Mean-density Bogoliubov description of inhomogeneous Bose-condensed gases

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A mean-density description of spatially-inhomogeneous Bose-condensed gases based on Bogoliubov’s method is introduced. The description assumes only a large mean atomic density and so remains valid when the mean field collapses due to phase diffusion. A spread in the number of particles in the condensate is shown to lead to an anomalous coupling between the condensate and excited modes. This coupling is due to the dependence of the condensate spatial wavefunction on particle number and it could, in principle, be used for reducing particle fluctuations in the condensate.

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There has been a surge of interest in Bose-Einstein condensation following the condensation of alkali gases in 1995 [1]. A defining feature of this recent work is the spatial inhomogeneity of the gases due to their confinement in relatively small magnetic and optical traps [2]. Inhomogeneous Bose condensates also occur in the presence of vortices [3] and in the surface region of superfluid helium [4]. Much theoretical work has focused on modifications of Bogoliubov’s mean-field method to include the inhomogeneity arising, in particular, from quadratic trapping potentials. For particles with a repulsive interaction the inhomogeneity leads to two important effects. One is that the mean energy per particle depends on the number of particles [5]. Wright et al. [6] and Lewenstein et al. [7] have shown that this can lead to rapid phase diffusion and collapse of the mean atomic field in a time much shorter than the lifetime of the condensate and so mean-field descriptions of the condensate in these cases remain valid only for relatively short times. The other effect is that the size of the ground-mode spatial wavefunction increases with the number of the particles [8] and so changing the number of particles in a condensate without correspondingly changing the spatial wavefunction will produce occupation of excited trap levels. This implies that a condensate with a nonzero mean field, and thus with a spread in the number of particles, is coupled in some way to the excited levels of the trap. However, such particle-fluctuation-dependent couplings are not included in descriptions of condensates to date. The aim of this Letter is to introduce a description of a condensed gas at zero temperature that takes account of these two important effects. The new description depends only on the condensate possessing a large mean atomic density and so changing the number of particles in the ground mode is assumed to be no larger than Poissonian. The effect of the spatial-dependence on particle number is most clearly seen by writing the atomic field operator in the form \( \hat{\Psi}(r) = \hat{a}_0 \xi_0(r) + \hat{a}_1 \xi_1(r) + \hat{\psi}_2(r) \) where \( \hat{a}_n \) is the annihilation operator associated with the spatial mode \( \xi_n(r) \) of the trapped gas with \( [\hat{a}_n, \hat{a}_m^\dagger] = \delta_{n,m}, [\hat{a}_n, \hat{a}_m] = 0 \) and \( \int d^3r \xi_n^*(r) \xi_m(r) = \delta_{n,m} \). The condensate is assumed to be in the “ground” mode represented by \( \hat{a}_n \) and \( \xi_n \) with \( n = 0 \) and so \( \langle \hat{a}_0^\dagger \hat{a}_0 \rangle = N_0 \gg 1 \) whereas all “excited” modes are weakly occupied, i.e. \( \langle \hat{a}_n^\dagger \hat{a}_n \rangle \ll N_0 \) for \( n \geq 1 \). Also, the spread in the number of particles in the ground mode is assumed to be no larger than Poissonian. The effect of the spatial-dependence on particle number is most clearly seen by writing the atomic field operator in the form \( \hat{\Psi}(r) = \hat{a}_0 \xi_0(r) + \hat{a}_1 \xi_1(r) + \hat{\psi}_2(r) \) where

\[
\hat{\psi}_n(r) = \sum_{m=1}^{\infty} \hat{a}_m \xi_m(r)
\]

Substituting into Eq. (1) yields

\[
\hat{H} = \hat{H}_{01} + \hat{H}_{\text{rem}}
\]
where \( \hat{H}_{01} \) contains all terms involving \( \hat{a}_0, \hat{a}_0^\dagger, \hat{a}_1 \) and \( \hat{a}_1^\dagger \) but not \( \hat{\psi}_2 \) nor \( \hat{\psi}_2^\dagger \).

