Hartree-Fock Theory for Double Condensates

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We present the first theoretical treatment that accounts in detail for a recent observation of overlapping Bose-Einstein condensates of two different ^{87}Rb hyperfine states [C. J. Myatt *et al.*, Phys. Rev. Lett. **78**, 586 (1997)]. Despite the complicated geometry, we have completed a three-dimensional Hartree-Fock calculation for the coupled condensates. The calculation explains a number of its key properties: (i) The manner in which one condensate partially wraps around the other, (ii) the mean separation between the two condensates including the effects of gravity and of their mutual interaction, and (iii) the surprisingly long lifetime of the trap. [S0031-9007(97)03154-2]

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In a recent experiment, Myatt *et al.* [1] have observed Bose-Einstein condensation (BEC) of ^{87}Rb atoms in a new dynamical regime. Two *interacting* condensates of atoms in different internal spin states, $|F, M_F\rangle = |1, -1\rangle$ and $|2, 2\rangle$, were formed using evaporative cooling in a magneto-optical trap (MOT) to cool only the $|1, -1\rangle$ state. Sympathetic cooling reduced the temperature of atoms in the other hyperfine state $|2, 2\rangle$ to form a second condensate of atoms that were "effectively distinguishable" from those in the $|1, -1\rangle$ condensate. Once condensed, the atoms were observed to separate into two distinct clouds with small spatial overlap, thus indicating an effectively repulsive interaction between the two species. By reducing the opportunity for inelastic interspecies (spin exchange) collisions, this separation makes possible the observed lifetime of seconds for the condensed phase.

In this Letter we show how the properties of this remarkable "double condensate" emerge from joint considerations of the identical particle collisions and the distinguishable particle collisions. The very existence of a metastable pair of interacting condensates was far from evident, *a priori*. In the s-wave domain that characterizes these collisions, spin exchange between unlike atoms can produce untrapped atomic hyperfine substates. We present theoretical evidence below for an unexpectedly low spin exchange loss rate of condensed trapped atoms from these collisions. We find that, in part, the loss is slow because the condensates repel each other rather than intermingling. Other predicted features of interacting condensates hinge on the values of the three relevant scattering lengths. We also obtain the two-body scattering length for collisions between the two atomic states studied in the recent experiment, and find the cross section for inelastic collisions between those states to be surprisingly small.

At least one study prior to ours has approached the subject, but, in the absence of a definite experiment, restricted itself to cylindrically symmetric condensates arranged concentrically, neglecting altogether the effects of gravity [2] (see also Refs. [3–6]). The experiment of Myatt *et al.* [1] requires a more detailed treatment since the symmetry axes were aligned perpendicular to gravity. In this case, the $|1, -1\rangle$ state, less strongly confined than the $|2, 2\rangle$ state because of its smaller total spin projection M_F, experiences a comparatively larger "sag" due to gravity. So, while each cloud individually remains in a cylindrically symmetric trap, the symmetry axes of the two traps do not coincide. This circumstance wrecks even the cylindrical symmetry of the individual clouds due to the interaction between the two species, as will become evident below.

Assuming that there is a fixed number N_1 of atoms in the hyperfine state $|1\rangle \equiv |1, -1\rangle$ and a fixed number N_2 in the state $|2\rangle \equiv |2, 2\rangle$, the Hartree-Fock equations for the corresponding single particle orbitals $\psi_1(\mathbf{x})$ and $\psi_2(\mathbf{x})$ are

$$\begin{aligned} &[h_1(\mathbf{x}) + (N_1 - 1)U_{11}|\psi_1(\mathbf{x})|^2 + \\ &\qquad N_2 U_{12}|\psi_2(\mathbf{x})|^2]\psi_1(\mathbf{x}) = \varepsilon_1 \psi_1(\mathbf{x}), \\ &[h_2(\mathbf{x}) + N_1 U_{12}|\psi_1(\mathbf{x})|^2 + \\ &\qquad (N_2 - 1)U_{22}|\psi_2(\mathbf{x})|^2]\psi_2(\mathbf{x}) = \varepsilon_2 \psi_2(\mathbf{x}). \end{aligned} \tag{1}$$

