Ground State and Excited States of a Confined Condensed Bose Gas

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Abstract

The Bogoliubov approximation is used to study the ground state and low-lying excited states of a dilute gas of $N$ atomic bosons held in an isotropic harmonic potential characterized by frequency $\omega$ and oscillator length $d_0$. By assumption, the self-consistent condensate has a macroscopic occupation number $N_0 >> 1$, with $N - N_0 << N_0$. For negative scattering length $-|a|$, a simple variational trial function yields an estimate for the critical condensate number $N_{0c} = (8\pi/25\sqrt{5})^{1/2} (d_0/|a|) \approx 0.671 (d_0/|a|)$ at the onset of collapse. For positive scattering length and large $N_0 >> d_0/a$, the spherical condensate has a well-defined radius $R >> d_0$, and the low-lying excited states are compressional waves localized near the surface. The frequencies of the lowest radial modes ($n = 0$) for successive values of orbital angular momentum $l$ form a rotational band $\omega_{0l} \approx \omega_{00} + \frac{1}{2} l(l+1) \omega (d_0/R)^2$, with $\omega_{00}$ somewhat larger than $\omega$.

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Recent experimental demonstrations of Bose-Einstein condensation in dilute confined $^{87}$Rb [1] and $^7$Li [2] have stimulated theoretical research into their physical properties, based largely on the Bogoliubov approximation [3], originally introduced as a model for bulk superfluid $^4$He. Although this simple description of liquid He has long been familiar, much of its application to Bose condensed dilute atoms has involved extensive numerical analysis [4-6]. In contrast, Baym and Pethick [7] provide a more physical description of the confined ground state, emphasizing the relevant dimensionless parameters for $^{87}$Rb, where the $s$-wave scattering length $a$ is positive. The present work extends this picture to include negative values of $a$ (as found, for example, in $^7$Li), along with the low-lying excited states for positive $a$.

The Bogoliubov model is most simply understood by considering the familiar second-quantized field operators that obey boson commutation relations $[\psi(r), \psi^\dagger(r')] = \delta(r - r')$. The dynamics follows from the “grand-canonical hamiltonian” operator

$$K \equiv H - \mu N = \int dV \, \psi^\dagger(T + U - \mu)\psi + 2\pi a\hbar^2 m^{-1} \int dV \, \psi^\dagger \psi^\dagger \psi \psi, \quad (1)$$

where $H$ is the hamiltonian, $N$ is the number operator, and $\mu$ is the chemical potential [8,9]. Here $T = -\hbar^2 \nabla^2 / 2m$ is the kinetic energy, $U(r)$ is the external confining potential, and the short-range interatomic two-body potential has been approximated by a pseudopotential with an $s$-wave scattering length $a$. The presence of Bose condensation implies that the field operator has a macroscopic ensemble average $\langle \psi(r) \rangle \equiv \Psi(r)$, identified as the (in general, temperature-dependent) condensate wave function. For a dilute system at low temperature, most of the particles are in the condensate, and the deviation operator $\phi(r) \equiv \psi(r) - \Psi(r)$ is treated as small (by definition, $\langle \phi(r) \rangle = 0$). An expansion of $K$ through second order in these small field amplitudes immediately yields $K \approx K_0 + K'$, where

$$K_0 = \int dV \, \Psi^\dagger(T + U - \mu)\Psi + 2\pi a\hbar^2 m^{-1} \int dV \, |\Psi|^4, \quad (2a)$$

$$K' = \int dV \, \phi^\dagger(T + U - \mu)\phi + 2\pi a\hbar^2 m^{-1} \int dV \, (4|\Psi|^2 \phi^\dagger \phi + \Psi^2 \phi^\dagger \phi^\dagger + \Psi^* \phi^2 \phi), \quad (2b)$$
and the first-order contribution vanishes because the first variation of $K_0$ provides the nonlinear Hartree equation for the condensate wave function [10,11]

$$(T + U - \mu)\Psi + 4\pi a\hbar^2 m^{-1}|\Psi|^2\Psi = 0. \quad (3)$$

In addition, the ensemble average of the total number operator $N \equiv N_0 + N'$ determines the temperature-dependent number of particles in the condensate $N_0 = \int dV |\Psi|^2$ and in the excited states $N' = \int dV \langle \phi^d \phi \rangle$. The Bogoliubov approximation assumes that $N' \ll N_0$, thus neglecting terms of third and fourth order in the deviation operators; this assumption clearly fails sufficiently close to the onset temperature $T_c$, since $N_0(T_c)$ vanishes.