The most significant contribution to \( \hat{H}_{01} \) are the terms involving only the operators \( \hat{a}_0 \) and \( \hat{a}_0^\dagger \) and these are given collectively by

\[
\hat{H}_g = \int d^3 r \hat{a}_0^\dagger \xi_0^* (r) \left[ \mathcal{L} + \frac{\mu}{2} \hat{a}_0^\dagger \hat{a}_0 |\xi_0 (r)|^2 \right] \hat{a}_0 \xi_0 (r). \tag{3}
\]

The normalised function \( \xi_0 (r) \) that minimizes the mean of this expression is a solution of the Gross-Pitaevskii equation

\[
[\mathcal{L} + \overline{N} u |\xi_0 (r)|^2] \xi_0 (r) = \mu \xi_0 (r) \tag{4}
\]

where \( \overline{N} \equiv \langle \hat{a}_0^\dagger \hat{a}_0 \rangle / \langle \hat{a}_0 \hat{a}_0 \rangle \approx N_0 \) and \( \mu \) is the chemical potential. Using Eq. (4) to remove \( \mathcal{L} \xi_0 (r) \) from Eq. (3) yields

\[
\hat{H}_g = \mu \hat{a}_0^\dagger \hat{a}_0 + \frac{\mu \alpha_0}{2} \hat{a}_0^\dagger (\hat{a}_0^\dagger \hat{a}_0 - 2 \overline{N}) \hat{a}_0,
\]

where \( \alpha_n \equiv \int d^3 r |\xi_0 (r)|^{2n} \). This result shows that the Gross-Pitaevskii equation (3) defines the minimum-energy spatial wavefunction \( \xi_0 (r) \) of the condensate for arbitrary states of the condensate (for a given \( \overline{N} \)) including those for which \( \langle \hat{a}_0 \rangle \), and thus the mean field \( \langle \hat{\Psi} \rangle \approx \langle \hat{a}_0 \rangle \xi_0 \), is zero.

The next most significant contribution to \( \hat{H}_{01} \) is given by terms which describe a coupling between the \( n = 0 \) and 1 modes. For example consider the terms containing the product \( \xi_1^* (r) \xi_0 (r) \) or its complex conjugate to first order, i.e., the terms \( \hat{a}_1^\dagger \hat{a}_0 \int d^3 r \xi_1^* (r) \mathcal{L} \xi_0 (r) + \text{h.c.} \), which, on replacing \( \mathcal{L} \xi_0 (r) \) using Eq. (4), become

\[
\hat{a}_1^\dagger \hat{a}_0 \int d^3 r \xi_1^* (r) [\mu - \overline{N} u |\xi_0 (r)|^2] \xi_0 (r) + \text{h.c.} \tag{5}
\]

The contribution of the first term in the square brackets is zero because \( \xi_0 (r) \) and \( \xi_1 (r) \) are orthogonal. If the contribution of the second term in square brackets was also zero then there would be no coupling of this type between the ground mode and the excited modes. Therefore the part of the function \( |\xi_0 (r)|^2 \xi_0 (r) \) which is orthogonal to \( \xi_0 (r) \) represents the spatial mode function coupled most strongly to the ground mode. \( \xi_1 (r) \) can be made to be this maximally-coupled mode by setting

\[
\xi_1 (r) = \beta (|\xi_0 (r)|^2 - \alpha_2 |\xi_0 (r)|) \tag{6}
\]

where \( \beta = (\alpha_2 - \alpha_2^2)^{-1/2} \) is a normalisation constant. Fig. 1 illustrates the mode functions \( \xi_0 \) and \( \xi_1 \) for typical experimental parameters. With this choice for \( \xi_1 (r) \) expression (3) becomes \( -\overline{N} \beta \hat{a}_1^\dagger \hat{a}_0 + \text{h.c.} \). Evaluating the integrals in the remaining terms in \( \hat{H}_{01} \) using \( \xi_1 (r) \) defined by Eq. (6) and the fact that \( \xi_0 (r) \) is a solution of Eq. (4) yields

