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Prediction of Feshbach resonances in collisions of ultracold rubidium atoms

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On the basis of recently measured Rb_2 bound-state energies and continuum properties, we predict magnetically induced Feshbach resonances in collisions of ultracold rubidium atoms. The resonances make it possible to control the sign and magnitude of the effective particle-particle interaction in a Rb Bose-Einstein condensate by tuning a bias magnetic field. For the case of ^{85}Rb they occur at field values in the range where these atoms can be magnetostatically trapped. For ^{87}Rb they are predicted to occur at negative field values. [S1050-2947(97)50208-3]

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The observation of Bose-Einstein condensation (BEC) in dilute ultracold gas samples of rubidium [1], lithium [2], and sodium atoms [3] has made it possible to study this macroscopic quantum phenomenon in its pure form without complicated modifications due to strong interactions. A variety of experiments has been proposed or already carried out, fascinating examples being the observation of collective shape oscillations and the observation of the relative phase of two Bose-Einstein condensates [4,5]. A rich variety of other experiments would come into reach if one could alter arbitrarily, possibly even in real time, the sign and magnitude of the atom-atom scattering length a. The scattering length occurs as the coefficient of the condensate self-interaction term in the condensate wave equation and has a profound effect on the stability and other properties of the condensate. An opportunity to change this parameter would arise if it were possible to tune the scattering length by means of external fields, i.e., either a static magnetic field [6] or a time-dependent optical [7] or rf field [8].

A situation where a can be changed between positive and negative values either through 0 or $\pm\infty$ by tuning a dc magnetic field is that of a Feshbach-type resonance between the initial two-atom continuum state and a quasibound molecular state at a common value of the energy [9]. Due to their different spin structures these states have different g factors, so that the continuum and bound-state energies can be tuned into resonance at specific values of B. If we can find a resonance at a field value for which the atoms can be magnetostatically trapped, the above situation of a tunable scattering length should be readily achievable experimentally. In particular, changing the sign of a from positive to negative would turn a stable condensate into a collapsing unstable one, the time development of which can be studied. A variety of other experiments would become possible too. For instance, a could be changed on the time scale of the resonance lifetime, or the particle interaction could be made repulsive in one part of space and attractive in another.

Rubidium atoms were the first atomic species for which BEC was realized. The purpose of this paper is to point out that they may also be the atomic species for which B-field tuning of the scattering length is first achieved. For rubidium atoms the information available on the atom-atom interaction has long been insufficient for a prediction of the kind we envisage. This situation has drastically changed by the observation of two coexisting ^{87}Rb condensates [10] and by the results of a two-color photoassociation (PA) experiment on a cold ^{85}Rb gas sample [11]. In the latter experiment the last 20 GHz of bound levels in the lowest molecular singlet and triplet states were measured, allowing us to precisely determine a complete set of Rb_2 interaction parameters.

Before these developments, important information on the low-energy triplet ($S=1$) collisional wave function had been obtained from cold-atom photoassociation work in our two groups on rubidium atoms, leading to the observation of its node structure [12] and the observation of shape resonances [13,14]. Due to the hyperfine interaction, pure singlet incident collision channels do not exist. As a consequence, information on the singlet interaction properties can only be obtained by studying mixed singlet-triplet collision channels. Very useful, but still insufficient, information of this kind came available [15] via a measurement of the absolute value of the scattering length $a_{1,-1}$ for elastic collisions of cold ^{87}Rb atoms in the $|f,m_f\rangle=|1,-1\rangle$ hyperfine state (see Fig. 1 for the ground-state hyperfine diagrams of ^{87}Rb and ^{85}Rb). As pointed out above, very important additional information came from the recent observation of overlapping $|2,2\rangle$ and $|1,-1\rangle$ Bose-Einstein condensates [10]. Three groups have independently pointed out that the extremely small rate con-

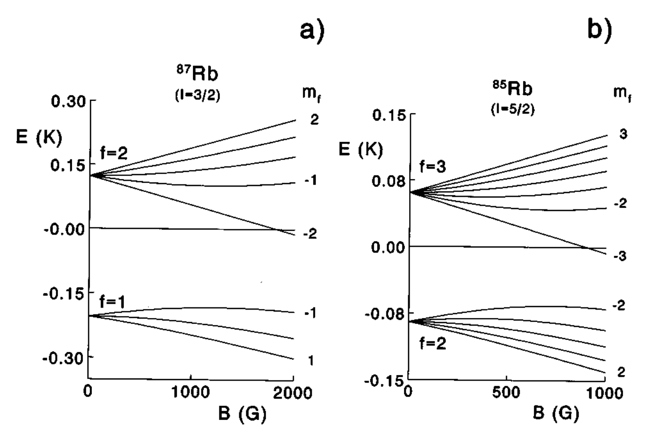

FIG. 1. Hyperfine diagrams for the electronic ground state of (a) ^{87}Rb, (b) ^{85}Rb.

