

# Properties of cold collisions of 39K atoms and of 41K atoms in relation to Bose-Einstein condensation

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## Properties of cold collisions of $^{39}\text{K}$ atoms and of $^{41}\text{K}$ atoms in relation to Bose-Einstein condensation

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We have determined properties of cold  $^{39}\text{K}+^{39}\text{K}$  and  $^{41}\text{K}+^{41}\text{K}$  collisions by a multichannel inverted perturbation approach applied to spectroscopic data of highly excited  $^{39}\text{K}$  singlet and triplet bound states. We predict positive scattering lengths for the  $^{39}\text{K}+^{39}\text{K}$  and  $^{41}\text{K}+^{41}\text{K}$  singlet potentials, as well as for the  $^{41}\text{K}+^{41}\text{K}$  triplet potential, and a negative value for  $^{39}\text{K}+^{39}\text{K}$  triplet scattering. From a study of the magnetic field dependence we conclude that  $^{41}\text{K}$  may be a bosonic atom with a Feshbach resonance in the magnetic field range where these atoms can be trapped in the  $f=1$ ,  $m_f=-1$  hyperfine state, thus providing a possibility to switch between stable and instable condensates in a Bose-Einstein condensation experiment. [S1050-2947(96)50211-8]

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The recent observation of Bose-Einstein condensation (BEC) in weakly interacting atomic gases of rubidium [1], lithium [2], and sodium [3] is an important step towards a more fundamental understanding of superfluidity and superconductivity in strongly interacting systems. A fascinating aspect of a Bose condensate in a dilute ultracold atomic gas is that its behavior is completely determined by one parameter only, the scattering length  $a$ , in contrast to the more complex systems. Recent work [4–6] shows that indeed various properties of a Bose condensate can be very well described by a nonlinear Schrödinger equation that contains  $a$  as a single parameter. In particular, it determines the stability of the condensate [7,8], a positive sign implying a stable and a negative sign an instable condensate [9]. The value of the scattering length is also a key ingredient of present methods to prepare the condensed phase, a large value being needed for efficient evaporative cooling [10]. Finally, two-body scattering properties play a crucial role also in other cold-atom experiments, for instance those dealing with laser-cooled atomic clocks [11].

In all successful BEC experiments thus far a cloud of atoms is trapped in a static magnetic field. In this kind of setup atoms can only be trapped for a reasonable time (larger than 1 s, for instance), when prepared in a specific hyperfine state. Figure 1 shows the ground-state hyperfine diagram for  $^{39}\text{K}$  and  $^{41}\text{K}$ , including the two states that are promising for observing BEC. The first of these is the  $f=2$ ,  $m_f=+2$  state with fully stretched electronic and nuclear spins, the second one is the highest state ( $f=1$ ,  $m_f=-1$ ) of the lower hyperfine manifold, trappable for  $B < B_0 = \frac{1}{2}a_{hf}/\mu_B$ , with  $a_{hf}$  the atomic hyperfine constant and  $\mu_B$  the Bohr magneton. An interesting aspect of atoms colliding in the  $f=1$ ,  $m_f=-1$  hyperfine state is the possibility to effect a large change of the scattering length by varying the magnetic field, if a Feshbach-type resonance shows up in the collision process. Changing the field would enable one to directly control the magnitude and sign of the scattering length and thus the stability properties and dynamical behavior of the condensate [8]. Changing the sign of  $a$  as a function of time by variations of  $B$ , for instance, would offer possibilities for

fascinating new experiments. Thus far theoretical predictions have been made for the locations of Feshbach resonances for  $^7\text{Li}$  and  $^{23}\text{Na}$  [12] with reliable interaction potentials and for  $^{133}\text{Cs}$  [13] with a less reliable interaction potential. Unfortunately, in  $^7\text{Li}$  and  $^{23}\text{Na}$  no resonances occur in the field regime where atoms can be trapped, while in the case of  $^{133}\text{Cs}$  the interaction potential is too uncertain to definitely predict the locations of resonances.

