Prospects for Mixed-Isotope Bose-Einstein Condensates in Rubidium

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We calculate binary collision parameters for mixtures of ultracold gases of ^{85}Rb and ^{87}Rb atoms. We predict a large positive triplet scattering length for mixed-isotope collisions, which implies that a stable mixed-isotope double condensate can be formed by sympathetic evaporative cooling. Moreover, collisions between ^{85}Rb and ^{87}Rb atoms in the lowest hyperfine manifold exhibit magnetic-field-induced Feshbach resonances which should allow partial control of the interaction between condensates. These considerations make Rb an ideal system for the study of *interpenetrating* bosonic superfluids. [S0031-9007(98)05522-7]

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For over two years, the properties of Bose-Einstein condensates (BEC) of dilute gases of alkali atoms have unfolded in a series of experiments. These experiments have probed the most basic properties of BEC, such as its transition temperature, condensate fraction [1], coherence [2], and low-lying collective excitation spectrum in its magnetic trap environment [3]. Also of interest have been studies of ^{7}Li condensates, whose negative s-wave scattering length implies instability for sufficiently large numbers of condensed atoms [4]. More recently, a new experimental possibility has emerged with the simultaneous production at JILA of a *pair* of condensates in the same trap, each in a different spin state of ^{87}Rb [5]. This intriguing experiment opens the possibility for observing the interaction between different condensates in the controlled environment of the magnetic atom trap.

The properties and stability of such double condensates have been of long-standing interest [6,7], revived recently by the atomic experiments [8]. An early proposal along these lines [7] considered ^{4}He-^{6}He mixtures, finding them untenable owing to the exceedingly low concentration of ^{6}He in ^{4}He. Our purpose in this Letter is to demonstrate that ^{87}Rb and ^{85}Rb atoms have suitable collision properties to make their double condensates both experimentally feasible and phenomenologically rich. Specifically, we identify collisions that afford (1) large elastic cross sections that favor the production of double condensates by evaporative cooling, (2) small inelastic rate coefficients that guarantee the condensates live long enough to be created and probed, and (3) an interspecies interaction that can be tuned by applying an external magnetic field.

We begin by reviewing the available spin states of the stable Rb isotopes. ^{87}Rb has a nuclear spin $i = \frac{3}{2}$, implying that its total spin $\vec{f} = \vec{i} + \vec{s}$ (nuclear plus electronic) can be in either the $f = 2$ or $f = 1$ state. These spin states diagonalize the atomic hyperfine interaction and are denoted as $|fm\rangle_{87}$. For ^{85}Rb, with nuclear spin $i = \frac{5}{2}$, the total spin can be either $f = 3$ or $f = 2$. Typical experiments trap atoms in a weak-field-seeking Zeeman sublevel of a particular hyperfine manifold such that $|m| = f$. For example, the majority of trapped ^{87}Rb atoms would be in either the upper manifold $|2,2\rangle_{87}$ or the lower manifold $|1,-1\rangle_{87}$ hyperfine state; the analogous states are $|3,3\rangle_{85}$ or $|2,-2\rangle_{85}$ for ^{85}Rb. We therefore focus only on these hyperfine states.

The collision properties hinge on accurate Born-Oppenheimer potential curves for the singlet $^1\Sigma_g^+$ and triplet $^3\Sigma_u^+$ diatomic states. The singlet potential was extracted in [9] from spectroscopic data, while the triplet potential was calculated in [10] by an *ab initio* method. These short-range potentials are joined onto long-range dispersion [11,12] and exchange [13] potentials, and suitably adjusted so that their near-threshold phase shifts are consistent with recent experimental determinations [5,12]. These constraints, along with their uncertainties, translate into a "most probable" range of scattering lengths as given in Table I. The largest source of uncertainties for the scattering lengths in Table I is due to incomplete information on the short-range $^3\Sigma_u^+$ potential. Adding the atomic hyperfine interaction, the spin-spin dipole interaction, and the second order spin-orbit interaction produces a realistic set of coupled molecular potentials. We use the second order spin-orbit term derived in the Mies *et al.* [14] *ab initio* calculation.

