Metastable Bose condensate made of atoms with attractive interaction

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Recent experiments with trapped cooled atoms have produced evidence for Bose-Einstein condensation (BEC). Among the atoms used are ^{7}Li, with attractive low-energy interaction. A potential barrier separating the condensed part from the collapse is studied and stability limits are established. The lifetime due to tunneling is estimated and is found to be very small. We further argue that BEC should have significant angular momentum $L/N \sim 1\hbar$ and thus both states with angular momentum $l_z = 0,1$ should be ''macroscopically'' populated. Eventually, as rotation is slowed down, collapse and strong reheating should occur, in amusing resemblance to a supernova explosion. [S1050-2947(96)10409-1]

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Bose-Einstein condensation (BEC) is a generic quantum phase transition discussed in most textbooks on quantum statistical mechanics. Recently several experiments [1,2] with atoms trapped in magnetic traps and cooled to temperatures as low as $T \sim 100$ nK have enabled this to be observed. Unlike liquid He, this condensate is in the low density domain. Since different atoms are used, we may learn more about the effects of the interaction.

In this paper we specifically discuss one experiment, performed by Bradley *et al.* [2] with ^{7}Li atoms. Li was chosen because of the *negative* sign of the scattering length of these atoms in the corresponding spin state, $a = -27.3 \pm 0.8 a_0$ [3] (a_0 is the Bohr radius). As a result of classic papers on the interacting Bose gas (e.g., [4]), it is known that a macroscopic system of bosons with attraction is *unstable against collapse*. However, it was repeatedly argued that the situation may be different for a *finite* number of atoms N trapped in a *finite* volume for *finite* time. In this paper we discuss the conditions under which a *metastable* Bose-condensed state exists.

We start with the $T=0$ case, in which all atoms are in the same quantum state, and present a simple argument why it *may* exist, based on a simple variational approach. Let $\psi(x)$ be the ground-state wave function [normalized by $\int d^D x |\psi(x)|^2 = 1$]. In the low-energy approximation one can describe interatomic interaction by the well-known Gross-Pitaevskii (or the *nonlinear* Schrödinger) equation [5], which follows from the Hamiltonian

$$H = N \int d^D x \left[\frac{\hbar^2}{2m} |\partial_x \psi(x)|^2 + V(x) |\psi(x)|^2 + N U_0 |\psi(x)|^4/2 \right], \tag{1}$$

where $V(x)$ is the trapping potential while $U_0 = 4\pi\hbar^2 a/m$ is the Fermi ''pseudopotential'' for pointlike interactions.

If atoms are in a state with a wave function which has size R, $\psi = f(r/R)$, their kinetic energy is $O(R^{-2})$, the potential energy is $O(R^2)$, while the interaction term is $O(R^{-D})$. So, for the *one-dimensional* case ($D=1$) the kinetic energy dominates at small R, always allowing for a stable solution. However, it is no longer so for higher dimensions. In the two-dimensional case kinetic and nonlinear terms may balance each other. For the $D=3$ case the interaction term takes over at small sizes, and if it is negative, collapse is inevitable. Nevertheless, the effective potential (which is obtained by the substitution of the trial function into the Hamiltonian)

$$V_{\rm eff}(R) = \langle H \rangle = C_1/R^2 + C_2 R^2 - C_3/R^3 \tag{2}$$

may have a minimum, provided C_3 (proportional to the number of atoms) is not too large.

However, in order to confirm its existence, one should show that the barrier separating it exists in all directions in a functional space of possible quantum states. That was the first problem we studied. Let us assume (for simplicity) that the trap is the three-dimensional isotropic oscillator, and introduce the dimensionless coordinates $r = x(m\omega/\hbar)^{1/2}$, measuring time in ω^{-1} units, etc. This leads to

$$H/(\hbar\omega N) = \int d^D r [|\partial_r \psi(r)|^2/2 + (r^2/2)|\psi(r)|^2 - (N/N_0)|\psi(r)|^4/2], \tag{3}$$

where $N_0 = (\hbar/m\omega)^{1/2}/(2\pi|a|)$ is some characteristic number of atoms. The experimental trap has an oscillator unit about 3 μm, which is much larger than the scattering length, so a large number $N_0 \gg 1$ appears. The corresponding equations, both static and time-dependent, were studied in some detail in [6,7]. Although these authors were mostly concerned with repulsive interactions, they obtained a very important result for the attractive case, namely that these equations allow for a solution in the attractive case below the critical point $N < N_{\rm crit} \approx 3.6 N_0$.

