Properties of Two-Species Bose Condensates

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We present theoretical studies of a two-species Bose condensate. Using a new numerical method, we have calculated ground state wave functions and show that, due to interspecies interactions, the condensate mixture displays novel behavior not found in a pure condensate. We compared our results with those of the Thomas-Fermi approximation (TFA) and find that under a broad range of conditions the TFA can be reliably used to predict many qualitative features of the condensates. Using our technique, we have modeled a recent JILA experiment on dual spin-state ^{87}Rb condensate. Finally, collective excitations of double condensates are discussed. [S0031-9007(97)05211-3]

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Since the realization of dilute alkali atomic vapor condensates in 1995 [1], we have seen a rapid development on the field of Bose-Einstein Condensation (BEC). New progress poses new questions to both experimentalists and theorists. One such questions is: What will the ground state density distribution be if we put two condensates of different atoms together? We have learned that the interactions between particles inside a pure condensate have huge effects on the properties of the condensate [2]. Thus, it is natural to conjecture that the interactions between different species will play an important role in a multispecies condensate. For example, one might guess that interspecies interactions could cause novel ground state structures that would not exist had only one species been present. Recently, the ground state wave functions of binary mixture of Bose condensates have been calculated by Ho and Shenoy [3], who devised an elegant algorithm to determine the density profiles of the mixtures within the Thomas-Fermi approximation (TFA).

A single-species Bose condensate can be described by the nonlinear Schrödinger equation, also known as the Gross-Pitaevskii Equation [4], which can be solved numerically [5]. However, in order to derive analytic results, some approximations must be applied. A commonly used one is the TFA, which ignores the kinetic energy terms. It has been shown that the TFA results agree well with numerical calculations for large particle numbers, except for a small region near the boundary of the condensate [6]. In fact, even for small particle numbers, the ground state wave function calculated within the TFA still usually gives qualitatively correct overall shapes. We find that this is also usually the case for a two-species condensate. For example, the TFA solution correctly predicts that "phase separation" will occur if there exists a strong repulsive interaction between the two species [3] and, indeed, it can reliably and efficiently estimate when this separation will occur. However, we do find that in many situations the TFA cannot be relied upon to predict *quantitative* features of the double condensate and in particular, the TFA solution can greatly underestimate the degree of overlap between the condensates. For example, the TFA does not accurately describe a new phenomenon which we describe here—that of density compression—nor can it be used to precisely evaluate collisional relaxation rates [7]. Therefore, we conclude that the solutions derived for the TBEC within the TFA are remarkably robust and provide an excellent starting point of study; however, we also stress the TFA should not be relied upon when a quantitative comparison of experiment and theory are important. Instead, a numerical approach becomes necessary. The realization of such an approach and examples of its application to the study of other novel properties of condensates mixtures, such as self-compression and collective excitations, are the subject of this Letter.

In the following, we will present our method of calculation. In the case of a two-species condensate inside an isotropic harmonic trap at zero temperature, letting $\psi_i(r)$ $(i = 1, 2)$ be the wave function of species i with particle number N_i (where r is the radial coordinate), we can write two coupled Schrödinger equations as [3]

$$\mathcal{H}_i\psi_i(r) = \mu_i\psi_i(r), \qquad i = 1, 2, \tag{1}$$

$$\mathcal{H}_1 = -\frac{\hbar^2}{2m_1}\nabla^2 + \frac{1}{2}m_1\omega_1^2 r^2 + N_1U_1|\psi_1|^2 + N_2U_{12}|\psi_2|^2, \tag{2}$$

$$\mathcal{H}_2 = -\frac{\hbar^2}{2m_2}\nabla^2 + \frac{1}{2}m_2\omega_2^2 r^2 + N_2U_2|\psi_2|^2 + N_1U_{12}|\psi_1|^2, \tag{3}$$

where m_i, ω_i, and μ_i are mass, trap frequency, and chemical potential for the ith species, respectively. We have assumed that the ground state wave functions are spherically symmetric [8]. The interaction between particles is described by a self-interaction term U_i and a term that corresponds to the interaction between different species U_{12} which have the following expressions:

