Role of attractive interactions on Bose-Einstein condensation

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The properties and stability of a trapped Bose-Einstein condensate are strongly influenced by attractive interactions between the particles. We describe the spatial distribution, stability, and collisional loss rates for a weakly interacting gas in the mean-field limit. We show how the condensate contracts and becomes unstable as the number of condensate atoms increases. We further show how the number of atoms is limited by the collisional loss rates associated with the contraction of the condensate; this loss is in addition to the particle ejection decay indentified by Kagan *et al.* [S1050-2947(96)09607-2]

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The recent production of trapped atomic vapors of ^{87}Rb [1], ^{7}Li [2], and ^{23}Na [3] at the temperatures and densities necessary to give Bose-Einstein condensation (BEC) in the ground state of a magnetic trap have generated significant interest in this area of physics. BEC generates a wave function with a macroscopic phase and makes possible many novel matter wave and light scattering experiments. Unlike the related case of superfluid helium, the interactions between particles in an alkali vapor are weak and the condensate wave function may be modeled in detail [4–6]. For ^{87}Rb and ^{23}Na, the scattering lengths are known to be positive and therefore to lead to condensates in which the mean interaction is repulsive. This in turn leads to stable condensate wave functions that are larger than the bare ground state of the harmonic trap and can be modeled well by a mean-field equation [4]. For ^{7}Li, the scattering length is known to be negative [2], which produces a net attractive interaction between the particles: a particularly interesting regime for BEC. In fact, a homogeneous condensate with negative scattering length is predicted to be unstable [7]. If, however, the condensate is spatially confined, it may be stable provided that the number of atoms it contains is sufficiently small [8]. Other discussions of the negative scattering length case have addressed the general issues of energetic stability and the possibility of a transition to a denser phase [5,9,10]. In this paper, we show explicitly how the mean-field solution for the trapped condensate becomes unstable as the number of condensed particles increases. We also show how two- and three-body collisional decay processes strongly limit the approach to this unstable regime for a case of experimental interest [2].

The instability and increased decay rates both arise due to the presence of a negative scattering length. The mean attraction brings the condensate into a region where quantum fluctuations are an essential aspect of its behavior, as the negative self-energy becomes comparable in magnitude to the ground-state kinetic energy. Furthermore, as atoms are added to the ground state of the trap, the self-consistent ground state contracts and the density of atoms increases very rapidly. This enhances the effect of a number of inelastic two- and three-body collisional processes, leading to greater trap loss for the low-temperature fraction of the cloud. The removal of low-energy atoms is an effective heating mechanism and must be balanced by the evaporative cooling in order to maintain a steady state. Kagan, Shlyapnikov, and Walraven [10] have indentified a fundamental loss rate of particles from a negative scattering length condensate that will add to the rates we find here. This rate is initially exceedingly small but has a very rapid onset close to the edge of stability of the condensate. It's presence does not require us to modify the nature of the conclusions we shall make.

In the region of stability, at the very low temperatures reached in the experiment, the condensate can be described using mean-field theory. All the particles in the condensate then have the same wave function $\psi(\mathbf{r},t)$, which is found using the following nonlinear Schrödinger equation, i.e., the Ginzburg-Pitaevskii-Gross equation [12],

$$i\hbar\,\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\,\nabla^2+V(\mathbf{r})+NU_0|\psi(\mathbf{r},t)|^2\right)\psi(\mathbf{r},t), \tag{1}$$

where $\mathbf{r}=(x,y,z)$ is the displacement from the trap center and m is the atomic mass, and for our case the trap potential may be written as $V(\mathbf{r})=m(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2)/2$. The

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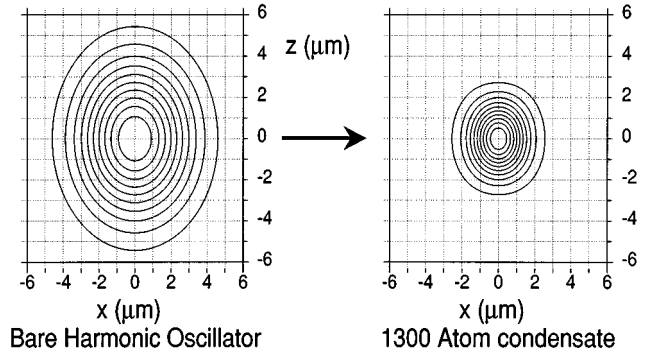