The molecular potentials are then transformed into a representation that diagonalizes the atomic hyperfine interaction; this representation is best suited for the limit of large interatomic separation R. The effect of the harmonic trapping magnetic field is negligible over

TABLE I. Range of singlet a_s and triplet a_t scattering lengths (in a.u.) for the different Rb isotopes given by our most probable Born-Oppenheimer potentials.

Isotope	a_t	a_s
^{87}Rb	101−108	95−104
^{85}Rb	−315−−520	−600−−4000
Mixed isotope	200−220	15−28

the length scale of an atomic collision. However, the magnetic field at the center of the trap can be nonzero. In calculations that also assess the influence of this bias field, the chosen representation diagonalizes the combined hyperfine plus magnetic field Hamiltonian at $R \to \infty$. The resulting coupled channel Schrödinger equations are then solved by a multichannel finite-element [15] R-matrix method [16] that gives the desired scattering matrix.

Table I gives a general indication of the types of double condensates to be expected in the mixed-isotope gases. Namely, a colliding pair of ^{87}Rb atoms has a positive s-wave scattering length a defined in terms of the elastic scattering phase shift δ as $a = \lim_{k\to 0} -\frac{\tan\delta}{k}$, where $k = \sqrt{2\mu E}$, μ is the reduced mass of the collision pair, and E is the relative collision energy. A positive scattering length implies an effective repulsive interaction between atoms and, in turn, a stable condensate. On the other hand, a colliding pair of ^{85}Rb atoms has a large negative scattering length, regardless of the detailed hyperfine states involved; this implies that the atoms exhibit a net effective attraction and that the ^{85}Rb condensate should be unstable for more than a certain critical number of atoms. Hartree-Fock calculations, based upon the weakest JILA baseball trap parameters $6 \times 12 \times 12$ Hz, have shown that this critical number is on the order of 90 atoms. Such a low number challenges the experimentalists severely, but the detection of a 90 atom condensate has been deemed feasible [17]. In addition, the Feshbach resonances predicted in a collision between two $|2,-2\rangle_{85}$ ^{85}Rb atoms [18] could, in principle, be used to produce a stable condensate with larger numbers of ^{85}Rb atoms. In the mixed-isotope collision, we again find a positive scattering length, and hence a repulsive interaction. We show below that for lower hyperfine manifold collisions the mixed-isotope scattering length should be a tunable function of applied magnetic field strength, so that various experimental scenarios might be explored.

The first issue facing the production of double condensates is whether the two species can be simultaneously evaporatively cooled. Figure 1 shows elastic scattering cross sections for the various combinations of Rb isotopes, over the several hundred μK energy range where evaporative cooling takes place. The results shown have been calculated for collisions between atoms in their "stretched" states $|2,2\rangle_{87}$ and $|3,3\rangle_{85}$, where electronic and nuclear spins are completely aligned; however, the other combinations of colliding spins give very similar results. Note that the ^{87}Rb elastic cross section remains uniformly high over the entire energy range; indeed, this is the isotope in which BEC was first produced. By contrast, the ^{85}Rb cross section is some 2 orders of magnitude smaller over much of the range, which will hamper its evaporative cooling. This minimum results from an unfortunately placed zero in the s-wave scattering cross section, also shown in Fig. 1. (This zero is analogous to that found in low-energy electron-atom scattering, where

