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 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 focussed 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 [5,6]. Wright et al. [5] and Lewenstein et al. [6,7] 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 [6,7] 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 without the necessity of a large mean field. Since in other respects it follows Bogoliubov’s method it could be called a mean-density Bogoliubov description [10]. The significant features that set it apart from conventional mean-field Bogoliubov descriptions are that it remains valid even when the mean field collapses and it includes an anomalous coupling between the condensate and excited modes which depends on the deviation of the condensate particle number from its mean value. This coupling could be used, in principle, to reduce the particle fluctuations in the condensate. The new description has important consequences for studies of the quantum-field nature of condensates such as state preparation [11], state reconstruction [12], weakly coupled condensates [13] and condensates as open systems [14] and atom lasers [15].

We begin with the Hamiltonian for a weakly interacting boson gas in second quantized form

\[ \hat{H} = \int d^3r \hat{\Psi}^\dagger(r) \left( \mathcal{L} + \frac{u}{2} \hat{\Psi}^\dagger(r) \hat{\Psi}(r) \right) \hat{\Psi}(r) \]  

(1)

where \( \hat{\Psi}(r) \) is the atomic field operator at position \( r \),

\[ \mathcal{L} = -\frac{\hbar^2}{2m} \nabla^2 + V(r), \]

\( V(r) \) is the trapping potential, \( u = 4\pi\hbar^2a_{sc}/m, a_{sc} \) is the s-wave scattering length and \( m \) is the atomic mass. The objective is to find an approximation to \( \hat{H} \) which is correct to order unity. It is convenient to expand \( \hat{\Psi}(r) \) in terms of an orthonormal basis of spatial modes \[ \hat{\Psi}(r) = \sum_{n=0}^{\infty} \hat{a}_n \xi_n(r) \]

where \( \hat{a}_n \) is the annihilation operator associated with the spatial mode \( \xi_n(r) \) of the trapped gas

\[ \langle \hat{a}_m \hat{a}_n \rangle = \delta_{n,m}, \quad \langle \hat{a}_n, \hat{a}_m \rangle = 0 \quad \text{and} \quad \int d^3r \xi_n^*(r) \xi_m(r) = \delta_{n,m}. \]

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 \( \hat{\Psi}(r) = \hat{\psi}_0^\dagger \xi_0(r) + \hat{\psi}_1 \xi_1(r) + \hat{\psi}_2(r) \)

where

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

Substituting into Eq. (1) yields

\[ \hat{H} = \hat{H}_{01} + \hat{H}_{\text{rem}} \]

(2)
where $\hat{H}_{01}$ contains all terms involving $a_0$, $a_0^\dagger$, $\hat{a}_1$, 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 $a_0$ and $a_0^\dagger$ and these are given collectively by

$$\hat{H}_g = \int d^3r a_0^\dagger \xi_0^*(r) \left[ \mathcal{L} + \frac{u}{2} a_0^\dagger a_0 |\xi_0(r)|^2 \right] a_0 \xi_0(r). \quad (3)$$

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

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

where $\overline{N} \equiv \langle a_0^\dagger a_0 \rangle / \langle a_0^\dagger a_0 \rangle \approx N_0$ and $\mu$ is the chemical potential. Using Eq. (4) to remove $\mathcal{L} \xi_0(r)$ from Eq. (3) yields

$$\hat{H}_g = \mu a_0^\dagger a_0 + \frac{u a_2}{2} a_0^\dagger a_0 - 2\overline{N} a_0$$

where $\alpha_n \equiv \int d^3r |\xi_0(r)|^{2n}$. This result shows that the Gross-Pitaevskii equation (4) 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 $\langle a_0 \rangle$, and thus the mean field $\langle \hat{\psi} \rangle \approx \langle a_0 \rangle \xi_0$, 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 $\xi_0^*(r) \xi_1(r)$ or its complex conjugate to first order, i.e., the terms $a_0^\dagger a_0 \int d^3r \xi_1^*(r) \mathcal{L} \xi_0(r) + \text{h.c.}$, which, on replacing $\mathcal{L} \xi_0(r)$ using Eq. (3), become

$$a_0^\dagger a_0 \int d^3r \xi_1^*(r) \left[ \mu - \overline{N} u |\xi_0(r)|^2 \right] \xi_0(r) + \text{h.c.} \quad (5)$$

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 $|\xi_0(r)|^2 |\xi_0(r)|^2$ 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

$$\xi_1(r) = \beta [\xi_0^*(r)^2 - \alpha_2] \xi_0(r) \quad (6)$$

where $\beta = (\alpha_1 - \alpha_2^2)^{-1/2}$ 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 $-\overline{N}^2 \beta a_1^\dagger a_0 + \text{h.c.}$ Evaluating the integrals in the remaining terms in $\hat{H}_{01}$ using $\xi_1(r)$ defined by Eq. (3) and the fact that $\xi_0(r)$ is a solution of Eq. (4) yields