Remarkably little has been published so far about the cold collision properties of K atoms. This is surprising because this element has the attractive feature of having the two above-mentioned stable bosonic isotopes, as well as an almost stable fermionic isotope  $^{40}\text{K}$ . In this paper we present a multichannel inverted perturbation approach of a combined set of singlet and triplet  $^{39}\text{K}$  bound states, including their coupling by the hyperfine interaction, that enables us to determine the  $C_6$  dispersion coefficient, exchange interaction parameters, and scattering lengths. A simple mass-scaling rule subsequently enables us to derive the corresponding scattering properties of  $^{41}\text{K}$ . Finally, we have used these potentials to predict the magnetic-field dependence of the scattering process of two  $^{39}\text{K}$  and two  $^{41}\text{K}$  atoms in the  $f=1$ ,  $m_f=-1$  hyperfine state.

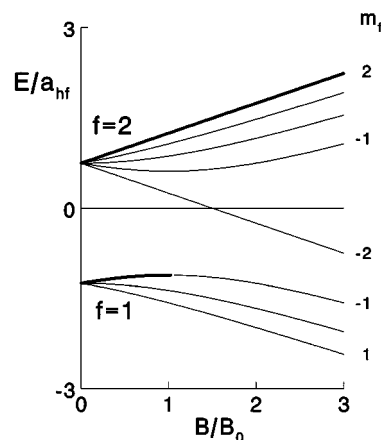


FIG. 1. Ground-state hyperfine diagram for  $^{39}\text{K}$  ( $B_0=82.4$  G,  $a_{hf}=11.079$  mK) and  $^{41}\text{K}$  ( $B_0=45.3$  G,  $a_{hf}=6.097$  mK). Trapable states are indicated by bold lines.

The long-range singlet ( $S=0$ ) and triplet ( $S=1$ ) interaction potentials between two K atoms are written as

$$V_S(r) = -C_6/r^6 - C_8/r^8 - C_{10}/r^{10} - (-1)^S A e^{-\alpha r}, \quad (1)$$

with dispersion coefficients  $C_n$  and exchange parameters  $A, \alpha$ . We select an interatomic distance  $r_0$  as far out as possible, such that inside  $r_0$  the energy separation between the  $S=0$  and  $S=1$  potentials is large enough for the singlet-triplet mixing by the hyperfine interaction to be negligible [12]. This enables us to summarize the entire  $r < r_0$  part of the interaction potentials in terms of accumulated phases  $\phi_S, \phi_T$  of the oscillating singlet and triplet radial wave functions, which serve as a boundary condition for Schrödinger's equation in the range  $r > r_0$ .

We start by improving the inner part of the singlet potential, determined by Amiot, Vergès, and Fellows [14], by a standard uncoupled inverted perturbation approach [15], making use of a code developed by Moerdijk *et al.* [12]. We use measured energy differences of levels up to and including  $v=74$  with outer turning points up to  $18.2a_0$ . This yields a potential reproducing the measured bound-state energies to within the experimental uncertainties. We use this singlet potential and a published Rydberg-Klein-Rees triplet potential [16] to determine  $\phi_S(E, l)$ ,  $\phi_T(E, l)$  for arbitrary combinations of energy  $E$  and relative orbital angular momentum  $l$  by integrating the singlet and triplet radial Schrödinger equations from the origin outward to  $r_0 = 16a_0$ . The variation with  $E$  and  $l$  of the radial phases at  $r_0$  is then used in the boundary condition for the  $r > r_0$  problem and the values of the phases  $\phi_T(0, 0)$ ,  $\phi_S(0, 0)$  at  $E = l = 0$  are varied together with the long-range potential parameters to optimally describe the highest energy levels [12], i.e., the singlet rovibrational levels of Ref. [14] with outer turning points between  $17a_0$  and  $29a_0$ , and the triplet rovibrational levels of Ref. [16] with outer turning points between  $17a_0$  and  $20a_0$ . The uncertainty in the variations of the phases over the  $E$  and  $l$  ranges involved in the following analysis has been estimated to be small and is included in the final error limits.