The first step is to determine the condensate wave function $\Psi$, which then provides a static interaction potential for the low-lying excitations. Although the actual experimental traps are anisotropic [1,2], it is simplest to consider an isotropic three-dimensional harmonic potential $U(r) = \frac{1}{2}m\omega^2 r^2$, with a characteristic oscillator length $d_0 = \sqrt{\hbar/m\omega}$ (the effect of the anisotropy can be treated in perturbation theory). Following Baym and Pethick [7], I use a Gaussian trial function $\Psi(r) = C \exp(-\frac{1}{2}r^2/d^2)$, where $C$ is a real normalization constant and the length scale $d$ serves as the variational parameter. Substitution into Eq. (2a) yields the variational quantity

$$K_0(\mu, d) = \frac{1}{2} \pi^{3/2} h \omega \left[ C^2 \left( \frac{3}{2} d d_0^2 + \frac{3}{2} d_5 d_0^{-2} \right) + C^4 \sqrt{2} \pi a d^3 d_0^2 \right] - \mu C^2 \pi^{3/2} d^3. \quad (4)$$

The thermodynamic identity [8] $\partial K_0 / \partial \mu = -N_0$ fixes the normalization $C^2 = N_0 / \pi^{3/2} d^3$, and the corresponding energy becomes

$$E(\lambda) \equiv K_0 + \mu N_0 = \frac{1}{2} N_0 h \omega \left[ \frac{3}{2} (\lambda^2 + \lambda^{-2}) + \sigma \lambda^3 \right], \quad (5)$$

where $\lambda \equiv d_0/d$ sets the spatial dimension of the spherical condensate, and

$$\sigma \equiv \sqrt{2/\pi} (N_0 a/d_0) \quad (6)$$

is a dimensionless parameter that characterizes the relative strength of the interparticle energy (note that $\sigma$ is proportional to the parameter $\zeta^5 \equiv 8\pi N_0 a/d_0 = \sqrt{32\pi^3} \sigma$ defined
in Ref. [7]). In Eq. (5), the three terms represent the kinetic energy, the confining energy, and the interparticle energy, respectively.

It is clear by inspection that $E(\lambda)$ becomes large for $\lambda \to 0$ (large $d/d_0$) because of the spatial confinement in the harmonic potential, but the detailed behavior for large $\lambda$ (small $d/d_0$) depends on the value of the parameter $\sigma$. In the absence of the interparticle interaction ($\sigma = 0$), the minimum of Eq. (5) occurs at $\lambda = 1$. For any positive $\sigma$ (repulsive scattering length with $a > 0$), the cubic term eventually dominates for $\lambda \to \infty$, and the local minimum of $E(\lambda)$ remains absolutely stable for all $\sigma \geq 0$. For negative $\sigma$ (attractive scattering length with $a < 0$), however, the function $E(\lambda)$ diverges to $-\infty$ for $\lambda \to \infty$, and the local minimum disappears entirely at some critical negative value $-|\sigma_c|$, signaling the onset of an instability.

The condition $E'(\lambda_0) = 0$ determines the location of the minimum, which satisfies the polynomial equation $1 = \lambda_0^4 + \sigma \lambda_0^5$. For $|\sigma| << 1$, the root is given approximately by $\lambda_0 \approx 1 - \frac{1}{4} \sigma$, with the corresponding energy $E_0 \approx \frac{3}{2} N_0 \hbar \omega (1 + \frac{1}{2} \sigma)$. As expected, a small repulsive (attractive) scattering length expands (contracts) the overall condensate size and raises (lowers) the overall energy. For large positive $\sigma$, it is straightforward to show that $\lambda_0 \approx \sigma^{-1/5} - \frac{1}{5} \sigma^{-1}$, with $E_0 \approx \frac{5}{4} N_0 \hbar \omega \sigma^{2/5}$, as found in Ref. [7].