FIG. 1. Contour plots, in the $y=0$ plane, of the evolution of a ^{7}Li condensate, with increasing population.

mean number of condensate atoms is denoted by N, and $U_0=4\pi\hbar^2a/m$ describes the elastic ground-state collisions in terms of the s-wave triplet scattering length a. The value of a for ^{7}Li was taken to be $-27.3a_0$, where a_0 is the Bohr radius, as reported in [2]. In the experiments to date, the gases are effectively dilute, i.e., the number of particles in a volume a^3 is very small ($\sim 10^{-5}$). This means that the depletion of the condensate purely due to interactions should be correspondingly small. There will, of course, be thermal excitations present, but they should have a very modest effect on the condensate in the cases studied. The experimental configurations in both [1] and [2] exhibit cylindrical symmetry ($\omega_x=\omega_y$), and so Eq. (1) can be solved in two dimensions. The details of this solution, in both time-dependent and time-independent form, have been described elsewhere [4,6].

In Fig. 1 we illustrate the density of the wave function at $y=0$ in the lithium trap. The harmonic trap frequencies used were 163 Hz in the radial direction and 117 Hz in the axial direction, corresponding to the experimental parameters in [2]. Figure 2 shows the rapid increase in peak density as the condensate contracts with increasing population.

When the condensate size is smaller than the extent of the harmonic ground state, the lowest-energy solution is nearly isotropic. The initial effect of adding atoms to the condensate is, therefore, to reduce the asymmetry associated with the anisotropic potential. As the number of atoms is increased further, the cloud approaches spherical symmetry and the chemical potential goes down. As this happens the fluctuations previously ignored in the mean-field description will become increasingly important and the condensate will be limited in the number of atoms it contains [10].

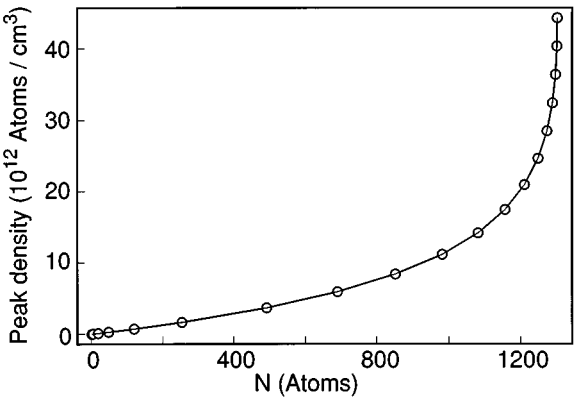

FIG. 2. Condensate peak density.

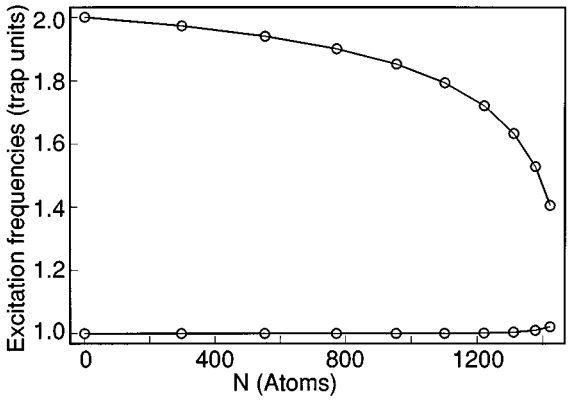

FIG. 3. Excitation frequencies, for a spherical trap ($\nu_r=108$ Hz), measured in trap units above the ground state.

Beyond approximately 1300 atoms, it is no longer possible to find stable numerical solutions to the time-dependent nonlinear Schrödinger equation for this potential. This corresponds to the point where the attractive interaction between the particles overwhelms the effective repulsive interaction [8,5,13]. The condensate in this region is to a very good approximation spherical. This means we can use the methods we have described elsewhere [14] to examine directly the nature of this instability. To do this, we have found the normal modes of a spherical condensate close to the experimental case. The frequencies of the two lowest frequency modes are plotted as functions of the number of condensed atoms in Fig. 3. The higher-frequency mode is the first radial excitation, i.e., the breathing mode of the condensate. The fact that its frequency goes down as the number of condensed atoms is increased shows that this breathing mode is going ''soft'' and that the mean field will become unstable with respect to collapse of the cloud. For the case of this spherical trap, $\nu_r=108$ Hz, it is no longer possible to find stable numerical solutions beyond approximately 1500 atoms.