In these equations, ε_i are single particle energies which represent the energy required to remove one particle from the condensate. As such, they correspond to the chemical potential in the grand canonical ensemble. The operators h_i are given by $h_i = T + V_i^{\text{trap}}(\mathbf{x})$ where T is the kinetic energy operator and $V_i^{\text{trap}}(\mathbf{x})$ is the trapping potential for the ith species,

$$V_i^{\text{trap}}(\mathbf{x}) = \frac{1}{2}M[\omega_{ix}^2 x^2 + \omega_{iy}^2 y^2 + \omega_{iz}^2 (z - z_{i0})^2].$$

In this expression, $\omega_{i\alpha}$ is the trap frequency along axis α for the ith species ($\omega_{ix} = \omega_{iz}$ and $\omega_{2\alpha} = \sqrt{2}\,\omega_{1\alpha}$ in the experiment of Myatt *et al.* [1]) and $z_{i0} = -g/\omega_{iz}^2$ is the displacement of the ith trap center due to the gravitational acceleration g. Note that the single particle *spin*-orbitals are orthogonal since they refer to different hyperfine states; thus, the spatial wave functions $\psi_i(\mathbf{x})$ need not be orthogonal. We have approximated the interatomic interactions as a pseudopotential whose strength is proportional to the s-wave scattering length a_{ij} between an i species atom and a j species atom:

$$U_{ij} = \frac{4\pi\hbar^2 a_{ij}}{M} \qquad (2)$$

with M the mass of ^{87}Rb. This approximation is appropriate at the extremely low collision energies and low densities in the trap [7].

The literature shows disagreement in factors of 2 that multiply the unlike atom interaction terms in Eq. (1): Ho and Shenoy [2] have $1/2$, Ballagh *et al.* [6] have 2, and Graham and Walls [5] have 1, in agreement with our expression. The correct factor can be understood most easily by recognizing that the scattering length a_{12} is calculated for symmetrized two-body wave functions. Thus, it is the symmetric combination of two particle interaction matrix elements $\langle 12|V|12\rangle + \langle 12|V|21\rangle$ that reduces to $U_{12}\int d^3x|\psi_1(\mathbf{x})|^2|\psi_2(\mathbf{x})|^2$ rather than each matrix element separately. In addition, the general expression for U_{ij}, $U_{ij} = 2\pi\hbar^2 a_{ij}/\mu$ where μ is the two-body reduced mass, must be used in order to obtain the correct factor. Errors in this factor of 2 can greatly affect the calculated overlap of the two states and, consequently, can greatly affect such experimentally measurable quantities as the calculated lifetimes of the condensates and their excitation frequencies. We have determined the scattering lengths a_{ij} from a multichannel scattering calculation that is presented in detail elsewhere [8]. Strictly speaking, the scattering length possesses an imaginary part which accounts for inelastic scattering processes. Here, we retain only its real part and assume that the fractional loss of atoms will be minimal over the time scale of the experiment.

We solve Eq. (1) for the fully three-dimensional geometry of the experiment using the method of steepest descents [9] which amounts to propagating the time-dependent version of Eq. (1) in imaginary time. In other words, we replace ε_i in Eq. (1) by $\partial/\partial\tau$ and solve for the normalized orbital $\psi_i(\mathbf{x}) = \psi_i(\mathbf{x}, \tau \to \infty)$ where $\tau = it$. With these solutions, all zero temperature condensate properties of interest can be calculated. Further, we can use these solutions as the initial state for the time-dependent version of Eq. (1) [replace ε_i in Eq. (1) by $i\hbar\partial/\partial t$] without the trapping potentials to simulate the expansion of the condensates necessary in experiment to perform measurements.