The situation is very different for negative $\sigma$, because $E(\lambda)$ no longer has a global minimum, and even the local minimum disappears at the critical values $\lambda_c$ and $\sigma_c$ determined by the simultaneous conditions $E'(\lambda_c) = E''(\lambda_c) = 0$. An elementary calculation yields the values

$$\lambda_c = 5^{1/4} \approx 1.495, \quad \text{and} \quad \sigma_c = -\frac{4}{5 \lambda_c} = -\frac{4}{5^{5/4}} \approx -0.535,$$

(7)

so that the interactions reduce the critical condensate size parameter $d_c \approx 0.669 d_0$ relative to that of the bare trap; the corresponding variational energy at the onset of the instability is $E_c \approx \frac{1}{2} \sqrt{5} N_0 \hbar \omega$. This calculation suggests that the energy becomes unbounded from below for $\sigma < \sigma_c$ through the disappearance of the local stable minimum rather than
through the onset of negative energy per particle. Since this variational calculation is merely an upper bound on the energy, the actual instability may well occur for less negative scattering lengths, and, indeed, numerical analysis from Ref. [5] gives the value $\sigma_c \approx -0.457$ for the vanishing of the ground-state energy per particle; the $\approx 15\%$ difference in these values can be taken to characterize the accuracy of the variational estimate.

As noted in Ref. [2], this estimate predicts a maximum condensate number $N_0 \approx 1440$ for the parameters ($a \approx -1.44$ nm and $d_0 \approx 3.13$ $\mu$m) appropriate to the $^7$Li experiment. This value is an order of magnitude less than the total number of trapped $^7$Li atoms reported in Ref. [2]. Even at zero temperature, however, the nonzero interparticle potential ensures that $N_0(T = 0) < N$, and finite-temperature excitation of quasiparticles (see below) further reduces $N_0(T)$ below $N$; hence it is unclear whether this discrepancy represents a failure of the Bogoliubov description. Although the effect of three-body clusters has recently been investigated [12], the small value of $|a|$ relative to the interparticle spacing suggests that two-body contributions dominate the physics of this many-body problem.

The next step is to consider the noncondensate, which is described by the boson fields $\phi$ and $\phi^\dagger$. Since $K'$ in Eq. (2b) is a quadratic form in these field operators, it can be diagonalized by a canonical transformation [9], as in the original work of Bogoliubov [3] for a uniform condensate. Assume that the condensate wave function has the general form

$$\Psi(r) = \sqrt{N_0} e^{iS(r)} f(r),$$

where the real amplitude function $f$ is normalized ($\int dV |f|^2 = 1$), and the phase $S$ produces a particle current $j = \hbar N_0 f^2 m^{-1} \nabla S$, as found, for example, in a singly quantized vortex [11,13,14], where the appropriate $S$ is the angle in cylindrical polar coordinates. Define the linear transformation [9]

$$\phi(r) = e^{iS(r)} \sum_j' \left[ u_j(r) \alpha_j - v^*_j(r) \alpha_j^\dagger \right],$$

$$\phi^\dagger(r) = e^{-iS(r)} \sum_j' \left[ u^*_j(r) \alpha^\dagger_j - v_j(r) \alpha_j \right],$$

where the primed sum means to omit the condensate mode from the sum. Here, the “quasi-particle” operators $\alpha_j$ and $\alpha_j^\dagger$ obey the usual boson commutation relations $[\alpha_j, \alpha_k^\dagger] = \delta_{jk}$,
\[ \alpha_j, \alpha_k = [\alpha_j^\dagger, \alpha_k^\dagger] = 0, \text{ ensuring that the transformation is canonical, and the wave functions } u_j \text{ and } v_j \text{ are chosen to satisfy the coupled "Bogoliubov" equations} \]

\[
Lu_j - 4\pi ah^2 m^{-1}|\Psi|^2 v_j = E_j u_j, \\
L^* v_j - 4\pi ah^2 m^{-1}|\Psi|^2 u_j = -E_j v_j,
\]

