Mean Field Calculations of Bose-Einstein Condensation of $^7$Li Atoms in a Harmonic Trap

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Abstract

A self-consistent mean-field theory for bosons for $T > 0$ is used to reconcile predictions of collapse with recent observations of Bose-Einstein condensation of $^7$Li. Eigenfunctions of a (non-separable) Hamiltonian that includes the anisotropic external trap field and atom-atom interactions are obtained by an iteration process. A sum over the Bose distribution, and the “alternating direction implicit” algorithm are used. Near $T_c$, the ensemble exhibits a localized condensate composed of atoms in the few lowest states. For lower $T$, numerical instability indicates collapse to a more dense phase.

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Recent observations of Bose-Einstein condensation in tenuous gases of alkali atoms have brought to concrete realization a text-book paradigm and a prediction by Einstein 70 years ago. These outstanding experimental achievements, coming after the rapid development of methods for cooling atoms by laser light and by evaporation in a trap, make it possible to test theories for weakly-interacting Bose gases. In contrast with superfluid helium, where the atoms interact strongly and thus depart from simple predictions, there is hope that BEC in dilute alkali atom gases can be usefully addressed by accessible theoretical methods.

Perhaps the experimental result that presents the greatest challenge to understanding is the reported Bose-Einstein condensation of $^7$Li, which is known to have a scattering length, $a = -27.2a_0$, indicating an attractive atom-atom interaction. It has been shown that in free space, BEC with $a < 0$ is not possible, because of the tendency to form a more dense phase. For a harmonic trap, recent computational results for $T = 0$ indicate that a stable condensate can be formed but with no more than about 1,400 atoms for the conditions of the experiment. When the number of atoms exceeds this value, it is expected that the cloud will collapse into a liquid or solid or into diatomic molecules. Since condensation of $^7$Li has been reported with as many as 20,000 atoms, there has been speculation on various mechanisms that might account for the observations.

In this report, we present a self-consistent mean field theory for trapped bosonic atoms. Whereas many previous theoretical studies concentrated on the condensate at $T = 0$, we report fully quantal results for $T > 0$, even for $T > T_c$. From these results, we can study the rapid changes in size and especially in the shape of the atomic cloud as the temperature goes through $T_c$ for comparison with experimental observations. We will show that mean-field theory calculations with $^7$Li parameters are consistent with the observed spatial distribution of cold atoms in the trap.

The Fermi-Thomas method or local density approximation (LDA) has yielded many useful results for BEC. This approximation is an appropriate and efficient method for large numbers of atoms and $a > 0$. On the other hand, the phenomena of interest with
a < 0 occur on a scale equal to or less than the dimension of the lowest quantum state, so the applicability of the LDA approach is severely limited in this case. Other approaches to BEC for ⁷Li have involved three-body collisions [10] and higher order terms in the atom-atom interaction constructed with derivatives of δ(⃗r₁₂) [11].

The mean field approach to BEC is based on the pseudopotential form of the atom-atom interaction [15,16]. We conjecture that the atom-atom interaction for densities of interest (an¹/³ ≪ 1) can be written

\[ V(⃗r₁₂) = \frac{4\pi a\hbar^2}{M} \delta(⃗r₁₂) \]

even for a < 0. From the Li₂ energies [4,14], the next term in the scattering series, the scattering range, may be computed. We find that it becomes significant at mK temperatures, but our concern here will be restricted to \( T < 1 \mu K \).

The discussion of the present computational approach can begin with the Gross-Pitaevskii equation (GPE) for \( T = 0 \) [17,18]. With the above form for the atom-atom interaction, the GPE for \( N \) atoms of mass \( M \) is

\[
\left[ -\frac{\hbar^2}{2M} \nabla^2 + V(⃗r) + \frac{4\pi a}{M} N|\psi(⃗r)|^2 \right] \psi(⃗r) = \bar{\mu}\psi(⃗r). \tag{1}
\]