A solution of the Schrödinger equation is an extremum of the Hamiltonian: but it may be either an unstable one (a saddle point) or a local minimum. Extensive variational studies of the nearby wave functions (trial functions of various shapes such as the sum of several Gaussians with variable amplitudes and widths) have led to the conclusion that the latter is the case. We have minimized the expectation value of H by steepest descent, and determined the ''basin of attraction'' to this minimum. (Such a ''relaxation'' approach has obvious advantages over studies of the time-dependent Schrödinger equation [6], which conserves energy and thus

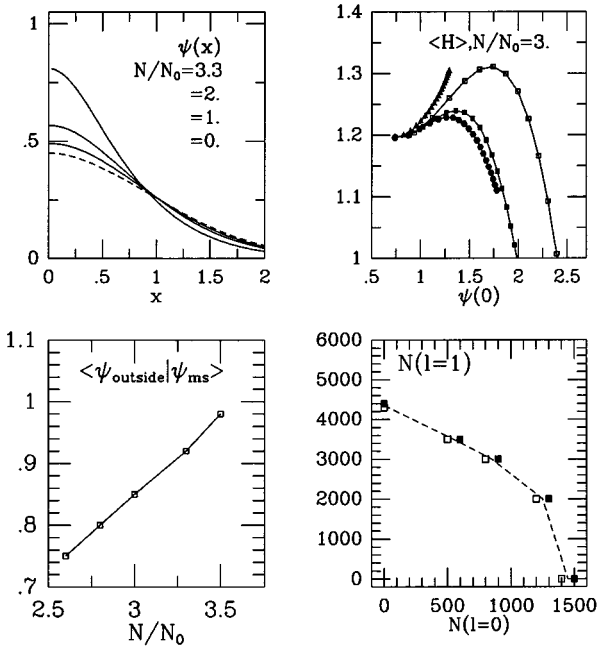

FIG. 1. (a) The wave function $\psi(x)$ of the metastable state, in oscillator units, defined in the text. Different curves correspond to four values of the number of atoms N given in the figure (from upper to lower one, at $x=0$). (b) Average energy for different trial functions (4), plotted as a function of the wave function at the origin $\psi(0)$. All curves are for $N/N_0=3$, for different spatial size of the perturbation: $1/R^2=10,5,4,3$ for open squares, closed squares, dots, and triangles. All of them show the existence of a barrier, separating the metastable state. (c) The projection of the state $\psi_{\text{outside}}(x)$ [which is outside the boundary of stability but has the same energy as the the metastable state $\psi_{ms}(x)$] versus the number of atoms N. At the critical point, the barrier disappears and here the projection becomes 1. (d) The condensate consisting of $N(l=0)$ and $N(l=1)$ atoms in states with orbital momentum $l=0,1$ is (meta)stable inside the domain shown by the dashed line. Out of a few dozen places where the wave functions were actually calculated, we show a few: closed squares indicate collapse and open ones correspond to stable solutions.

makes it difficult to penetrate into local minima.) We have also studied what happens near the critical point. The wave function found in [6] is shown in Fig. 1(a): note that, although the density at the origin grows by a significant factor, it is not singular. Nothing in the wave function itself suggests that, as one approaches the critical point, a qualitative change should occur. Those changes, however, are well seen when one looks at the instability threshold, or the barrier around the metastable state. Consider, for example, a wave function of the form of the metastable one ψ_{ms} plus a perturbation of *finite* magnitude; e.g.,

$$\psi(x)\sim[\psi_{ms}+C\exp(-x^2/R^2)], \tag{4}$$

where C,R are variable parameters (a common multiplier is determined by normalization to 1). A typical result for $N=3N_0$ is shown in Fig. 1(b): it displays energy versus $\Psi(0)$ for variable size R. The barrier is observed in all cases. Furthermore, we have found that at the critical point (4) the simplest ''opening of the pocket'' scenario takes place: for larger N the system may roll down *classically* into a collapse.