The instability of the mean field occurs because the kinetic energy can no longer stabilize the wave function and prevent collapse to a denser state. Kagan, Shlyapnikov, and Walraven [10] and Stoof [11] have shown how such a transition can take place by tunneling even before the stability edge for mean field of the whole condensate is reached. Kagan, Shlyapnikov, and Walraven further showed that this rate is initially very small and does not compete strongly with the two- and three-body loss rates until close to the edge of stability. As this is approached it will rise, initially at a high power of the density, and overwhelm any other rates. Describing this region accurately will require far more than mean-field theory plus corrections [15]. Even in the absence of such an analysis we can be sure that it will not be possible to achieve stable solutions beyond the numbers found here.

Even before the region of instability of the mean field is reached, the kinetic loss rates become very large indeed. We now show explicitly how two- and three-body interactions will limit the approach to the densities at which the instability becomes an issue. These losses can be thought of as a kinetic obstacle to getting a large enough number of atoms to

see the onset of instability in the condensate. The two processes we will look at are two-body dipolar loss collisions and three-body recombination collisions. These occur predominantly between the lower-energy atoms, i.e., those in the ground translational state of the trap. This loss acts in the opposite sense to the evaporative cooling and therefore there is the possibility for a kinetic steady state to develop. There has been some casual discussion to the effect that the instability, caused by $a<0$, would lead to a transition to a solid or liquid state. It is clear that in our analysis (or in any reasonable extension) no such thing will happen for magnetically trapped atoms; dipolar loss will heat and eject atoms, reducing the density of the gas. Three-body recombination will similarly lead to heating and loss of atoms from the trap, but it is unlikely that many clusters larger than diatomic molecules will be formed.

The two-body dipolar loss rates that we used were found using the coupled Schrödinger equation for the following dipolar relaxation process:

$$^7\mathrm{Li}(F_a=2,m_{F_a}=2)+{}^7\mathrm{Li}(F_b=2,m_{F_b}=2)$$

$$\rightarrow {}^7\mathrm{Li}(F_a',m_{F_a}')+{}^7\mathrm{Li}(F_b',m_{F_b}'). \qquad (2)$$

The calculations were done in the zero-magnetic-field limit, in which case the Hamiltonian separates into individual blocks of good parity p and total angular momentum F. Thus, for the process described above we need only to consider the $F=4$ positive-parity Hamiltonian. A more extensive description of the Hamiltonian and resulting close-coupled equations is found in [18] and are equivalent to those reported in [19]. As expected, the predominant loss processes are due to spin-spin dipole relaxation. Because the incoming channel is a pure $a\ {}^3\Sigma_u^+$ state, the rates are only weakly affected by the $X\ {}^1\Sigma_g^+$ scattering length. Thus, it is unlikely that these rates will change drastically and, in fact, the numbers presented here are consistent with recent calculations of lithium loss rates by Moerdijk and Verhaar using a slightly different potential [16]. The calculations described here use the potential and potential subroutines described by Côté, Dalgarno, and Jamieson [17].

The dominant dipolar loss processes, $|22\rangle+|22\rangle\rightarrow|F_a'm_{F_a}'\rangle+|F_b'm_{F_b}'\rangle$, are independent of collision energy in the range of 1–1000 nK. The rates for the four largest dipolar loss processes are 3.2×10^{-15} cm^3 s^{-1} for $|11\rangle+|11\rangle$, 4.8×10^{-15} cm^3 s^{-1} for $|21\rangle+|11\rangle$, 2.5×10^{-16} cm^3 s^{-1} for $|22\rangle+|10\rangle$, and 3.6×10^{-15} cm^3 s^{-1} for $|22\rangle+|11\rangle$, where the states listed are the final magnetic hyperfine states of the two fragments. For the three-body recombination rates, we have used the recent calculations of Moerdijk, Boesten, and Verhaar [20]. The actual collisional-loss process is totally dominated by the two-body dipolar loss except for condensates approaching 1300 atoms.