\[
\hat{H}_{01} = \mu \hat{a}_0^\dagger \hat{a}_0 + \frac{\mu \alpha_2}{2} \hat{a}_0^\dagger (\hat{a}_0^\dagger \hat{a}_0 - 2 \overline{N}) \hat{a}_0
\]

\[
+ \left[ \frac{\mu}{\beta} \langle \hat{a}_0 \hat{a}_0 - \overline{N} \rangle \right] \hat{a}_1^\dagger \hat{a}_1 + \mu_1 \hat{a}_1^\dagger \hat{a}_1
\]

\[
+ \gamma \hat{a}_1^\dagger \hat{a}_1 (2 \hat{a}_0^\dagger \hat{a}_0 - \overline{N}) + \frac{\gamma}{2} (\hat{a}_1^\dagger \hat{a}_1 \hat{a}_0 \hat{a}_0 + \text{h.c.}) \tag{7}
\]

where \( \gamma = \frac{\beta^2 (\alpha_4 - \alpha_2^2) - 2 \alpha_2 |u|}{\overline{N}} \) and \( \mu_1 = \mu + \frac{\hbar^2}{2m} \int d^3 r |\xi_1|^2 \langle \xi_0 | \nabla^2 \xi_0 - \nabla^2 |\xi_0|^2 \xi_0 \rangle \). Terms of order one or lower in \( \hat{a}_0 \) or \( \hat{a}_1 \) have been neglected because their magnitude, being \( O(1/\sqrt{\overline{N}}) \), is relatively small. The second term in Eq. (7) produces phase diffusion of the mean field [17]. This term is quite distinct from the corresponding “momentum”-squared term in Lewenstein and You’s mean-field model [18]. In fact, the “momentum”-squared term in [18] is essentially a linearized version of the above term for the special case where the condensate has a large mean field and a phase of zero. The next term in Eq. (7) represents one of the main results of this work: it describes an anomalous coupling between the ground mode and mode 1 whose strength depends on the particle fluctuations in the ground mode. This term embodies the coupling to the excited modes mentioned in the opening paragraph. The last three terms represent the “usual” terms for excited modes in the sense that replacing \( \hat{a}_0 \) with \( \sqrt{\overline{N}} \) gives the corresponding terms in the mean field approach.

We can get some idea of the effect of the coupling between the ground mode and mode 1 by considering the action of the Hamiltonian term \( \hat{H}_{01} \) alone. This ignores the effect of the other excited modes, however, these effects should be small if the system is in an approximate stationary state of \( \hat{H}_{\text{rem}} \) in Eq. (3). \( \hat{H}_{01} \) conserves the total particle number and so one easy way to follow its effect is to consider the evolution of a fixed number of

![FIG. 1. Spatial mode functions as a function of the radial coordinate r = |r|, in units where r0 = \( \sqrt{\hbar/m \omega} \approx 1 \), for a spherical harmonic trap of frequency 1000Hz with a condensate containing 105 rubidium atoms (\( m = 1.44 \times 10^{-25} \) kg, \( a_0 = 10 \) nm). The solid and dashed curves are the Lambert function approximation and Thomas-Fermi approximation, respectively.](https://example.com/figure1.png)
particles, for example, with initially $M$ particles in the ground mode and 0 particles in mode 1. The value of $N$ need not be equal to $M - 1$, i.e. $\xi_0(\mathbf{r})$ need not be the lowest energy wavefunction. (The general solution for an arbitrary state $|A\rangle$ with a spread in the number of particles in the ground mode can then be obtained by an appropriate linear superposition of the solutions for different values of $M$ but the same value of $N = \langle A|\hat{a}_0^\dagger\hat{a}_0|A\rangle/\langle A|\hat{a}_0^\dagger\hat{a}_0|A\rangle$.) It is not difficult to show for $M \gg 1$ that the evolution of the mean particle number in mode 1 is given to a close approximation by