(9)

where \( L = -(2m)^{-1} h^2 (\nabla + i\nabla S)^2 + U - \mu + 8\pi ah^2 m^{-1}|\Psi|^2 \) is a hermitian operator. It is easy to verify that the eigenvalues \( E_j \) are real and that the eigenfunctions obey the normalization \( \int dV (u_j^* u_k - v_j^* v_k) = \delta_{jk} \). Substitution of Eq. (8) into Eq. (2b) yields the simple and physical result [9]

\[
K' = -\sum_j' E_j \int dV |v_j|^2 + \sum_j' E_j \alpha_j^\dagger \alpha_j,
\]

(10)

so that the canonical transformation indeed diagonalizes the operator \( K' \). In addition, if \( u_j \) and \( v_j \) are a solution with energy \( E_j \), then the pair \( v_j^* \) and \( u_j^* \) are also a solution with energy \(-E_j\); since the quasiparticle number operator \( \alpha_j^\dagger \alpha_j \) has nonnegative integral eigenvalues, it is necessary to take \( E_j \geq 0 \). Finally, Eq. (9) also has the solution \( u_0 = v_0 = f \) with \( E_0 = 0 \), verifying that the Bose condensation does occur in the lowest self-consistent single-particle mode. Although these equations are easily rewritten in terms of two-component vectors (see, for example, pp. 477 and 501 of Ref. [8]), such formalism is unnecessary here.

The structure of \( K' \) in Eq. (10) leads to a very simple description of the equilibrium states of the condensed Bose system. The quasiparticle ground state \(|0\rangle\) satisfies the condition \( \alpha_j|0\rangle = 0 \) for all \( j \neq 0 \), and the excited states follow by applying arbitrary number of quasiparticle creation operators \( \alpha_j^\dagger \) to \(|0\rangle\). In addition, the well-known properties of these harmonic-oscillator operators mean that the low-temperature properties are determined entirely by the eigenvalues and eigenfunctions of the Bogoliubov equations (9). If \( \langle \cdots \rangle \equiv \text{Tr} [\cdots \exp(-\beta K')] / \text{Tr}[\exp(-\beta K')] \) denotes a self-consistent ensemble average at temperature \( T = (k_B\beta)^{-1} \), then the only nonzero averages of one- or two-quasiparticle operators are \( \langle \alpha_j^\dagger \alpha_k \rangle = \langle \alpha_k^\dagger \alpha_j \rangle - \delta_{jk} = \delta_{jk} f_j \), where \( f_j \equiv [\exp(\beta E_j) - 1]^{-1} \) is the usual
Bose-Einstein distribution function. For example [9], the total number density $n(r)$ has a condensate contribution $n_0(r) = |\Psi(r)|^2$ and a noncondensate contribution

$$n'(r) = \sum_j' \left[ f_j |u_j(r)|^2 + (1 + f_j) |v_j(r)|^2 \right],$$

(11)

where the condition $N = N_0(T) + \int dV n'(r)$ determines the temperature-dependent condensate fraction $N_0(T)/N$.

In the present case of a spherical condensate in a spherical confining potential $U(r)$, where $\Psi(r) = \sqrt{N_0} f(r)$ satisfies Eq. (3), the Bogoliubov equations simplify greatly because the states can be characterized by the usual angular-momentum quantum numbers $(l, m)$ associated with the spherical harmonics $Y_{lm}$, along with a radial quantum number $n$. Given a solution for $\Psi(r)$, standard numerical techniques can determine the eigenvalues $E_{nlm}$ and associated radial eigenfunctions $u_{nlm}(r)$ and $v_{nlm}(r)$ [6]. In order to gain more physical insight, however, it is valuable to consider a special limiting case in which the kinetic energy of the condensate wave function is negligible compared to the confining energy and the repulsive interparticle interaction energy. As discussed in [7] (see also Refs. [4] and [15]) this condition holds for a harmonic confining potential when the dimensionless parameter $\sigma = \sqrt{2/\pi} (N_0 a/d_0)$ from Eq. (6) is large and positive, because the kinetic energy is then of order $\sigma^{-4/5}$ relative to the other two contributions. As a result, the Hartree equation (3) for the condensate wave function then has the simple solution

$$4\pi a \hbar^2 m^{-1} |\Psi(r)|^2 = \left[ \mu - U(r) \right] \theta \left[ \mu - U(r) \right],$$