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stant $G_{(2,2)+(1,-1)}$ for decay due to collisions between atoms in the two different states, implied by the stability of the double Bose condensates, should be a strongly constraining factor in the determination of the remaining cold collision properties [16–18]. In the following we will show that this and all other available $^{85}Rb+^{85}Rb$ and $^{87}Rb+^{87}Rb$ cold-collision observations fit into a consistent picture, which can be derived from the bound states of the two-color PA experiment [11]. This allows us to make a reliable and accurate prediction of Feshbach resonances.

In order to calculate bound or continuum state wave functions, we write the Rb_2 long-range interaction potentials in the form

$$V_S(r) = -C_6/r^6 - C_8/r^8 - C_{10}/r^{10} + V_{exch}, \qquad (1)$$

with the exchange part taken from Smirnov and Chibisov [19], the dispersion coefficients C_8 and C_{10} from a calculation by Marinescu *et al.* [20], and C_6 from previous photoassociation work [14]. We do not need the full information on the short-range singlet ($S=0$) and triplet ($S=1$) interaction potentials. Rather, this information is summarized in a boundary condition on the $S=0$ and $S=1$ radial wave functions at the interatomic distance $r=r_0=20a_0$, on the basis of which Schrödinger's equation is solved for $r>r_0$. The boundary condition takes the form of a specific choice of the phases ϕ_S, ϕ_T of the oscillating singlet and triplet radial wave functions in a small region of energy E and interatomic angular momentum l near $E=l=0$ [21]. This phase information was extracted from an analysis of the energies of the highest $^{85}Rb_2$ bound states [11] and of the g-wave shape resonance observed in Ref. [14]. We also used available information on the total number of Rb_2 singlet and triplet bound states in this analysis [22,23,14].

With the parameters thus determined we can calculate the continuum quantities of interest. For the $^{85}Rb+^{85}Rb$ triplet and singlet scattering lengths, we find [11] $a_T(^{85}Rb)=-440\pm140a_0$ [corresponding fractional s-wave vibrational quantum number v_D at dissociation (modulo 1)=0.95 ±0.01] and $+4500a_0<a_S(^{85}Rb)<+\infty$ or $-\infty<a_S(^{85}Rb)<-1200a_0$ ($v_D=122.994\pm0.012$). A coupled-channel calculation allows us to predict a value for the scattering length of a pair of ^{85}Rb atoms in the $|2,-2\rangle$ state. We find $a_{2,-2}(B=0)=-450\pm140a_0$. Mass scaling the phases to ^{87}Rb enables us to predict bound-state and ultracold scattering properties for this isotope too, in particular the mixed hyperfine decay rate constant $G_{(2,2)+(1,-1)}$. In this mass-scaling transformation we correct for the different local de Broglie wavelengths, multiplying $\phi_{S/T}(E,l)$ by a square root of the atomic mass ratio and taking into account the total phase change from the inner turning point to r_0. We find excellent agreement between the bound-state and continuum properties. As an illustration, Fig. 2 shows the calculated $G_{(2,2)+(1,-1)}$ as a function of the ^{87}Rb singlet scattering length, which corresponds directly with the singlet phase. The two-sided arrow indicates the maximum a_S range $\pm5a_0$ obtained from the two-color PA bound-state energies, including the uncertainty in the dispersion coefficients. The position of the G curve along the a_S axis is uncertain by $\pm6a_0$, with the error bar $\pm3a_0$ due to the uncertainty in the number of bound triplet states (38 ± 1 for $^{85}Rb_2$ [14]) as an important contribution. Clearly, there is a preference for the a_S interval along the right-hand slope of the G minimum. Good agreement is obtained between the calculated and measured rate constant (range between horizontal lines) with the *same* set of parameters determined above.