We show in Fig. 1 the single particle probability densities $|\psi_i(\mathbf{x})|^2$ for $N_1 = N_2 = 10^5$ and $\nu_{2x} = \nu_{2z} = 400$ Hz, $\nu_{2y} = 11$ Hz, corresponding to the JILA baseball trap in which overlapping condensates have recently been observed [1]. Note that we have chosen the z direction to be parallel to gravity. Approximately 1.5 μm of the distance between the centers of the states along the z axis is due to gravitationally induced sag; the remaining 0.5 μm arises from the repulsive interaction U_{12} between the atoms in the two condensates. We have adjusted the ^{87}Rb singlet potential such that its scattering length is 89.3 a.u. which, in turn, fixes two of the three scattering lengths in Eq. (2) to $a_{11} = 108.8$ a.u. and $a_{12} = 108.0$ a.u.—the third scattering length a_{22} is purely triplet in character and has the value 109.1(10) a.u. [8,10]. With this choice, we calculate a spin exchange decay rate (the rate at which atoms are lost from the trap due to inelastic collisions between atoms in different spin states) of 2.15×10^{-14} cm^3/s which is consistent with the measured value of $2.2(9) \times 10^{-14}$ cm^3/s [1]. Arbitrarily varying the unknown singlet scattering length changes the calculated spin exchange rate by 4 orders of magnitude *via* a remarkable suppression mechanism [8]; its variation within the limits set by the experimental rate, however, amounts to no more than a 2% change in either a_{11} or a_{12}.

Figure 1 shows how the more tightly confined $|2,2\rangle$ state pushes the $|1,-1\rangle$ state out of its way. Further, for this value of a_{12}, the overlap between the two condensates, as measured by $\int d^3x|\psi_1|^2|\psi_2|^2$, is an order of magnitude smaller than either $\int d^3x|\psi_1|^4$ or $\int d^3x|\psi_2|^4$. These quantities, when multiplied by N $(= N_1 = N_2)$ and the appropriate rate constant, can be used to estimate the lifetime of the condensate assuming exponential decay. The overlap of the states shown in Fig. 1 leads to a lifetime of 6 s for each condensate if spin exchange were the only loss mechanism. We emphasize that the Thomas-Fermi approximation badly underestimates this overlap, yielding instead an inflated lifetime of 450 s.

In reality, spin exchange competes with other loss processes such as dipolar relaxation (the dominant inelastic two-body loss process for like atoms) and three-body recombination. For the conditions of Fig. 1 relevant to the recent JILA experiment [1], the lifetimes due to dipolar

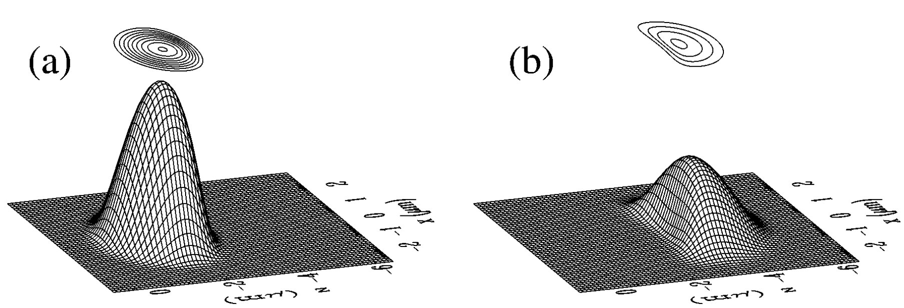

FIG. 1. The single particle densities $|\psi_i(\mathbf{x})|^2$ in the $y = 0$ plane: (a) $|2,2\rangle$ and (b) $|1,-1\rangle$, shown separately for clarity. Note that the z axis increases from right to left. The $|2,2\rangle$ is more tightly confined and is therefore closer to the nominal trap center, $z = 0$.

loss alone are 2 and 16 s for the $|2,2\rangle$ and $|1,-1\rangle$ states, respectively, assuming dipolar loss rates of 3×10^{-15} cm^3/s for the $|2,2\rangle$ state and 6×10^{-16} cm^3/s for the $|1,-1\rangle$ state [11]. If we further assume a three-body recombination loss rate of 4×10^{-30} cm^6/s [12] and consider only collisions between like atoms, then the lifetimes due to this process alone are 8 and 19 s for the $|2,2\rangle$ and $|1,-1\rangle$ states, respectively. The density factors weighting the rates for three-body recombination between *unlike* atoms are smaller by a factor of at least 30 and so can effect only a 10% decrease in these estimates assuming the rates are comparable to the like atom recombination rate. We have, then, the interesting situation in which the lifetime of each species is limited by a different process although the dominance of each particular mechanism is not overwhelming.