$$U_i = 4\pi\hbar^2 a_i/m_i, \tag{4}$$

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$$U_{12} = \frac{2\pi\hbar^2 a_{12}}{m_1 m_2/(m_1 + m_2)}, \tag{5}$$

where a_i is the scattering length of species i and a_{12} that between species 1 and 2. If we denote $\phi_i(r) = r\psi_i(r)$, and let $\sqrt{\hbar/2m_1\omega_1}$ and $\hbar\omega_1$ be the units for length and energy, respectively, Eqs. (2) and (3) can be rewritten as

$$H_1 = -\frac{d^2}{dr^2} + V_1(r), \tag{6}$$

$$H_2 = -\frac{1}{a_m}\frac{d^2}{dr^2} + V_2(r), \tag{7}$$

$$V_1 = \frac{1}{4}r^2 + 8\pi N_1 a_1 \frac{|\phi_1|^2}{r^2} + \frac{1 + a_m}{a_m} 4\pi N_2 a_{12} \frac{|\phi_2|^2}{r^2}, \tag{8}$$

$$V_2 = \frac{1}{4} a_m a_\omega^2 r^2 + \frac{8\pi N_2 a_2}{a_m}\frac{|\phi_2|^2}{r^2} + \frac{1 + a_m}{a_m} 4\pi N_1 a_{12} \frac{|\phi_1|^2}{r^2}, \tag{9}$$

where $a_m = m_2/m_1$ and $a_\omega = \omega_2/\omega_1$. Our numerical solution requires some discretization of continuum space. Let δ be the mesh length in the r direction and approximate $\phi(r)$ by ϕ_l for $l\delta < r \le (l + 1)\delta$. Free-boundary conditions have been applied, i.e., $\phi_l = 0$ if $l \le 0$ or $l > L$. Replacing the second derivative with respect to r by its simplest finite-difference approximation $d^2\phi(r)/dr^2 = (\phi_{l+1} - 2\phi_l + \phi_{l-1})/\delta^2$, we can write H_1 in a tridiagonal matrix of the form

$$H_1 = \begin{pmatrix} v_1^1 & -\delta^{-2} & & & \\ -\delta^{-2} & v_1^2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & v_1^{L-1} & -\delta^{-2} \\ & & & -\delta^{-2} & v_1^L \end{pmatrix}, \tag{10}$$

where $v_1^l = V_1(l\delta) + 2\delta^{-2}$, and similarly for H_2. The eigenproblem of these matrices can be solved by the FORTRAN subroutine package EISPACK (the Eigenvalue Analysis Package) in a CRAY supercomputer system. Since the Hamiltonians themselves contain the wave function ϕ_i, iteration is necessary. In detail, we start from a set of trial wave functions $\phi_i^{(0)}$. Using H_i, we find the eigenvector ϕ_i corresponding to the smallest eigenvalue of H_i. (In this way, we can ensure that the wave function we find is the ground state.) Let $\phi_i^{(1)} = \sqrt{\epsilon(\phi_i^{(0)})^2 + (1 - \epsilon)(\phi_i)^2}$ (with ϵ being a positive number between 0 and 1) be the new trial function. Repeat the above procedures until ϕ_i agrees with its trial function within a certain range. Then, $\psi_i = \phi_i/r$ is the ground state wave function for species i. We find that this method is very stable. The largest particle number used in our calculation is 10^8. However, we find no principle upper bound on N.