For this optimization problem we use a multichannel inverted perturbation approach, which will be explained in more detail elsewhere [17]. Like the standard inverted perturbation approach (IPA), it searches for potential corrections that eliminate deviations between theoretical and experimental energy eigenvalues, using the expression for the first-order energy shift in perturbation theory. The essential difference is that the potential contains in addition singlet-triplet coupling terms, in our case the sum of the single-atom hyperfine interactions. Another advantage of the method compared to the standard IPA is that triplet and singlet levels are included simultaneously, the parameter search comprising both dispersion and exchange parts and the triplet and singlet phases. It is emphasized that our analysis uses *differences* of experimental energy levels only [12]. On the other hand, our analysis predicts *absolute* energies relative to the continuum.

We follow an iterative procedure in applying our multichannel IPA program to search for successively better singlet and triplet potentials. As a starting point we use long-range potentials described by the dispersion coefficients of Marinescu, Sadeghpour, and Dalgarno [18], which are believed to

TABLE I. Triplet ( $a_T$ ) and singlet ( $a_S$ ) scattering lengths in  $a_0$  for  $^{39}\text{K}$  and  $^{41}\text{K}$ .

Isotope	Scattering length
$^{39}\text{K}$	$-1200 < a_T < -60$
$^{39}\text{K}$	$+132 < a_S < +144$
$^{41}\text{K}$	$+25 < a_T < +60$
$^{41}\text{K}$	$+80 < a_S < +88$

be correct to within 4% [19], and the exchange coefficients of Magnier [20]. With our multichannel IPA code we then search for the optimum phase values  $\phi_S(0, 0)$ ,  $\phi_T(0, 0)$ . In the following step, using these as a starting point, we search for the optimum combination of  $C_6$  and the phase values. It turns out that the data are not sensitive enough to  $C_8$  and  $C_{10}$  to determine these higher-order dispersion coefficients. In further iterative steps these parameters are varied within their theoretical uncertainty bounds. Finally we vary  $C_6$ , the exchange parameters, and the phase parameters simultaneously to search for a least-squares minimum. As a result we find  $C_6 = 3960 \pm 40$  a.u., in good agreement with the theoretical value of Marinescu, Sadeghpour, and Dalgarno [18] but with an error bar of only 1%, and  $\alpha = 0.845 \pm 0.015 a_0^{-1}$ ,  $A = (2.75 \pm 0.25) 10^{-6} \times \exp(-\alpha \cdot 20a_0)$  a.u., in reasonable agreement with Magnier's values [20]. We find that the terms included in the potential (1) give an excellent description in the radial range considered. It turns out that an analysis with  $r_0$  shifted to  $17a_0$  leads to values of  $C_6$ ,  $A$ , and  $\alpha$  within the above error limits.

From these coefficients and the corresponding phase parameters we then determine the scattering lengths for the collision of  $^{39}\text{K} + ^{39}\text{K}$  atoms via a pure triplet or a (hypothetical) pure singlet collision channel. The results are summarized in Table I. A simple mass-scaling law [21–23], transforming the phase values at  $r_0$ , enables us to transform these results into the corresponding values for a  $^{41}\text{K} + ^{41}\text{K}$  collision. The results are also presented in Table I. We thus predict that the stability condition for the Bose condensate under homogeneous circumstances is fulfilled in the case of doubly spin-polarized  $^{41}\text{K}$  atoms. For the analogous case of  $^{39}\text{K}$  we predict that it is not fulfilled.

The other state that can be trapped in a static magnetic trap, the  $f=1$ ,  $m_f = -1$  hyperfine state, is a field-dependent superposition of singlet and triplet eigenstates. The scattering length  $a_{1,-1}$  will therefore depend on  $B$ . It is well known that this dependence cannot be calculated by simply averaging  $a_S$  and  $a_T$  with weight factors equal to the singlet and triplet probabilities in the spin state of the incoming channel. This is only true in the degenerate internal states (DIS) limit, i.e., when the influence of the hyperfine splitting is negligible during a two-body collision [24]. The averaging prescription would lead to a smooth dependence on  $B$  with no resonances. A more realistic picture suggesting where Feshbach resonances might be expected arises as follows. For a fixed value of the field we separately diagonalize the spin Hamiltonian  $V_{hf} + V_Z$ , consisting of the hyperfine and Zeeman interactions, in the singlet and triplet two-atom subspace; i.e., we neglect the hyperfine-induced singlet-triplet mixing, replacing  $V_{hf}$  by its ‘‘symmetric’’ part  $V_{hf}^+$