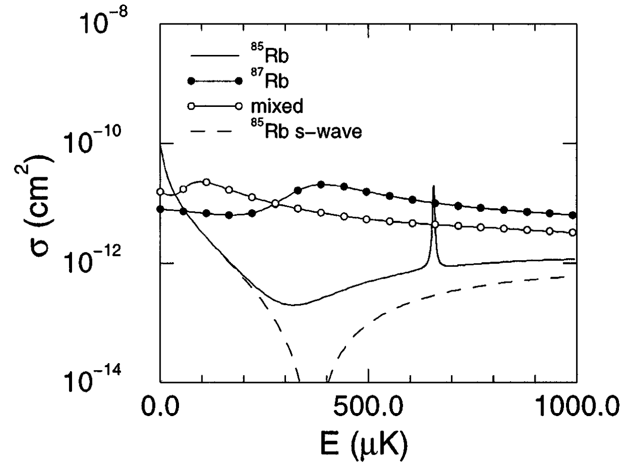

FIG. 1. Elastic cross sections for collisions between a pair of $|3,3\rangle_{85}$ ^{85}Rb atoms, a pair of $|2,2\rangle_{87}$ ^{87}Rb atoms, and a mixed-isotope collision ($|3,3\rangle_{85} + |2,2\rangle_{87}$) in cm^2 as a function of collision energy E. The pure ^{85}Rb collision suffers a suppression in the s-wave partial cross section (dashed line). Note the g-wave shape resonance in the ^{85}Rb cross section at roughly 660 μK and the broad d-wave shape resonance in the ^{87}Rb cross section starting at roughly 200 μK as previously determined [12]. In addition, we find a broad p-wave shape resonance in the mixed-isotope collision cross section starting at roughly 50 μK. The uncertainty in the position of the ^{85}Rb s-wave suppression is ± 30 μK.

it has long been known as the Ramsauer-Townsend effect [19].) The inelastic cross section is not suppressed over the same energy range, and, therefore, using an extremely long evaporative cooling cycle, as in ^{7}Li, would still not necessarily be successful. Figure 1 also illustrates that the mixed-isotope case fares quite well for evaporative cooling, maintaining a high elastic cross section over the energy range shown. It therefore should be possible to evaporatively cool only the one species, ^{87}Rb, and use the thermal contact between the two isotope clouds to cool the ^{85}Rb atoms "sympathetically." This was the method which produced the double condensate of Ref. [5].

In addition to large elastic collision rates, successful evaporative cooling also requires small inelastic rates, so that the atom cloud has a chance to rethermalize before being destroyed by inelastic processes. Typical elastic rate coefficients are of order 10^{-10}–10^{-11} cm^3/s for Rb atoms at sub-mK temperatures; a general rule of thumb requires that inelastic rate coefficients K_e should be about 100 times smaller, at the 10^{-13} cm^3/s level or below. Table II summarizes the $B = 0$ values of K_e for various collision partners. Note that dipole-induced inelastic collisions have a strong magnetic field dependence at low fields $B < 20$ G (see Fig. 2) [20]. For all collision pairs shown in Table II, however, the low-field dipole rates remain acceptable given the above criteria.

In general, collisions between upper and lower manifold hyperfine states suffer large spin-exchange losses. A notable exception is ^{87}Rb, where it has been shown [21]

TABLE II. $B = 0$ inelastic event rate constants K_e, in units of cm^3/s, and scattering lengths a given in a.u. are calculated for an incident energy of 1 μK above threshold. Uncertainties are determined by varying the scattering lengths over the ranges given in Table I and the C_6 coefficient over the range 4450–4650 a.u. [13].

Entrance Channel	K_e	a
^{87}Rb		
$\|2,2\rangle + \|2,2\rangle$	$(2.0-2.1) \times 10^{-16}$	102–107
$\|2,2\rangle + \|1,-1\rangle$	$(0.5-3.5) \times 10^{-14}$	102–107
$\|1,-1\rangle + \|1,-1\rangle$	$(3.1-3.2) \times 10^{-18}$	105–110
^{85}Rb		
$\|3,3\rangle + \|3,3\rangle$	$(0.8-1.4) \times 10^{-14}$	−320−−470
$\|3,3\rangle + \|2,-2\rangle$	$(0.4-5.9) \times 10^{-12}$	−340−−510
$\|2,-2\rangle + \|2,-2\rangle$	$(3.1-3.4) \times 10^{-18}$	−335−−490
Mixed isotope		
$\|3,3\rangle_{85} + \|2,2\rangle_{87}$	$(1.0-1.2) \times 10^{-15}$	201–216
$\|2,-2\rangle_{85} + \|2,2\rangle_{87}$	$(3.3-4.2) \times 10^{-11}$	214–230
$\|3,3\rangle_{85} + \|1,-1\rangle_{87}$	$(1.2-4.5) \times 10^{-12}$	216–247
$\|2,-2\rangle_{85} + \|1,-1\rangle_{87}$	3.4×10^{-18}	230–265