In our calculations, we take Rb as species 1 and Na as species 2, with scattering lengths taken as 6 and 3 nm, respectively. For the trap, we assume $\omega_1 = 2\pi \times 160$ Hz and $\omega_2 = 2\pi \times 310$ Hz. In Fig. 1, we compare our results with those of Ho and Shenoy's [3]. Figures 1(a)–1(c) correspond to $a_{12} = 1.8$ nm, or relatively weak interaction between the two species. In

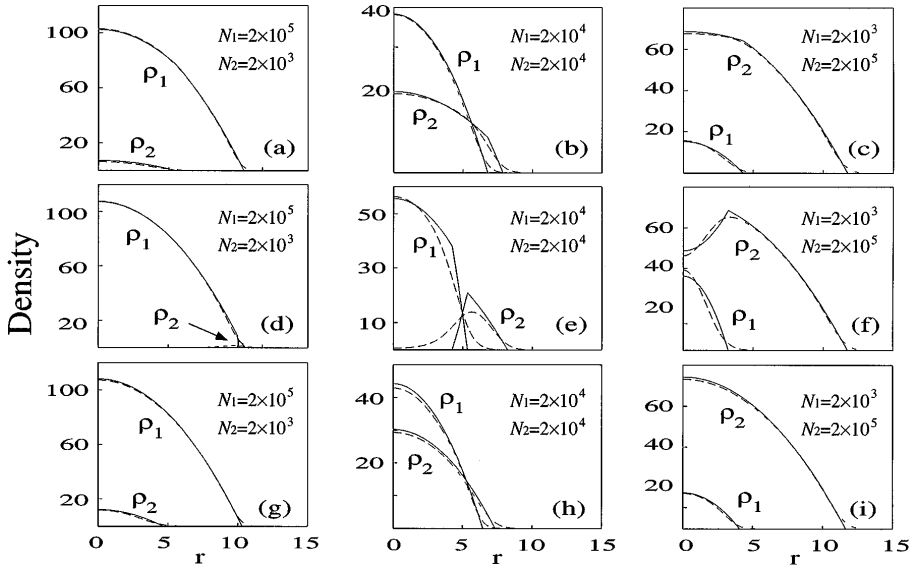

FIG. 1. Ground state density profiles. Solid curves—TFA results; dashed curves—numerical results. The units for density and length are $(2m_1\omega_1/\hbar)^{3/2}$ and $(\hbar/2m_1\omega_1)^{1/2}$, which have numerical values of 4.6×10^{12} cm^{-3} and 0.6 μm in our calculations, respectively. The interspecies scattering length is as follows: (a)–(c) $a_{12} = 1.8$ nm; (d)–(f) $a_{12} = 3.6$ nm; (g)–(i) $a_{12} = 0$.

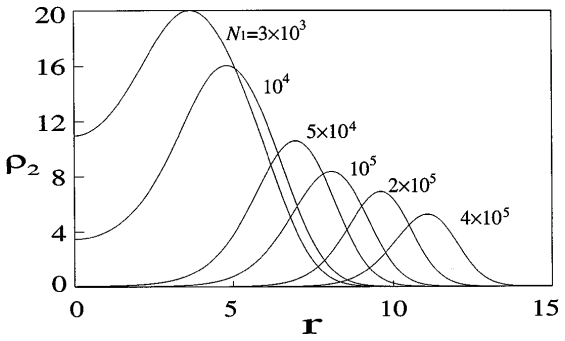

FIG. 2. Ground state density profiles of species 2 (Na). $N_2 = 2 \times 10^4$, $a_{12} = 3.6$ nm. From left to right, $N_1 = 3 \times 10^3$, 10^4, 5×10^4, 10^5, 2×10^5, and 4×10^5. Same units as in Fig. 1.

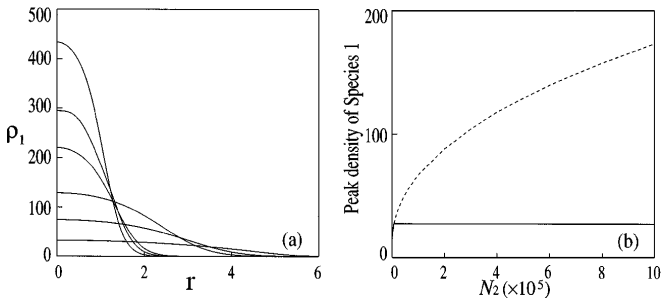

FIG. 3. (a) Ground state density profiles of species 1 (Rb). $N_1 = 10^4$, $a_{12} = 3.6$ nm. In ascending order, $N_2 = 0$, 10^5, 5×10^5, 2×10^6, 4×10^6, and 10^7. (b) Peak density of Rb as a function of N_2. Calculated with numerical method (dashed line) and the TFA (solid line). Same units as in Fig. 1