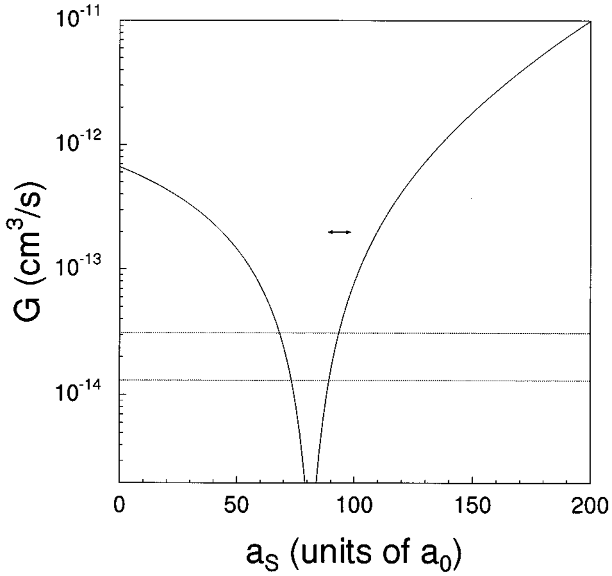

FIG. 2. Rate constant $G_{(2,2)+(1,-1)}$ for decay due to collisions between ^{87}Rb atoms in different hyperfine states as a function of the singlet scattering length. The horizontal lines indicate the experimental range. The two-sided arrow indicates the a_S range following from the two-color PA experiment.

On the basis of this consistency we are now able to predict the field-dependent scattering lengths for a further comparison with experiment and to search for Feshbach resonances. Figure 3 shows the calculated B dependence of

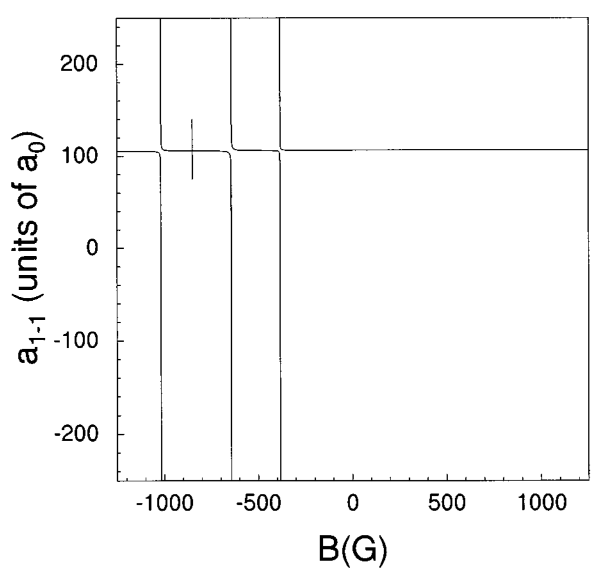

FIG. 3. Predicted field-dependent scattering length for collisions of ^{87}Rb atoms in $|1,-1\rangle$ state. Three broad Feshbach resonances occur for negative fields at 383, 643, and 1018 G. A narrow resonance occurs at 850 G.

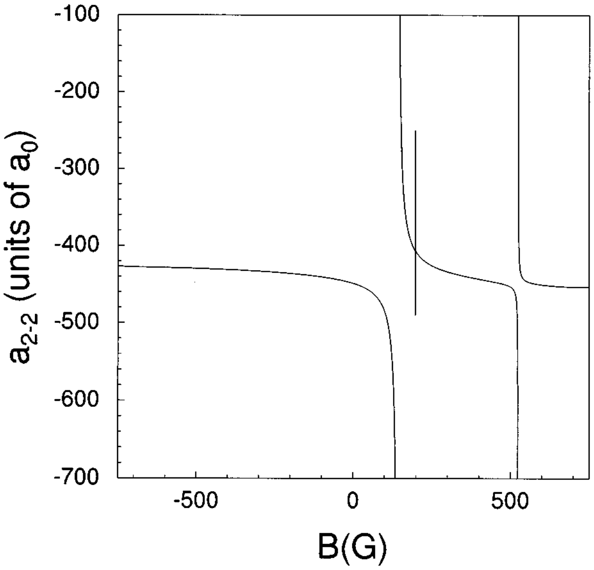

FIG. 4. Predicted field-dependent scattering length for collisions of ^{85}Rb atoms in the $|2,-2\rangle$ state. Two broad Feshbach resonances occur in the weak-field seeking range at 142 and 524 G, and a narrow one at 198 G.

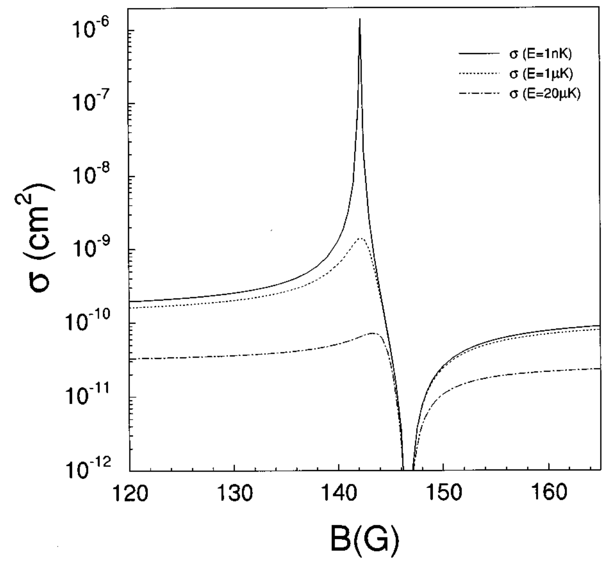

FIG. 5. Resonance structure of the elastic cross section in the ^{85}Rb $|2,-2\rangle+|2,-2\rangle$ channel as a function of B for three collision energies. For each energy σ increases from a background value to the quantum limit $8\pi/k^2$, then decreases to 0, and finally returns to background value.