$$
(\hat{a}_1^\dagger\hat{a}_1(t)) = c_1 \sin^2(\omega t) + c_2[\cos(\omega t) - 1]^2 \quad (8)
$$

which indicates that particles oscillate between the two modes. Here $c_1 = [(M\gamma)^2 + u^2(M - N)^2M/\beta^2]/(\hbar\omega)^2$, $c_2 = u^2(M - N)^2M[(M - N)(\gamma - \omega_0) + \mu_1 - \mu_1^2]/\beta^2(\hbar\omega)^2$ and $(\hbar\omega)^2 = [\gamma(2M - N) - (M - N)\omega_2 + \mu_1 - \mu_1^2 - \gamma^2M^2].$

In the Thomas-Fermi regime $\bar{N}$ the ground state for a harmonic trap of angular frequency $\omega$ is approximated by $\xi_0(\mathbf{r}) = [(|\mu|/\hbar\omega)^2/2r_0^2]/(N\mu)^{1/2}$ where $r_0 \equiv \sqrt{\hbar/m\omega}$ for which $\mu = B\hbar\omega/2$, $\omega_0 = B\hbar\omega/2\bar{N}$, $u/\beta = B\hbar\omega/\sqrt{67\bar{N}}$, $\gamma = B\hbar\omega/2\bar{N}$ and $\mu_1 = \mu + 63\hbar\omega/2B$ where $B \equiv (15\bar{N}a_{sc}/r_0)^{2/5}$. Taking $\gamma \approx \omega_0 \approx 2u/\beta$ and $\bar{N} \approx N_0$ leads to the simplifications

$$
c_1 \approx [M + 1/4(M - N_0)^2](a_{sc}/r_0)^{4/5}(28N_0^{1/5})^{-1}
$$

and

$$
c_2 \approx (M - N_0)^2(16M)^{-1}
$$

and $\omega' \approx 4\sqrt{M/N_0}\omega \approx 4\omega$ for $r_0/N_0a_{sc} \ll 1$. For a condensate of rubidium atoms tightly confined in a trap of frequency 1000Hz the number of atoms oscillating between the two modes is of the order of $c_1 \approx N_0^{1/2}/470$.

This can be a significant number for large condensates containing $N_0 \gg 500$ atoms, e.g. $N_0 = 10^6$ gives approximately 200 = $\sqrt{N_0}/5$ atoms oscillating between the modes. For a Poisson-distributed occupation of the condensate a quarter of these atoms are due to the anomalous term.

The dependence of the coefficients $c_1$ and $c_2$ on the difference $M - N_0$ suggests a method for reducing particle fluctuations in the ground mode that, despite its practical limitations at present, serves to illustrate the nature of the anomalous coupling. Imagine that after evolving according to Eq. (3) for a time $\pi/\omega'$ the population of mode 1 is rapidly depleted by some means. Although difficult in practice, in principle it would be possible to do this without simultaneously depleting the ground mode using the method proposed by Walsworth and You [13]. This removes $4c_2$ particles, on average, from the system. After repeating this process many times the population of the ground mode either approaches $N_0$ or decays rapidly to zero depending on whether initially $M > N_0$ or $M < N_0$, respectively. Evidently this cyclic process is a measurement of the occupation of the ground mode that distinguishes only between initial occupations $M$ that are above and below $N_0$. Thus, by linearity, if the ground mode begins in a pure state which has, e.g., a symmetrical spread in particle number $M$ about the mean $N_0$ it will eventually be transformed into a state which has, with equal probability, either approximately $N_0$ or zero particles. This method, therefore, has a 50% efficiency in reducing particle fluctuations in the ground mode.