this case, Ho and Shenoy's results agree remarkably well with our calculations: compared with the $a_{12} = 0$ case [i.e., no interactions between different species, Figs. 1(g)–1(i)], the density profiles for both Rb and Na have lower peak values and wider widths. When we increase a_{12} [as in Fig. 1(d)–1(f) where $a_{12} = 3.6$ nm] we see that the peak density of Na does not occur at $r = 0$ any more. It is as if Na has been squeezed out and forced to form a shell around the trap center which holds Rb, while Rb is compressed—it has a higher peak density and narrower width compared to its pure condensate. This is because the Rb gets extra confinement from the Na shell surrounding it. In other words, the coupling term $N_2 U_{12} |\psi_2|^2$ in Eq. (2) acts as an effective attraction potential for the Rb. The formation of this central Rb core and outside Na shell is analogous to the phase separation in a two-component fluid—different components occupy different regions of space. Here we see that in regions of overlap, the density profiles predicted within the TFA become less satisfactory for larger a_{12}. The detailed nature of this overlap is important because it influences quantities such as the ground state system energy, the excitation spectrum, and the collisional relaxation rates [7].

Besides the interaction strength, the density profiles also depend on particle numbers N_1 and N_2. Figure 2 displays the density profile of Na, ρ_2, as a function of N_1 when N_2 is fixed. The Na is pushed further out as the number of Rb atoms increases. In Fig. 3(a), we show the density distribution of Rb, ρ_1, when we change N_2 while holding N_1 fixed. We see that, with the increase of N_2, the Rb condensate is compressed further and further. Figure 3(b) shows the peak value of ρ_1 as a function of N_2 as calculated with both our numerical method and the TFA. With the increase of N_2, the peak density of Rb increases. For small values of N_2 ($N_2 < 7 \times 10^4$), the results from the TFA qualitatively agree with our numerical results. However, at larger values of N_2, ρ_1 remains unchanged as N_2 changes. The reason for this is that, for large particle numbers, the strong interspecies interactions cause both wave functions to vary rapidly in space, especially in the region of coexistence. In the coexistence region it is not at all appropriate to neglect the derivative terms (or the kinetic energy terms) in the Hamiltonian and hence there, the TFA becomes rather unsatisfactory. Figure 4 contrasts the quantitative differences between the two results. The peak density of Rb can be enhanced by more than 1 order of magnitude by varying N_2 from 0 to 10^7. This provides us with the possibility of making a condensate with extraordinarily high densities, so high that the condensate may become unstable due to the effects of spin relaxation [7] and/or three-body recombination [9]. A true two-species condensate is a very attractive system in which to study this phenomenon, since the density of one species can be easily controlled by adjusting the particle number of the other.

Although a condensate composed of two different species of atoms remains to be realized, experimentalists in JILA have already successfully demonstrated a two-state condensate [10]. That is, a ^{87}Rb condensate composed of two different spin states $|F = 2, m = 2\rangle$ and $|F = 1, m = -1\rangle$. Because atoms in these two states have different values of magnetic moment, under the influence of gravity, the two pure condensates made of each

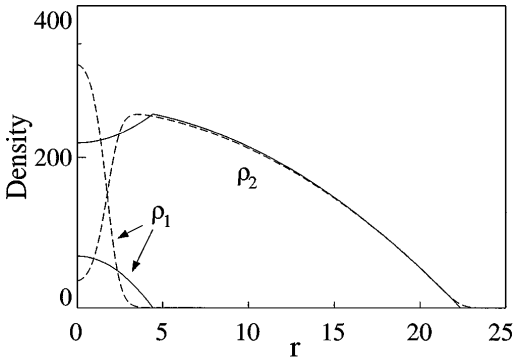

FIG. 4. Ground state density profiles. $N_1 = 10^4$, $N_2 = 5 \times 10^6$, $a_{12} = 3.6$ nm. Solid curves—TFA results; dashed curves—numerical results. Same units as in Fig. 1.

