shift does now agree quantitatively with the experimental data for the lower energy excitation, but does not agree with the stated shifts in the higher energy $m = 0$ mode.

In this letter we have shown how to improve consistently upon the Popov approximation to the HFB treatment of the collective excitations of a trapped condensate and that the corrections to the results previously obtained (within the Popov approximation) are small. These corrections are in quantitative agreement with the observed downward shift in the frequency of the $m = 2$ mode in the JILA experiment near $T_c$. If the upper mode observed in the experiment is indeed the $m = 0$ mode at all $T$, then an extension to the theory that treats the thermal cloud of atoms in a dynamical manner is going to be needed to explain the upward shift in the higher energy mode.

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[1] A. Griffin, Phys. Rev. B 53, 9341 (1996).
[2] D. A. W. Hutchinson, E. Zaremba and A. Griffin, Phys. Rev. Lett. 78, 1842 (1997); R. J. Dodd, M. Edwards, C. W. Clark and K. Burnett, Phys. Rev. A 57, R32 (1998).
[3] S. Stringari, Phys. Rev. Lett. 77, 2360 (1996).
[4] Eric Cornell, Private Communication.
[5] S. A. Morgan, Private Communication; N. P. Proukakis, S. A. Morgan and K. Burnett, to be published.
[6] Hua Shi, Doctoral Thesis, University of Toronto (1997).
[7] M. Girardeau and R. Arnowitt, Phys. Rev. 113, 755 (1959).
[8] E. M. Lifshitz and L. P. Pitaevskii, Statistical Physics Part 2, Landau and Lifshitz Course of Theoretical Physics, vol. 9, (Pergamon Press, Oxford, 1980).
[9] H. T. C. Stoof and M. J. Bijlsma, Phys. Rev. E, 47, 939 (1993), M. Bijlsma, Phys. Rev. A, 55, 498 (1997) and references therein.
[10] N. P. Proukakis and K. Burnett, Phil. Trans. R. Soc. Lond. A, 355 (1997).

FIG. 1. The calculated excitation frequencies for 2000 $^{87}$Rb atoms in a 200 Hz spherical harmonic trap. The ideal gas (solid line), GHBF (‘+’), HFB (‘×’), and HFB-Popov (‘◦’) results.
FIG. 2. The experimental, temperature dependent excitation spectrum in the JILA TOP trap (filled circles) versus the HFB-Popov predictions for the $m = 0$ mode (top, labelled by "+"") and the $m = 2$ mode (bottom, labelled by "×") and the GHFB results (‘◦’). The solid curves are excitation frequencies for a zero-temperature condensate having the same number of condensate atoms as the experimental condensate in the finite-$T$ cloud.
Reduced Temperature, $T' = \frac{T}{T_0}$