Here \( V(⃗r) \) is the external harmonic potential and \( \bar{\mu} \) the chemical potential. \( \psi \) is normalized so that \( \int dτ |ψ|^2 = 1 \). For applications to the trap used for ⁷Li atoms, the external potential,

\[ V = \left( \frac{M}{2} \right) (ω_z^2 z^2 + ω_ρ^2 ρ^2) = \left( \frac{Mω^2}{2} \right) (λ_z^2 z^2 + λ_ρ^2 ρ^2), \]

where \( ω = (ω_z + 2ω_ρ)/3 \) is the average oscillator frequency and \( λ_i = ω_i/ω \) for \( i = z \) or \( ρ \). For a convenient distance scale, we let \( ⃗r = α⃗r \), with \( α^2 = \hbar/(2Mω) \) and then let \( μ = \bar{μ}/hω \). With \( \int dτ |φ(⃗r)|^2 = 1 \), and since \( dτ = α^3 dτ \), \( φ(⃗r) = α^{3/2}ψ(⃗r) \). Thus the scaled GPE equation is

\[
\left[ -\nabla^2 + \frac{1}{4}(λ_z^2 z^2 + λ_ρ^2 ρ^2) + gN|φ(⃗r)|^2 \right] φ(⃗r) = μφ(⃗r) \tag{2}
\]

The coefficient is \( g = 8πa/α = 8πa√(2Mω/ℏ) \). ⁷Li is notable not simply because \( a < 0 \), but also because \(|g|\) is relatively small. For ²³Na, \(|g|\) is about 6 times, and for ⁸⁷Rb, \(|g|\) is about 14 times the value for ⁷Li. So in this respect, ⁷Li is significantly closer to an ideal gas than the heavier alkali atoms.

For \( T > 0 \), one needs to obtain the wavefunctions for many orbitals self-consistently, analogous to the Hartree-Fock theory of atoms. Basic equations for this approach can be
found in Ref. [19]. With the pseudopotential approximation, the Hamiltonian equation for each basis state in a self-consistent set is \( H \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}) \), with

\[
H = -\nabla^2 + \frac{1}{4} \lambda_z^2 z^2 + \frac{1}{4} \lambda_\rho^2 \rho^2 + g \sum_j N_j |\phi_j(\vec{r})|^2
\]  

(3)

In the sum over states, the Bose distribution law applies:

\[
N_i = \frac{g_i}{\exp \left[ (\epsilon_i - \epsilon_0) \hbar \omega - \mu \right]/kT - 1}
\]  

(4)

where \( g_i \) is the degeneracy and \( \epsilon_i \) the energy eigenvalue of the \( i \)th state. The chemical potential, \( \mu \), is determined from the condition \( \sum_i N_i = N \).

The distribution law, Eq. (4), is often derived from the grand canonical distribution based on an exchange of particles and energy between a large ensemble and a subensemble. This situation seems irrelevant to a gas of trapped atoms, which (after the evaporative cooling is turned off) ideally exchanges neither particles nor energy with the surroundings. We have therefore considered a microcanonical ensemble defined to include all configurations of harmonic oscillator quantum states consistent with a given (small range of) total energy and atomic number. The number of such possibilities increases very rapidly, so that with only 5 atoms and \( T = 20 \) nK for the trap of Ref.[2], more than \( 10^7 \) configurations were found. The distribution obtained strongly resembled the Bose distribution with slight differences not likely to affect the present discussion. Since it is difficult to extend this microcanonical distribution analytically to thousands of atoms, we have adopted the Bose distribution. However, this point warrants further study.

Solutions to (3) are obtained by two stages of iteration. For a chosen \( T \) and \( \mu \), it is first assumed that \( \phi_i(\vec{r}) \) is given by harmonic oscillator eigenfunctions for each set of quantum numbers \( N_x(i), N_y(i), N_z(i) \). The mean field is computed from the sum. Since the Schrödinger equation for \( H \) (Eq. (3)) is nonseparable, the alternating direction implicit (ADI) method is used with successive scans in the \( x, y \) and \( z \) directions [20]. ADI iterations have the effect of transforming a function \( \phi_x(x)\phi_y(y)\phi_z(z) \) into a non-factorizable eigenfunction \( \phi(x, y, z) \) of \( H \). With cylindrical coordinates, factors of \( \rho^{m+1/2} \) make numerical
differentiation near $\rho = 0$ unreliable, so Cartesian coordinates are used. For $a < 0$, the atom-atom interactions produce a potential well that is typically smaller in spatial extent than the lowest orbital, so only the lowest quantum states are significantly affected by the term in $g$. Therefore, we needed to apply ADI to only the 4 to 50 lowest states. Other states are retained in the sum in the form of the harmonic oscillator (HO) functions. Typically states up to $E = 6kT$ are needed, so as many as $10^7$ HO states were included.