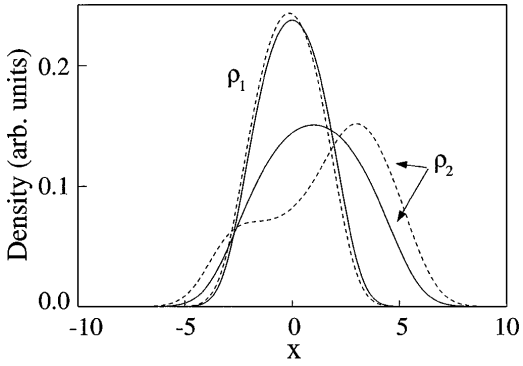

FIG. 5. A qualitative explanation of the experiment of Ref. [6]. Density profiles of the two spin states of ^{87}Rb without interaction (solid line) and with repulsive interaction (dashed line) between them. States 1 and 2 correspond to spin state $|2,2\rangle$ and $|1,-1\rangle$, respectively.

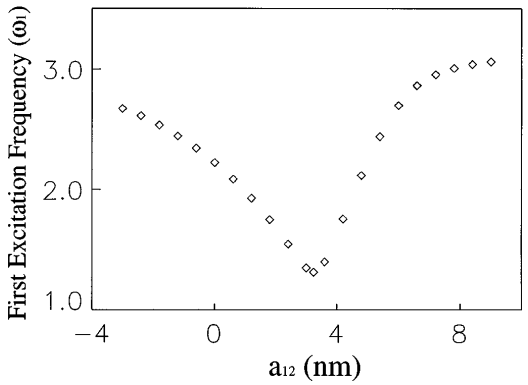

FIG. 6. The angular frequency of the lowest isotropic breathing mode as a function of a_{12}. $N_1 = N_2 = 10^4$.

single state have a slight offset in space, i.e., the two density peaks do not coincide with each other. If these two condensates are formed together, the repulsive interaction between them will separate them farther away. This has been observed experimentally. Using the numerical method outlined above, we made a one-dimensional calculation to simulate this phenomenon [7]. Suppose we have two condensates with the respective trapping potentials $m\omega_1^2 x^2/2$ and $m\omega_2^2(x - x_0)^2/2$, respectively, where x_0 is the initial spatial offset. Figure 5 shows the density profiles for the two condensates with and without interspecies interaction. Obviously, the separation between the two peaks is significantly widened due to the presence of interaction. Hence, our simple model agrees qualitatively with the experimental results.

Finally, we want to mention our results for negative a_{12}. In this case, both wave functions are compressed as compared to the case of $a_{12} = 0$, and phase separation will not occur. Furthermore, if the magnitude of a_{12} becomes larger than a certain value which depends on N_i, a_i, etc., the condensates mixture eventually collapses.

Currently, we are undertaking the study of the collective excitations of a two-species condensate. The frequencies of the excitation modes can be verified by studying the response of the condensates to external probes [11,12]. We observe two types of breathing modes—out-of-phase modes (i.e., at a given time, one condensate is compressed while the other being decompressed) and in-phase modes (i.e., both condensates are compressed or decompressed at the same time); modes which are analogous to the two normal modes of a coupled pendulum. The excitation spectra of these modes can be obtained by solving the Bogoliubov equations [11] with the input of the ground state wave functions calculated with our numerical method. Figure 6 shows the excitation angular frequency of the lowest isotropic breathing mode as a function of a_{12}. It can be seen that the presence of interspecies interactions dramatically changes the resonance condition. In fact, this shows that a precise measurement of excitation frequencies can help us determine the value of a_{12}. Further studies on this subject will be reported in a separate paper [13].

With the present rapid development in the field of BEC, the goal of making a condensate composed of two different types of atoms does not seem to be far-fetched. Our work will help us understand the properties of the Bose condensates mixtures and broaden our knowledge of coupled macroscopic quantum states.

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