Figure 2(a) shows our calculated single particle energies for each hyperfine state and also the result in the noninteracting limit $a_{12} \to 0$ [9,13,14]. The effectively repulsive interspecies interaction boosts the single particle energies above their noninteracting limit as can be seen in Fig. 2(a). Figure 2(b) shows the expectation value of z for each hyperfine state as a function of particle number. The behavior is qualitatively as expected: for smaller numbers of atoms, the values nearly coincide with the gravity displaced trap centers, while for larger numbers of atoms the mutual repulsion of the atoms in each hyperfine state forces the condensates farther apart. The separation of the condensates cannot currently be measured directly, but their separation after some period of expansion can be measured. We can thus compare the separation after 20 ms for our time-dependent solution of Eq. (1), 60 μm, with the experimental result of 70–80 μm [15].

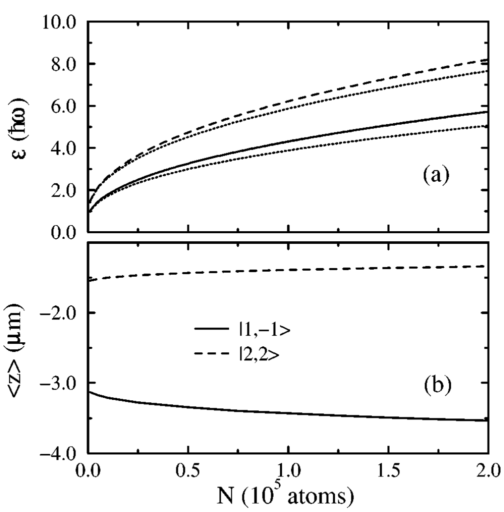

FIG. 2. (a) The single particle energies as a function of $N = N_1 = N_2$. (b) The expectation value of z for each cloud. In both (a) and (b), the solid lines correspond to the $|1,-1\rangle$ state; and the dashed lines, to the $|2,2\rangle$ state. In (a), the dotted lines are the single particle energies for noninteracting ($a_{12} = 0$) condensates.

In addition to the above example directly relevant to ^{87}Rb experiments, other values of scattering lengths—which can be realized for other atoms—can provide insight into qualitatively different experiments. The behavior of the two condensates as a function of a_{12} is particularly interesting given the predicted instability of single condensates for negative scattering lengths within the mean field approximation. For double condensates with positive a_{11} and a_{22} one can calculate within the Thomas-Fermi approximation, which neglects the kinetic energy in Eq. (1), a critical value of $|a_{12}|$ above which the condensates cannot coexist [3,4],

$$|a_{12}^c| = \left(\frac{N_1 - 1}{N_1}\,\frac{N_2 - 1}{N_2}a_{11}a_{22}\right)^{1/2} \approx \sqrt{a_{11}a_{22}}\,.$$

For $a_{12} \leq -a_{12}^c$, the attraction between the condensates overwhelms the repulsive interactions within each condensate, causing their collapse; for $a_{12} \geq +a_{12}^c$, the mutual repulsion of the two condensates dominates, and the two condensates no longer overlap at all within the Thomas-Fermi approximation. It is interesting to note that this critical behavior also manifests itself in the more complete Hartree-Fock solutions. Of course, with the kinetic energy retained in the coupled equations, the condensates still overlap by a nonzero but negligible amount for $a_{12} \geq +a_{12}^c$. The single particle energies, for instance, exhibit this critical behavior. Near $-a_{12}^c$, they decrease rapidly as the mean field each "sees" due to the other deepens in accordance with the increasing dominance of the interspecies attraction relative to same species repulsion. At $+a_{12}^c$, the energies approach equilibrium values since the overlap decreases with further increases in a_{12} at such a rate as to keep the interaction energy essentially constant.