The final task in developing this mean-density Bogoliubov description is to identify the quasiparticle modes. The expansion of the Hamiltonian in Eq. (2) was chosen to express most clearly the coupling between the ground mode and mode 1. It is more appropriate here, however, to write the atomic field operator as $\hat{\Psi}(\mathbf{r}) = \hat{a}_0\xi_0(\mathbf{r}) + \hat{\psi}_1(\mathbf{r})$ and expand the Hamiltonian to second order in $\hat{\psi}_1(\mathbf{r})$. Transforming off the uninteresting chemical potential gives the Hamiltonian in grand canonical form, $\hat{H}' = \hat{H} - \int d^3\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})$, for which the required expansion can be written as

$$
\hat{H}' = \hat{H}_g' + \hat{H}_{ge} + \hat{H}_e
$$

where $\hat{H}_g'$, $\hat{H}_{ge}$ and $\hat{H}_e$ are, respectively, independent, linear and bilinear in $\hat{\psi}_1(\mathbf{r})$ and $\hat{\psi}_1^\dagger(\mathbf{r})$. Choosing $\xi_0(\mathbf{r})$ to minimize the mean of $\hat{H}_g'$ as before, yields

$$
\hat{H}_g' = \frac{u_0a_2^2}{2}\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_0 - 2\bar{N}\hat{a}_0 . \quad (10)
$$

The foregoing analysis also shows that $\hat{H}_{ge}$ represents the coupling between the ground mode and mode 1 as given by the third term on the right side of Eq. (5), i.e.

$$
\hat{H}_{ge} = \frac{u}{\beta}(\hat{a}_0^\dagger\hat{a}_0 - \bar{N})\hat{a}_1^\dagger\hat{a}_0 + h.c. . \quad (11)
$$

It is useful to consider this coupling term as a perturbation on a system whose Hamiltonian is given by $\hat{H}_g' + \hat{H}_e$.

In this perturbative approach the quasiparticle modes are those that diagonalize $\hat{H}_e$,

$$
\hat{H}_e = \int d^3\mathbf{r} \left[ \hat{\psi}_1^\dagger(\mathcal{L} - \mu)\hat{\psi}_1 + \frac{u}{2}\hat{\psi}_1^\dagger\hat{a}_0^\dagger\hat{a}_0\xi_0^2 + h.c. \right] + 2u\hat{\psi}_1^\dagger\hat{\psi}_1\hat{a}_0\hat{a}_0|\xi_0^2|^2 . \quad (12)
$$

The diagonalization can be carried out by generalizing the method used by Fetter [3] to accommodate the ground mode operators $\hat{a}_0^\dagger$, $\hat{a}_0$ in Eq. (12) which are absent from Fetter’s mean-field treatment. Since $\hat{H}_e$ conserves total particle number the required Bogoliubov transformation must also conserve particle number. We therefore adopt the ansatz [19]

$$
\hat{\psi}_1(\mathbf{r}) = \sum_{k=1}^{\infty}[U_k(\mathbf{r})\hat{b}_k - V_k^*(\mathbf{r})\hat{b}_k^\dagger] \quad (13)
$$
where \( \{ \hat{b}_k \}_k \) are a set of independent quasiparticle operators with \( [\hat{b}_k, \hat{b}_j^\dagger] = 0 \) and \( [\hat{b}_k, \hat{b}_j^\dagger] = \delta_{kj} \). Eq. (13) implies that \( U_k(\mathbf{r}) \) and \( V_k(\mathbf{r}) \) are orthogonal to \( \xi_0(\mathbf{r}) \); this fact can be made more transparent by defining

\[
U_k(\mathbf{r}) = u_k(\mathbf{r}) - \xi_0(\mathbf{r}) \int d^3r \xi_0^\dagger(\mathbf{r}) u_k(\mathbf{r}) \tag{14a}
\]

\[
V_k(\mathbf{r}) = v_k(\mathbf{r}) - \xi_0(\mathbf{r}) \int d^3r \xi_0^\dagger(\mathbf{r}) v_k(\mathbf{r}) \tag{14b}
\]