The next issue is a *lifetime* of the metastable state. We have seen that a finite increase in density at the origin leads to an instability. Such perturbation may appear spontaneously, as a result of quantum fluctuation.

Usually one solves such problems semiclassically, by finding a solution of the time-dependent Schrödinger equation with inverted potential. This solution should start (and end) with the minimum ψ_{ms}, and describe a ''bounce'' from the state ψ_{outside} on the outside part of the barrier, with the energy identical to the original one. The penetration probability is then obtained in terms of the action for that solution $\sim\exp(-S[\psi])$. Such an approach is known in many similar cases; see, e.g., Coleman's solution for ''the fate of a false vacuum'' [8] of the ϕ^4 relativistic field theory. Unfortunately, in the present nonrelativistic problem there is no symmetry between the time and space coordinates, which simplify it so that an analytic solution becomes possible.

Instead of looking for a numerical solution, we propose an estimate of the collapse rate based on *projection* of the wave functions in question, $\psi_{ms}(x)$, onto the state at the other end of the tunnel, $\psi_{\text{outside}}(x)$:

$$P_{\text{collapse}}/\omega\sim|\langle\psi_{\text{outside}}|\psi_{ms}\rangle|^{2N}. \tag{5}$$

We do not know which $\psi_{\text{outside}}(x)$ is connected with $\psi_{ms}(x)$ by the classical path (of *minimal* action), but in fact the transition may happen along any path, and in Eq. (5) one should sum over them. We have evaluated the projection probability for a number of $\psi_{\text{outside}}(x)$, which can be found for any direction in the functional space [e.g., for any curve shown in Fig. 1(b)]. Fortunately, the projection is in fact rather insensitive to the details of the density fluctuation, such as its size R and shape. Typical results are shown in Fig. 1(c): they can then be translated into an estimate $P_{\text{collapse}}/\omega\sim\exp[-0.57\times(N_{\text{crit}}-N)]$. Although for a few atoms it would not be an improbable fluctuation, for the condensate made of $N\sim1000$ particles the tunneling is strongly suppressed. In such experimental conditions the tunneling is very improbable (except maybe very close to the critical point).

Now we proceed to the nonzero temperature case. Although the temperature T is not reliably measured in the experiment under consideration, it is suggested to be about $T\sim150$ nK by the observed size. As $T\gg\hbar\omega\sim5$ nK, one can use a very simple classical approximation for the noncondensate particles. Ignoring self-interaction and setting the chemical potential to zero (thus looking for the *maximal* noncondensate particle density) one gets

$$\rho_{nc}(x)=\int\left(\frac{dp}{2\pi\hbar}\right)^D\frac{1}{\exp(p^2/2mT+V/T)-1}. \tag{6}$$

The total number of noncondensate particles $N_{nc}=(T/\hbar\omega)^3\zeta(3)$ is about $\sim2\times10^4$ atoms for the tem-

perature mentioned above, and it is consistent with the total number of particles actually observed. Furthermore, the noncondensate particles cannot significantly affect the stability condition for the spherically symmetric condensate derived above for $T=0$ because their density at the origin $\rho_{nc}(0)=(mT/2\pi\hbar^2)^{3/2}\zeta(3/2)$ is small compared to $\rho_c=N|\psi_{ms}(0)|^2$. So, in the *equilibrium* state of the experimental trap the fraction of the atoms in BEC cannot exceed several percent, and this conclusion seems to contradict the observations.