In Fig. 3, we show the expectation value of z for each species as a function of a_{12}, and in Fig. 4, we show the lifetimes due to dipolar loss and spin exchange processes also as a function of a_{12}. We have set $N_1 = N_2 = 10^5$ atoms, $a_{11} = 108.8$ a.u., and $a_{22} = 109.1$ a.u. (which

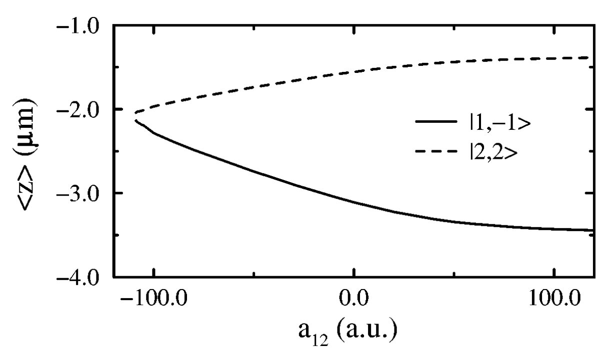

FIG. 3. The expectation value of z for each hyperfine state as a function of a_{12} for $N_1 = N_2 = 10^5$ atoms. The solid line corresponds to the $|1,-1\rangle$ state; and the dashed line, to the $|2,2\rangle$ state.

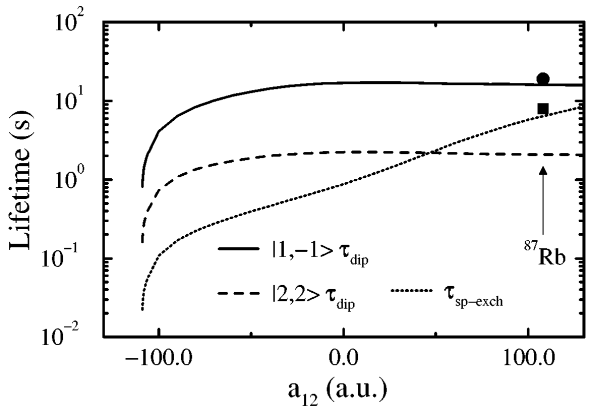

FIG. 4. The lifetimes due to dipolar relaxation, $\tau_{\rm dip}$, and spin exchange, $\tau_{\rm sp\text{-}exch}$, as a function of a_{12} for $N_1 = N_2 = 10^5$ atoms. The thick solid line corresponds to the dipolar relaxation lifetime of the $|1,-1\rangle$ state; and the dashed line, to the $|2,2\rangle$ state. The dotted line represents the spin exchange lifetime of either species. The arrow marks the calculated value of a_{12} for ^{87}Rb, and the solid square and circle mark the lifetimes due to three-body recombination for this value of a_{12} for the $|2,2\rangle$ and $|1,-1\rangle$ states, respectively.

gives $a_{12}^c = 109.0$ a.u.). We see that at $-a_{12}^c$, the attraction has pulled the center of the condensates together, greatly increasing their density overlap so that the spin exchange lifetime has shrunk to tens of milliseconds while the dipolar lifetime of each species remains on the order of seconds. As a_{12} increases, the condensates move farther from each other and live longer. Finally, at $+a_{12}^c$, the mean field has reached its maximum effectiveness, and the condensate centers are essentially stationary with respect to further increases in a_{12}. At the same time, the lifetimes have increased for both states with dipolar losses dominating the $|2,2\rangle$ lifetime and spin exchange dominating the $|1,-1\rangle$ lifetime. The physical value of the scattering length $a_{12} = 108.0$ a.u. is quite near the critical value and is indicated in Fig. 4. The 2% variations in a_{12} possible due to the uncertainty in the ^{87}Rb singlet scattering length will not affect these conclusions.

In summary, we have reported the first realistic calculations for a double condensate experiment like the one reproted in Ref. [1]. We have found the Thomas-Fermi solutions to be unable to represent the condensates' overlap adequately even though they predict many other quantities such as the single particle energies and the positions of the clouds to within better than 10% of the Hartree-Fock values. It follows that quantities that depend critically on the overlap such as excitations of the condensate [5] must be studied within the Hartree-Fock (or better) approximation. Such a study is currently underway [16]. We finally remark that condensate profiles like those shown in Fig. 1 are not directly observed at present. Preliminary studies of the double condensates' expansion suggest, however, that these distinctive profiles may be observable in expanded clouds [17].

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