and working instead with \( u_k(\mathbf{r}) \) and \( v_k(\mathbf{r}) \) which are elements of the whole space spanned by \( \{ \xi_n(\mathbf{r}) \}_{n=0,1,\ldots} \). Since the magnitude of \( \hat{H}_c \) is of order unity one can make approximations of relative error of order \( 1/\sqrt{N_0} \) such as replacing the operator \( \hat{a}_0^\dagger \hat{a}_0 \) with its mean value \( \bar{N}_0 \). Multiplying the first term in Eq. (12) by \( \hat{a}_0^\dagger \hat{a}_0 / \sqrt{N} = 1 + O(1/\sqrt{N_0}) \), which is effectively unity here, and then substituting for \( \frac{\hat{a}_0^\dagger}{\sqrt{N}} \hat{v}_1(\mathbf{r}) \) and its hermitian conjugate using Eq. (13) yields an approximate expression for \( \hat{H}_c \) which does not involve \( \hat{a}_0 \) nor \( \hat{a}_0^\dagger \). It can be shown using an analysis similar to that of Fetter [3] that

\[
\hat{H}_c = C + \sum_{k=1}^{\infty} \hbar \omega_k \hat{b}_k^\dagger \hat{b}_k \tag{15}
\]

to order unity, where \( \omega_k \), \( u_k(\mathbf{r}) \) and \( v_k(\mathbf{r}) \) satisfy the Bogoliubov-de Gennes equations

\[
\hat{L} u_k(\mathbf{r}) - u_N |\xi_0(\mathbf{r})|^2 v_k(\mathbf{r}) = \hbar \omega_k u_k(\mathbf{r})
\]
\[
\hat{L} v_k(\mathbf{r}) - u_N |\xi_0(\mathbf{r})|^2 u_k(\mathbf{r}) = -\hbar \omega_k v_k(\mathbf{r})
\]

with \( \hat{L} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) - \mu + 2uN |\xi_0(\mathbf{r})|^2 \), and where

\[
C = -\sum_{k=1}^{\infty} \hbar \omega_k \int d^3r |V(\mathbf{r})| v_k^\dagger(\mathbf{r}) + c.c. / 2.
\]

It is now possible to find the decomposition of mode 1 in terms of the quasiparticle modes via the overlap

\[
\frac{\hat{a}_0^\dagger}{\sqrt{N}} \hat{v}_1(\mathbf{r}) = \int d^3r \xi_1^\dagger(\mathbf{r}) \frac{\hat{a}_0^\dagger}{\sqrt{N}} \hat{v}_1(\mathbf{r}).
\]

Using Eqs. (13) and (14) with the approximate expressions for \( u_k \) and \( v_k \) in the Thomas-Fermi regime found by Öhberg et al. [20] for the physical parameters used in Fig. 1 gives \( \frac{\hat{a}_0^\dagger}{\sqrt{N}} \hat{a}_1 \approx 1.755 \hat{b}_1 - 1.443 \hat{b}_1^\dagger - 0.986 (\hat{b}_2 - \hat{b}_2^\dagger) \), that is, mode 1 is composed of the first two quasiparticle modes only [21].

In conclusion, this Letter introduces a new description of inhomogeneous Bose-condensed gases which is based on Bogoliubov’s method but assumes a large mean density \( \langle \hat{N}/\hat{N} \rangle = (\hat{a}_0^\dagger \hat{a}_0) |\xi_0|^2 \) instead of a large mean field. The description remains valid, therefore, when the mean field collapses due to phase diffusion. Eq. (3) together with Eqs. (10), (11) and (13) represent its main result: an approximate Hamiltonian which is valid for arbitrary states of the condensate and which includes an anomalous coupling between the ground and quasiparticle modes. This coupling, which has not been described previously, is due to the dependence of the ground-mode spatial wavefunction on particle number. It vanishes on taking the mean of \( \hat{H}' \) with respect to a coherent state of the ground mode, i.e. it vanishes in the mean-field approach. The mean-density description thus accommodates the two important effects of inhomogeneous condensed gases that have come to light recently: rapid phase diffusion and the dependence of the ground-mode spatial wavefunction on particle number.

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