$a_{1,-1}$ for ^{87}Rb in the range $-B_0<B<B_0$, where B_0 is the maximum field for which an atom in the $|f=i-\frac{1}{2}, m_f=-(i-\frac{1}{2})\rangle$ hyperfine state, with i the nuclear spin, is weak-field seeking and thus trappable. The figure is extrapolated to negative fields to include collisions of ultracold $|1,+1\rangle$ atoms [24]. Note that reversing the field direction for constant m_f is equivalent to reversing m_f for a fixed field. Four Feshbach resonances are found at negative field values (383, 643, 850, and 1018 G) and none at positive fields smaller than 1250 G. The latter as well as the flat B dependence in this range are consistent with the results of Newbury *et al.* [15], in particular with the absence of Feshbach resonances with magnetic field width $\geqslant 2$ G over the field range 15–540 G. Also, the calculated $a_{1,-1}$ value 106 $\pm 6a_0$ in this range agrees with the measured absolute magnitude $87\pm 21a_0$. We find $a_{1,-1}$ to be positive, in agreement with the apparent stability of a large condensate of ^{87}Rb $|1,-1\rangle$ atoms [10,15]. The occurrence of Feshbach resonances at negative fields is also consistent with the field dependence of the highest $^{87}Rb_2$ s-wave bound-state energies, calculated by means of our coupled-channels method. The threshold of the elastic $|1,-1\rangle+|1,-1\rangle$ collision channel intersects with bound-state energy curves at four negative B values, which agree with the four values given above.

Figure 4 shows similar results for ^{85}Rb. This time we find two broad Feshbach resonances at positive fields 142 and 524 G, and a very narrow one at 198 G, all three in the weak-field-seeking B range. From the shape of the excursions through $\pm\infty$ it appears that the resonances are due to molecular states crossing the threshold of the incoming channel from above with increasing B. Again this is consistent with a calculation of coupled-channels bound-state energies. An interesting phenomenon in both Figs. 3 and 4 is the occurrence of a very narrow resonance. It arises from a molecular state with the electronic spins and the nuclear spins adding up to the maximum possible F value at $B=0$. Their narrow width is due to the selection rule $\Delta F=0$, by which the transition from the incoming channel with F lower by 2 can only take place via the Zeeman interaction in second order.

We finally give the values of the singlet and triplet scattering lengths deduced in the analysis, including error bars on the various experimental and theoretical input parameters. We find: $a_T(^{87}\mathrm{Rb})=102\pm 6a_0$ and $a_S(^{87}\mathrm{Rb})=93\pm 5a_0$. We also find that the predicted field positions of the Feshbach resonances are reliable to within about 10 G for ^{85}Rb and 40 G for ^{87}Rb. To give an impression of the resonance behavior to be expected for $^{85}\mathrm{Rb}+{}^{85}\mathrm{Rb}$ scattering, Fig. 5 shows the elastic cross section for three collision energies as a function of B in the range of the first resonance at 142 G. For the lowest energies the background value is almost equal to $8\pi a_{2,-2}^2$. For each energy σ increases to the quantum limit $8\pi/k^2$ close to the resonance field value and subsequently decreases to 0 before returning to the background value. Apparently, although the maximum gradually disappears with increasing energy, the resonance shape is sufficiently pronounced to be observable in an experiment similar to that of Ref. [15].

An important conclusion of our work is that we can account for all presently known properties of Rb_2 bound and continuum states with a single set of parameters. These include the triplet scattering lengths from earlier experiments [13,14], the highest bound $^{85}Rb_2$ states measured in the two-color PA experiment [11], the double condensate stability [10], the measured scattering length $a_{1,-1}(^{87}\mathrm{Rb})$, and the absence of resonances in that quantity wider than 2 G in the range 15–540 G [15]. This enables us to deduce scattering lengths and positions of Feshbach resonances. The prediction of such resonances in an interesting field range should be readily verifiable experimentally. If confirmed, they will give rise to a variety of fascinating possibilities for studying Bose condensates.

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