In Fig. 4 we show the loss rate of the condensate, calculated using condensate densities as in Fig. 1 and the loss rate equations given in [20,21]. The total loss rate is given by

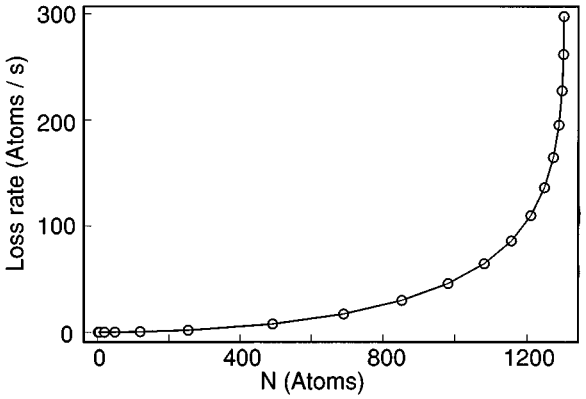

FIG. 4. Total condensate loss rate due to two- and three-body collisions.

$$R(N)=\alpha N^2\int d\mathbf{r}|\psi(\mathbf{r})|^4+LN^3\int d\mathbf{r}|\psi(\mathbf{r})|^6. \qquad (3)$$

These calculations used a two-body dipolar loss rate coefficient α of 1.2×10^{-14} cm^3 s^{-1} and a three-body recombination loss rate coefficient L of 2.6×10^{-28} cm^6 s^{-1} [20]. Our results give a lower limit of the loss rate, since the interaction with the thermal and background gas has been neglected.

We have shown, in the mean-field limit, that in the case of the negative scattering length the rapid increase in the density of the atoms will result in a very large loss rate for the condensate in the case of a large number of particles. The precise number of particles that may be condensed will depend on the details of the confining potential and the evaporative cooling mechanism, but we do not expect it to exceed 1300 for the case of Ref. [2]. We should point out that the analysis we have given here does not take into account the possibility of observing other types of phase transitions as described by Stoof [9]. In the case of a trapped gas the onset of Bardeen-Cooper-Schrieffer pairing in the atoms could occur in a different way than that which occurs in a homogeneous gas. The characterization of the interaction potential by the s-wave scattering length, i.e., U_0, is only valid for the system when the dominant interactions are long-range elastic collisions, this may no longer be completely true as we approach the instability point. In any case, for reasonable parameters it does not appear that it will be possible to generate a large macroscopic field. The negative scattering length case is, however, very much worthy of further study because of the large range of subtle issues it brings up.

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[1] M. H. Anderson *et al.*, Science **269**, 198 (1995).
[2] C. Bradley, C. Sackett, J. Tollett, and R. Hulet, Phys. Rev. Lett. **75**, 9 (1995).
[3] K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995).
[4] M. J. Holland and J. Cooper, Phys. Rev. A **53**, 1954 (1996).
[5] G. Baym and C. Pethick, Phys. Rev. Lett. **76**, 6 (1996).
[6] Mark Edwards *et al.*, Phys. Rev. A **53**, 1950 (1996).
[7] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics* (Pergamon, Oxford, 1980), Part 2.
[8] P. A. Ruprecht, M. J. Holland, K. Burnett, and Mark Edwards, Phys. Rev. A **51**, 4704 (1995).
[9] H. Stoof Phys. Rev. A **49**, 3824 (1994).
[10] Y. Kagan, G. Shlyapnikov, and J. Walraven, Phys. Rev. Lett. **76**, 2670 (1996).
[11] H. Stoof (unpublished).
[12] V. L. Ginzburg and L. P. Pitaevskii, Zh. Éksp. Teor. Fiz. **34**, 1240 (1958) [Sov. Phys. JETP **7**, 858 (1958)]; E. P. Gross, J. Math. Phys. **4**, 195 (1963).
[13] A. L. Fetter, Phys. Rev. A (to be published).
[14] Mark Edwards, P. A. Ruprecht, K. Burnett, and C. Clark (unpublished).
[15] A. Griffin, *Excitations in a Bose-Condensed Liquid* (Cambridge University Press, Cambridge, 1993).
[16] A. J. Moerdijk and B. J. Verhaar, Phys. Rev. A **53**, 19 (1996).
[17] R. Côté, A. Dalgarno, and M. J. Jamieson, Phys. Rev. A **50**, 399 (1994).
[18] C. J. Williams and P. S. Julienne, Phys. Rev. A **47**, 1524 (1993).
[19] H. T. C. Stoof, J. Koelman, and B. J. Verhaar, Phys. Rev. B **38**, 4688 (1988).
[20] A. J. Moerdijk, H. M. J. M. Boesten, and B. J. Verhaar, Phys. Rev. A **53**, 916 (1996).
[21] T. W. Hijmans, Yu. Kagan, G. V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. B **48**, 12 886 (1993).