FIG. 1. Spatial mode functions as a function of the radial coordinate $r = |\mathbf{r}|$, in units where $r_0 = \sqrt{\hbar/m\omega} = 1$, for a spherical harmonic trap of frequency 1000Hz with a condensate containing $10^3$ rubidium atoms ($m = 1.44 \times 10^{-25}$ kg, $a_c = 10$ nm). The solid and dashed curves are the Lambert function [23] and Thomas-Fermi [6] approximations, respectively.

$$\hat{H}_{01} = \mu a_0^\dagger a_0 + \frac{u a_2}{2} a_0^\dagger a_0 - 2\overline{N} a_0$$

+ $\left[ \frac{u}{\beta} (a_0^\dagger a_0 - \overline{N}) a_1^\dagger a_1 + \text{h.c.} \right] + \mu_1 a_1^\dagger a_1$

+ $\gamma a_1^\dagger a_1 (2a_0^\dagger a_0 - \overline{N}) + \gamma \left( a_0^\dagger a_1^\dagger a_0 a_0 + \text{h.c.} \right) \quad (7)$

where $\gamma = [\beta^2 (\alpha_1 - \alpha_2^2) - 2\alpha_2] u$ and $\mu_1 = \mu + \frac{\hbar^2}{2m} \int d^3r \xi_1^2 (\beta |\xi_0(r)|^2 \nabla^2 \xi_0 - \nabla^2 (|\xi_0(r)|^2 \xi_0))$. Terms of order one or lower in $a_0$ or $a_0^\dagger$ have been neglected because their magnitude, being $O(1/\sqrt{\overline{N}_0})$, 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 [3]. In fact, the “momentum”-squared term in [3] 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 $a_0$ 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
particles, for example, with initially $M$ particles in the ground mode and 0 particles in mode 1. The value of $\overline{N}$ 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 $M$ 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 $\overline{N} = \langle A|a_0^\dagger a_0 a_0 a_0|A\rangle / \langle A|a_0^\dagger a_0|A\rangle$.) 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

$$\langle a_1^\dagger a_1(t) \rangle = c_1 \sin^2(\omega' t) + c_2 \{ \cos(\omega' t) - 1 \}^2 \quad (8)$$

which indicates that particles oscillate between the two modes. Here $c_1 = [(M\gamma)^2 + u^2(M - N)^2 M/\beta^2/(\hbar \omega')^2]$, $c_2 = u^2(M - N)^2 M[(M - N)(\gamma - u \omega_0) + \mu_1 - \mu_2]^2/(\hbar \omega')^4$ and $(\hbar \omega')^2 = [(2M - N) - (M - N) u \omega_0 + \mu_1 - \mu_2]^2 - \gamma^2 M^2$. In the Thomas-Fermi regime the ground mode is rapidly depleted by some means. $\xi_0(\mathbf{r})$ suggests a method for reducing particle fluctuations in the ground mode that, despite its...
where \( \{\hat{b}_k\}_k \) are a set of independent quasiparticle operators with \( \{\hat{b}_k, \hat{b}_j^\dagger\} = 0 \) and \( \{\hat{b}_k, \hat{b}_j\} = \delta_{kj} \). 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 \( \hat{H}_e \) is of order unity one can make approximations of relative error of order \( 1/\sqrt{N_0} \) such as replacing the operator \( \hat{a}_0\hat{a}_0\) with its mean value \( N_0 \). Multiplying the first term in Eq. (12) by \( \hat{a}_0^\dagger\hat{a}_0/N = 1 + O(1/\sqrt{N_0}) \), which is effectively unity here, and then substituting for \( \hat{a}_0\hat{a}_0/N \xi_1(\mathbf{r}) \) and its hermitian conjugate using Eq. (13) yields an approximate expression for \( \hat{H}_e \) 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

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

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

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

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

with \( \hat{L} = -\hbar^2 \nabla^2 + V(\mathbf{r}) - \mu + 2u_N \xi_0(\mathbf{r})^2 \), 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

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

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 \( \sqrt{N} \xi_1 \approx 1.755 \hat{b}_1 - 1.443 \hat{b}_1 - 0.986(\hat{b}_2 - \hat{b}_2) \), 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 \( \langle \hat{\Psi}^\dagger \hat{\Psi} \rangle = \langle \hat{a}_0\hat{a}_0 \rangle \xi_0^2 \) 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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[10] It is important to distinguish the description introduced here from that of Gardiner [3], and equivalently Castin and Dum [22], which could also be called a mean-density description. The main difference is that the latter does not allow for a coherent spread in condensate particle number (and thus a nonzero mean field) which underpins the main result of this work.
[19] This definition of the quasiparticle operators is equivalent to that of Refs. [20,22]; see also note [3].
[21] Note that \( \langle \hat{a}_0^\dagger \hat{a}_1, \hat{a}_0 \hat{a}_1 \rangle/N = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle/\sqrt{N} = 1 + O(1/\sqrt{N_0}) \) and so effectively \( \hat{a}_1 \sim 1.755 \hat{b}_1 - 1.443 \hat{b}_1 - 0.986(\hat{b}_2 - \hat{b}_2) \).