that the near equivalence of singlet and triplet phase shifts produces a suppression in spin-exchange losses. The possibility exists that this is also the case with ^{85}Rb, but experimental uncertainties in the singlet-triplet phase shift difference do not yet allow a conclusive prediction. This ambiguity does not exist with mixed-isotope collisions. The singlet-triplet phase shift difference remains large within the experimental uncertainties and therefore spin-exchange loss rates are quite high (see Table II).

Given the criteria above, the most viable candidates for mixed-isotope condensates are the $|3,3\rangle_{85} + |2,2\rangle_{87}$ and $|2,-2\rangle_{85} + |1,-1\rangle_{87}$ combinations of hyperfine states. Spin-exchange processes are forbidden in both of these combinations, which means loss rates are governed by weaker two- and three-body interactions. Of these two candidates, the most interesting is the $|2,-2\rangle_{85} + |1,-1\rangle_{87}$ combination because the scattering length *between* isotopes can be controlled by applying a magnetic field $\vec{B}$, taking advantage of Feshbach resonances similar to those explored Ref. [18]. The basic idea is that the magnetic field distorts the long-range scattering potentials through the Zeeman interaction. Within the distorted potentials a bound state may become degenerate with the total incident energy of the colliding atom pair. The resonance thus generated can significantly alter the effective interatomic interaction, parametrized by a $\vec{B}$-dependent scattering length. Figure 3 illustrates a pair of these resonances. The scattering length can be tuned from positive to negative by sweeping the applied bias field across the resonance. A variety of double condensates can thus be generated for these species and, in principle, one can produce *interpenetrating* quantum fluids. Note, however, that the inelastic rates often grow quite large at resonant field strengths (see Fig. 2). This would limit the double condensate lifetime for configurations with a large overlap of the respective wave functions. (Figure 2 also shows a rich resonance structure which we will investigate in detail in a subsequent publication.)

These resonances are not ubiquitous, but occur at reasonable fields only for certain pairs of collision partners. For example, an applied bias field can only grow to

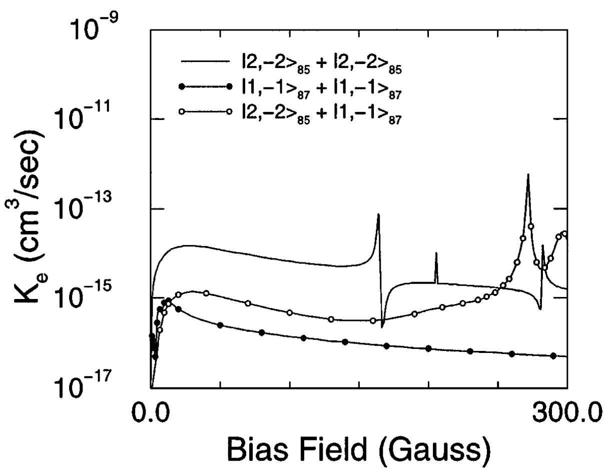

FIG. 2. Magnetic field dependence of the inelastic event rate constant K_e for collisions of atoms in the lowest hyperfine manifold. A collisional energy of 1 μK above threshold was used for the calculation. Narrow resonance features are not mapped in detail. We find agreement within the stated uncertainties with the resonance positions predicted in Ref. [18]. Note that the extremely narrow resonance found at 200 G in that paper is not resolved in this graph. We also find additional narrow resonances associated with dipole coupled channels which are not shown in Ref. [18]. The uncertainties in the positions of the ^{85}Rb resonances are roughly ±20 G and in the mixed-isotope resonance are ±20 G. It should be cautioned that both the line shapes and widths are extremely sensitive to the particular details of the potentials used.