In comparing calculations with experimental observations, it is pertinent to recall features of Bose distributions that differ from the more familiar Boltzmann forms. For a given $T$, there is a range of possible $\mu$ values, and the spatial distribution of the ensemble will depend on $\mu$ as well as on $T$. This is illustrated in Fig. 1, which shows the distribution over $\rho$ calculated for a harmonic trap with the parameters of the permanent magnet trap used for $^7$Li. The frequency is is 112 Hz in the axial direction and 149 Hz in the transverse direction [2]. In this figure, the lighter curves are for $a=0$ (an ideal gas), while for the heavier curves, $a = -27.2a_0$, as for $^7$Li. The attractive interaction slightly narrows the distribution at large $N$. In the limit $-\mu \to \infty$, one has effectively a Boltzmann distribution. As $\mu$ approaches 0, $N$ increases and the distribution shrinks due to the onset of condensation. Thus from Fig. 1, it is apparent that $T$ cannot be accurately deduced from the size of an atom cloud in a trap unless $N$ is also known. A similar statement applies to measurements of the width of the velocity distribution, since the transformed wavefunctions $\tilde{\phi}_i(\vec{p})$ could have been used in place of $\phi_i(\vec{r})$ in the summation over discrete states.

Formation of a condensate with a fixed number of atoms as $T$ is varied is shown in Fig. 2, for 20,000 atoms and $a = -27.2 \ a_0$. The condensate peak develops over a very narrow range of $T$. As $T$ is reduced to slightly below 162 nK, the computation becomes numerically unstable due to the attractive atom-atom interactions. Similarly, for 1D calculations at $T = 0$ [3, 4], no eigenfunction can be found beyond a certain critical value of $gN$. The maximum number of atoms in the ground state with the anisotropic trap and with the ADI algorithm is about 1,000, or somewhat less than obtained with an isotropic trap of the same mean harmonic frequency.
Because of this instability, the calculations indicate that for more than about 1,000 atoms, phase-coherent BEC in a trap cannot be achieved with \(^7\)Li. However, the term “Bose-Einstein condensation” often refers to phenomena occurring over the entire range \(T \leq T_c\) rather than simply at \(T = 0\) \(^{10}\). In a harmonic trap, the signature of BEC is the rapid decrease of cloud size or narrowing of the velocity distribution, and these phenomena occur as the temperature is lowered through \(T_c\). A general view of this phenomenon is shown in Fig. 3. The filled circles on this figure represent \(\rho(1/e)\) values taken from the distributions shown in the previous figure (calculated with \(a=-27.2 \, a_0\)), while all the curves are for \(a=0\). The temperature at which the transition occurs is little affected by an \(a\) of this magnitude. For \(a = 0\), \(\rho(1/e)\) drops to a limiting value equal to the size of the ground state, but for \(a = -27.2 a_0\), the collapse has no limit. Determination of the ultimate minimum \(T\) for a given \(N\) would require an investigation of fluctuation effects, which are beyond the scope of this study.

The long dashed line in Fig. 3 shows that the sharp decrease in \(\rho(1/e)\) occurs while \(N_0/N < 10^{-2}\). Thus it does appear that with \(^7\)Li, there is a regime of \(N\) or \(T\) in which a “condensate peak” might be observable but in which there is no threat of collapse into a more dense phase because the accumulation of atoms in the ground state is far short of the critical number. From Fig. 3, the most obvious choice for a critical temperature \((T_c)\) is 161 nK, which marks the limit of numerically stable solutions for \(a = -27.2 a_0\). This is close to the value \(T_c = 167\) nK from semiclassical theory \(^{21}\) with the present trap parameters and \(N\).

A consideration of Fig. 1-3 might suggest that \(\rho(1/e)\) as a measure of cloud size accentuates the condensate. If instead one plots the average energy, \(\langle E \rangle\), results for \(a=0\) are shown in Fig. 3 as the short dashed line and inner left scale. (We have divided by \(3k\) for easy comparison with \(T\).) As discussed by deGroot et al. \(^{22}\), when there is a finite number of atoms in the ground state, \(\langle E \rangle < 3kT\). In Fig. 3 there is a discontinuity in the slope of \(\langle E \rangle\) vs. \(T\) at \(T_c\), so for \(a=0\), the most significant decrease of \(\langle E \rangle/3k\) occurs below \(T_c\). \(\langle E \rangle/3k\) does not mimic the sharp variation in \(\rho(1/e)\) because the condensate peak involves
relatively few atoms.