However, experiments deal with finite time and thus one has to look more carefully at the dynamics of the condensate formation and possible deviation from equilibrium. We propose that axial symmetry of the trap is very important here because (similar to the birth of stars from nebulas) the BEC follows a compression of an atomic cloud: as a result of angular-momentum conservation it should significantly spin up. A typical angular momentum (in $\hbar$ units) of an atom is $l\sim T/\hbar\omega$. So a *random* sum for N atoms should result in the total angular momentum per atom $L/N\sim T/(\hbar\omega\sqrt{N})$. For large N (which is the case in some other Bose-condensation experiments), L/N is small, and the adequate picture is similar to that in macroscopic systems (e.g., rotating liquid helium): a (nonrotating) condensate is formed, with a relatively small density of vortices [10]. However, if N is only about a few thousand atoms, separate vortices cannot actually exist. Furthermore, due to a play of numbers, L/N estimated above happens to be of the order of $1\hbar$. This implies that BEC starts with a spinning condensate, eventually going into a ''dual'' state in which both $l=0$ and $l=1$ collective states are ''macroscopically''populated. The energy functional (1) should then be rewritten, with two wave functions $\psi_{l=0}(x),\psi_{l=1}(x)$ to be optimized, and $N=N_{l=0}+N_{l=1}$. The initial value of N_1 is fixed by the total angular momentum at the formation stage.

We have performed the corresponding calculations for arbitrary $N_{l=0},N_{l=1}$, for the axially symmetric trap used in the Rice experiment. The resulting (meta)stability domain is shown in Fig. 1(d). Our results for those states occupied *separately* agree very well with those in [9]. If both states are populated together, the stability line is about linear, keeping the largest number of atoms in the condensate at about 4000. (This happens because two functions have very different shape, ψ_0 has a maximum at the origin, while ψ_1 has zero there.) This total number roughly matches the typical expected L evaluated above, so the system should form predominantly the $l=1$ condensate first. Certainly, the $l=1$ condensate has a different spatial distribution (including a hole going along the symmetry axis), so one can test this proposal by direct observation of BEC shape.

This dual condensate is still a nonequilibrium state: for how long may it exist? The relevant processes are scattering on noncondensate particles, in which an atom originating in the $l=1$ component ends up in the $l=0$ one. The total collision rate of a condensate particle with the noncondensate ones can easily be estimated from densities, velocities, and the cross section $\sigma=\pi a^2$: it is of the order of 1 Hz. Therefore, the angular-momentum transfer reaction (which includes some suppression factors such as small spatial overlap of ψ_0 and ψ_1, special kinematic required, etc.) should take time at least on the order of minutes. Only then is the stability boundary [the dashed line in Fig. 1(d)] crossed, and collapse should take place.

We do not study the collapse in this work, which is a formidable task in itself. Let us only add a few comments about it. First of all, it certainly is there in the low-energy approximation only, in which the interaction is assumed to be represented by the scattering length. The next term in the Hamiltonian $\sim(\partial\psi)^2(\psi^2)$ (and others indicated repulsion of atoms at small distances) should stop the collapse and result in a condensed ground state, solid or liquid. The collapse is related to many other phenomena in physics, from sonoluminescence to supernovas, which are also not yet well understood. The energy per particle released in the collapse is very small in absolute units, but it is still many orders of magnitude higher than the intial temperature, so strong reheating of the system is expected. For Li atoms used in experiment [2], the binary potential in the appropriate state is deep enough to cause reheating up to temperatures of the order of degrees K (compared with 150 nK at the beginning). A ''minisupernova'' event would include a tiny cluster (which is no longer a Bose condensate, but an ordinary liquid), which would blow up the noncondensate cloud (in a few seconds).

In summary, we have established that N trapped atoms with attractive interaction have a metastable state, surrounded by a barrier. We have obtained the stability conditions and studied the barrier when it exists. We have estimated the tunneling probability: it is very unlikely that tunneling could occur in experiment, but it can be studied in future ones. We then argue that in an equilibrium ensemble with the observed temperature most particles cannot be in the Bose condensate, but the kinetics of its formation favor formation of a ''dual'' condensate, starting with a rapidly rotating $l=1$ state. Stability of such a dual system was found to occur for $N<$ 4000 atoms, but, as friction eventually stops rotation of the system, it leaves the stability domain and collapses. Finally, we speculate that collapse should lead to strong reheating of the small drop of ordinary liquid and evaporation of noncondensate atoms.

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