(12)

where $\theta(x)$ denotes the unit positive step function. If the oscillator length $d_0$ is used to scale dimensionless lengths, the normalization condition on $\Psi$ then yields the radius $R$ of the spherical condensate

$$R^5 = 15N_0 a/d_0 = 15(\pi/2)^{1/2} \sigma,$$

(13)

with chemical potential given by $\mu = \frac{1}{2} \hbar \omega R^2$. Although this approximation clearly fails in the immediate vicinity of the condensate surface (see, for example, Fig. 1 of Ref. [4]), its use in the Bogoliubov equations leads to only a small error in the limit $\sigma >> 1$. 

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A combination of Eqs. (9) and (12) yields the following coupled eigenvalue equations

\[
\begin{align*}
[D_x + V(x)] u_{nl}(x) - V_<(x) v_{nl}(x) &= \epsilon_{nl} u_{nl}, \\
-V_<(x) u_{nl}(x) + [D_x + V(x)] v_{nl}(x) &= -\epsilon_{nl} v_{nl},
\end{align*}
\]

(14)

where \( x = r/R \) and \( \epsilon_{nl} = 2E_{nl}/\hbar \omega \). Here,

\[
D_x \equiv -\frac{1}{R^2} \left[ \frac{1}{x^2} \frac{d}{dx} x^2 \frac{d}{dx} + \frac{l(l+1)}{x^2} \right]
\]

(15a)

is the kinetic-energy operator, and \( V(x) \equiv V_<(x) + V_>(x) \) is the potential energy, where

\[
V_<(x) = R^2 (1 - x^2) \theta(1 - x^2), \quad \text{and} \quad V_>(x) = R^2 (x^2 - 1) \theta(x^2 - 1)
\]

(15b)

are both positive. Apart from the coupling between \( u \) and \( v \), which occurs only for \( x < 1 \) through \( V_<(x) \), these equations look like those for radial eigenstates with orbital angular momentum \( l \) in an isotropic repulsive potential \( V(x) = R^2 |1 - x^2| \), which has a central peak at the origin, vanishes linearly at \( x = 1 \), and rises quadratically for \( x >> 1 \). Thus the low-lying eigenfunctions are expected to be “surface” modes localized in the vicinity of the condensate surface at \( x = 1 \).

In principle, these coupled differential equations can be solved numerically, but more physical insight comes from recognizing that they have a variational basis. If \( U(x) \) denotes a two component vector with elements \( u(x) \) and \( v(x) \), then Eq. (14) has a matrix representation

\[
[D_x + V(x)] U(x) = \epsilon \tau_3 U(x),
\]

(16)

where \( D_x = D_x \mathbf{1} \), \( V(x) = V(x) \mathbf{1} + V_<(x) \tau_1 \), \( \mathbf{1} \) is the \( 2 \times 2 \) unit matrix, and \( \tau_i \) are the familiar \( 2 \times 2 \) Pauli matrices. It follows immediately that the variational quantity

\[
\epsilon_{0l} \leq \frac{\int_0^\infty x^2 dx U^\dagger(x) [D_x + V(x)] U(x)}{\int_0^\infty x^2 dx U^\dagger(x) \tau_3 U(x)}
\]

(17)

provides an upper bound on the lowest eigenvalue \( \epsilon_{0l} \) for each separate \( l \). As a very simple model, take

\[
U(x) = \begin{pmatrix} \cosh \chi \\ \sinh \chi \end{pmatrix} g(x),
\]

(18)
with $\int_0^\infty x^2\,dx\,|g(x)|^2 = 1$. Substitution into Eq. (17) gives

$$\epsilon_{0l} \leq A \cosh 2\chi - B \sinh 2\chi,$$

where

$$A = \int_0^\infty x^2\,dx\,g(x)^*\left[D_x + V(x)\right]g(x) \quad \text{and} \quad B = \int_0^1 x^2\,dx\,g(x)^*V_<(x)g(x).$$