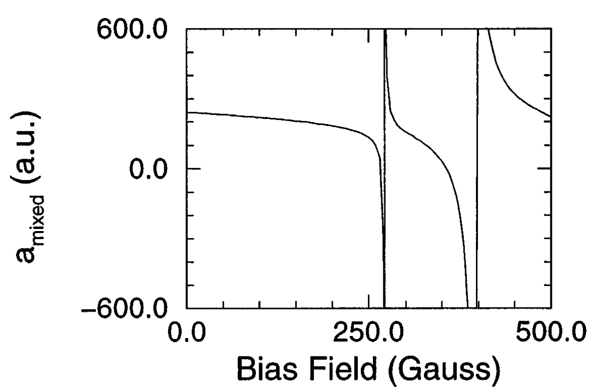

FIG. 3. Magnetic field dependence of the scattering length a_{mixed} for collisions between ^{85}Rb $|2,-2\rangle_{85}$ and ^{87}Rb $|1,-1\rangle_{87}$ atoms. A collisional energy of 1 μK above threshold and nominal values of the singlet ($a_s = 23.7$ a.u.) and triplet ($a_t = 208$ a.u.) scattering lengths were used for the calculations. The uncertainties in the positions of the resonances are 267 ± 20 and 356 ± 30 G.

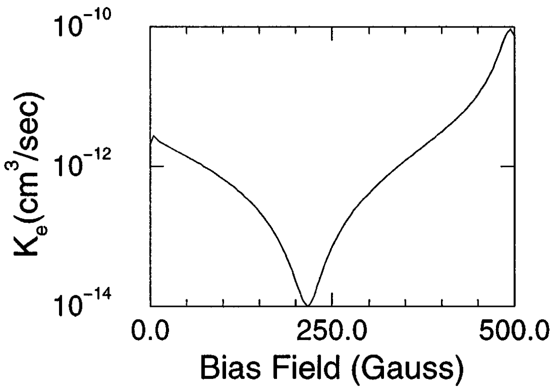

FIG. 4. Magnetic field dependence of the inelastic event rate constant K_e for collisions between ^{85}Rb $|3,3\rangle_{85}$ and ^{87}Rb $|1,-1\rangle_{87}$ atoms. A collisional energy of 1 μK above threshold and nominal values of the singlet ($a_s = 23.7$ a.u.) and triplet ($a_t = 208$ a.u.) scattering lengths were used for the calculations. The graph shows a nonresonant suppression of the rate as well as a dramatic increase in the rate which is due to a Feshbach resonance. The uncertainty in the position of the suppression is approximately 215^{+50}_{-40} G.

$\approx$1200 G before the $|1,-1\rangle_{87}$ spin state becomes untrapped. Below this field value, there are no Feshbach resonances in collisions of the type $|2,2\rangle_{87} + |1,-1\rangle_{87}$. Thus the interaction potential relevant to the original double condensate experiment [5] cannot be tuned in this way. In addition, the mixed-isotope resonances predicted in Li [22] also occur at magnetic field strengths for which the hyperfine states are untrapped.

Finally, Fig. 4 shows the inelastic event rate coefficient for collisions of the type $|1,-1\rangle_{87} + |3,3\rangle_{85}$ versus an applied bias magnetic field. Ordinarily, these two species would eject one another from the trap by spin-exchange processes. In a magnetic field, however, we find a surprising interference between singlet and triplet channel components, similar to that which occurs at zero field in $|2,2\rangle_{87} + |1,-1\rangle_{87}$ collisions [21]. At an applied field strength of $\approx$215 G, the $|1,-1\rangle_{87} + |3,3\rangle_{85}$ inelastic rate plummets by 2 orders of magnitude, implying that these species might then be simultaneously condensed. This destructive interference, which is not associated with any resonance structure, raises the possibility that a *triple* condensate could be formed with the species $|1,-1\rangle_{87}$, $|2,2\rangle_{87}$, and $|3,3\rangle_{85}$.

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