In the experiments [2], the evolution of a fixed ensemble as temperature is lowered is not observed. Rather, atoms are repeatedly placed in the trap and evaporatively cooled. After each load and cool cycle, the total number of atoms, \( N \), is measured by optical absorption, and also the size of the cloud is measured by imaging a probe beam. The size can be stated in terms of \( \rho(1/e) \), the value of \( \rho \) for which the optical density is \( 1/e \) times the maximum. Since this value is necessarily deduced from a two-dimensional image of the cloud and thus includes the effects of all atoms in the line of sight, it is not exactly equivalent to the \( \rho(1/e) \) parameter extracted from calculations as above. Nevertheless, we examine in Fig. 4 how BEC is manifest with data on \( N \) and \( \rho(1/e) \), as defined above, for various assumed temperatures. These computational results are for \( T > T_c \) and were obtained with \( a=0 \). Over the range of interest, the \( N \) vs. \( \rho(1/e) \) curves are quite flat due to the condensation process shown in Figs. 2 and 3. To characterize the quantum state distribution, we have plotted a few values of \( N_0/N \) as an orthogonal grid. The data point reported in Ref. [2] is clearly within the condensation regime.

An alternative discussion of the observations on \(^7\)Li has been developed in terms of rotation of the cloud [3]. It has been found (and we confirm) that if all atoms have, for example, 3 quanta of angular momentum around the symmetry axis, about 8,000 atoms in the ground state will be stable. We find further that if all atoms have \( J_z = 30 \), a condensate of about 50,000 atoms will be stable. However if the total value of \( J_z \) were not an integer times \( N \), there will be differing rates of rotation, hence a possibility for collisions, in which case the distribution over \( m_i \) would be statistical. To consider such a distribution, we have added an angular velocity term to the Bose distribution law, Eq. (3), giving an exponent 

\[
[(\epsilon_i - \epsilon_0)\hbar\omega - \mu - \gamma m_i]/kT,
\]

where \( m_i \) is the value of \( J_z \) for the \( i \)th level and \( \gamma \) is an additional Lagrange multiplier analogous to that used for fermions in the “cranking model” of nuclear physics [23]. With this distribution, one does not obtain a concentration of atoms at a single high value of \( m_i \). It seems possible that the cloud of atoms in the trap may randomly acquire angular momentum when loaded, but this is not needed to explain the observations.
In conclusion, one may debate the semantic question as to what constitutes BEC, but self-consistent mean field results presented here for $^7$Li atoms show that a “condensate peak” in the spatial distribution develops rapidly for $T$ near $T_c$. The experimental data on $N$ vs. $\rho(1/e)$ span the region of rapid decreasing $\rho(1/e)$. It is predicted that over a small range of $N$ for a given $T$, a condensate peak does occur, but for $N$ slightly greater or $T$ slightly less, the cloud will collapse. Confirmation of this and other predictions with experimental data would be useful tests of $T > 0$ mean field theory for bosons.

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FIGURES

FIG. 1. Calculated distribution of $^7$Li atoms in a harmonic trap as at Rice University, with $T = 150$ nK. The plotted curves show distributions for several values of the chemical potential, $\mu$, which determines the atom number, $N$. The light lines are for an ideal gas with $a=0$, while the heavy lines pertain to $a=-27.2\ a_0$, as for $^7$Li. The curve with smallest $N$ is identical to that for a Boltzmann distribution.

FIG. 2. Calculated spatial distribution of 20,000 $^7$Li atoms in a trap as in Fig. 1, with $a = -27.2a_0$. The “condensate peak” arises over a small range of $T$. The peak includes atoms in the several lowest quantum states, not simply the ground state.

FIG. 3. Condensation phenomena near $T = T_c$, for 20,000 $^7$Li atoms in a trap as in Fig. 1. The solid line gives the $\rho$ value at $1/e$ times the maximum density (whether the distribution is Gaussian or not) as a function of intensity for $a=0$ (ideal gas), while the circles give the same parameter calculated with $a = -27.2a_0$, taken from the distributions shown in Fig. 2. (Both refer to the outer left axis.) The long dashed line gives $N_0/N$ on a logarithmic scale (right axis). The short dashed line and inner left axis show $\langle E \rangle/3k$ from averaging over all quantum states in the distribution.

FIG. 4. Computational results obtained with $a=0$, plotted in the form of parameters measured experimentally, namely the total number of atoms $N$ and the $1/e$ width of the distribution in the $\rho$ direction. The roughly horizontal lines are for constant $T$ as shown at the left, while the approximately vertical lines indicate various values of $N_0/N$. A data point from Ref. 2 is shown. The rapid variation of $\rho(1/e)$ with $N$ for a given $T$ reflects the occurrence of Bose-Einstein condensation.