Minimization with respect to $\chi$ yields the condition \(\tanh 2\chi = B/A\), with

$$\epsilon_{0l} \leq \sqrt{A^2 - B^2}. \quad (21)$$

If $g$ also depends on some parameters, they can be varied to find the minimum of Eq. (21). For example, take $g(x) \propto x^\gamma \theta(1-x) + x^{-\gamma-1} \theta(x-1)$. The integrals in $A$ and $B$ are easily evaluated (with an integration by parts in the case of $A$), as is the normalization integral, and the minimum with respect to $\gamma$ was found numerically for several different values of $l$ and $R$. Since the description is expected to hold best for larger $R$, only the case of $R = 5$ will be considered in detail, corresponding to a value $\sigma \approx 168$ for the dimensionless parameter $\sigma$ that determines the relative importance of the kinetic contribution in the energy balance for the condensate wave function. To a good approximation, the 11 lowest eigenvalues $\epsilon_{0l}$ for $l = 0, \ldots, 10$ can be fit to a quadratic polynomial $\epsilon_{0l} \approx 5.83 + l/25.05 + l^2/25.25$, which effectively has the intuitive form $\epsilon_{0l} \approx \epsilon_{00} + l(l+1)/R^2$ of a radial zero-point energy $\epsilon_{00}$ plus rotational energy $l(l+1)/R^2$ of a rigid rotor; similar calculations for other values of $R$ show that $\epsilon_{00}(R)$ depends only weakly on $R$, as expected from the form of the potential $V(x)$. For comparison, the eigenvalues of the bare confining harmonic potential (here assumed isotropic) are $4n + 2l + 3$ in the same units of $\frac{1}{2}\hbar\omega$ [16]. The most striking conclusion here is that the low-lying elementary excitations of the Bose condensate for relatively large condensate radius $R$ and condensate number $N_0$ should have a rotational band of states (those for $n = 0$ and $l = 0, 1, 2, \ldots$) lying somewhat above the lowest state of the bare confining potential. With the values $a \approx 10$ nm and
\( d_0 \approx 1.4 \mu m \), which are appropriate for the experiment in Ref. [1], the radius \( R = 5 \) corresponds to a condensate number \( N_0 \approx 29,000 \), about an order of magnitude larger than the value estimated in Ref. [1]. In Ref. [6], where the Bogoliubov equations were solved numerically in the presence of the “exact” condensate density, the corresponding dimensionless parameter is \( \sigma \approx 9.7 \); thus it is not surprising that their eigenvalues (Ref. [6] reports only those for \( l \leq 4 \)) differ considerably from the simple rigid-rotor form given above.

The particle density operator \( \rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \) plays a central role in the response of a physical system to external perturbations. In the present case of a dilute Bose condensate, the noncondensate density \( \rho' \equiv \rho - |\Psi|^2 \) has an unusual and characteristic form

\[
\rho' \approx \Psi^* \phi + \Psi \phi^\dagger \tag{22}
\]

that follows from the Bogoliubov approximation introduced below Eq. (1). Since the operators \( \phi(\mathbf{r}, t) \) and \( \phi^\dagger(\mathbf{r}, t) \) oscillate harmonically at the frequencies given by the eigenvalues of the Bogoliubov equations, Eq. (22) shows that the normal modes of the condensate can be identified as density (compressional) waves. In particular, the noncondensate part of the density-density correlation function becomes simply a correlation function of the deviation operators, given by

\[
\frac{\langle \rho'(\mathbf{r}, t)\rho'(\mathbf{r}', 0) \rangle}{|\Psi(\mathbf{r})\Psi(\mathbf{r}')|} \approx \sum_j \left\{ (1 + f_j) \left[ u_j(\mathbf{r}) - v_j(\mathbf{r}) \right] \left[ u_j^*(\mathbf{r}') - v_j^*(\mathbf{r}') \right] e^{-iE_j t/\hbar} \right.
\]

\[
+ f_j \left[ u_j^*(\mathbf{r}) - v_j^*(\mathbf{r}) \right] \left[ u_j(\mathbf{r}') - v_j(\mathbf{r}') \right] e^{iE_j t/\hbar} \}
\]

\( \tag{23} \)

thus a measurement of the frequency spectrum of density oscillations (for example, by studying the resonant response to small modulations of the trapping potential) would directly characterize the eigenvalues \( E_j \).

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