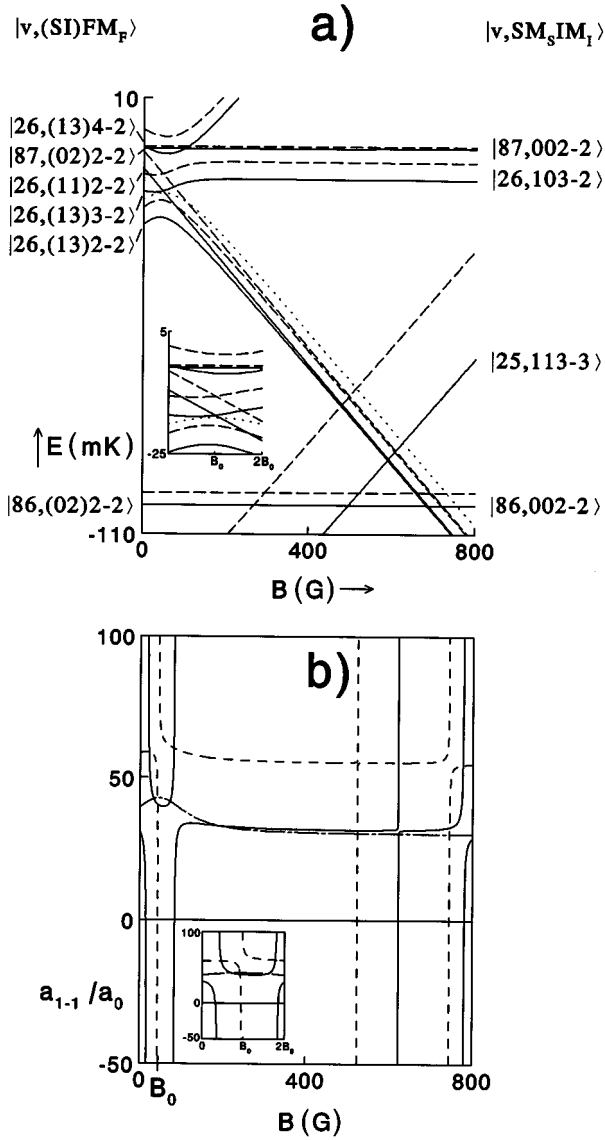


FIG. 2. (a) Energies of highest singlet and triplet bound states for  $^{41}\text{K}$  as a function of magnetic field for model neglecting  $V_{hf}^-$ . At  $B=0$  the splitting of the  $S=1$  levels is given by  $V_{hf}^+ = \frac{1}{4}a_{hf}\{F(F+1) - S(S+1) - I(I+1)\}$ . For each bound state two lines (drawn and dashed) are presented, corresponding to two extremes for the potential parameters. The dotted line shows the threshold energy of the  $|1-1,1-1\rangle$  collision channel. Resonances for ultralow collision energy occur where this line intersects with a bound-state energy curve. (b) Value of the scattering length for the  $f=1$ ,  $m_f=-1$  state following from coupled-channel calculation. The two lines are extreme results for different choices of the potentials. The dash-dotted line shows  $a_{1,-1}$  in the DIS limit for one extreme choice.

$= \frac{1}{4}a_{hf}\{F(F+1) - S(S+1) - I(I+1)\}$ , depending on the two-atom spin quantum numbers  $S, I, F$ . For  $^{41}\text{K}$  the result is presented in Fig. 2(a). We restrict ourselves to the relevant highest vibrational levels  $v$  and to states with the two-atom magnetic quantum number  $M_F$  equal to the value  $-2$  in the incident channel. Note that the singlet levels are only weakly field dependent via the nuclear Zeeman term. We give an indication for the error limits due to the uncertainties in the potential parameters and phase values by giving two extreme sets of curves (drawn and dashed lines). Also, we indicate

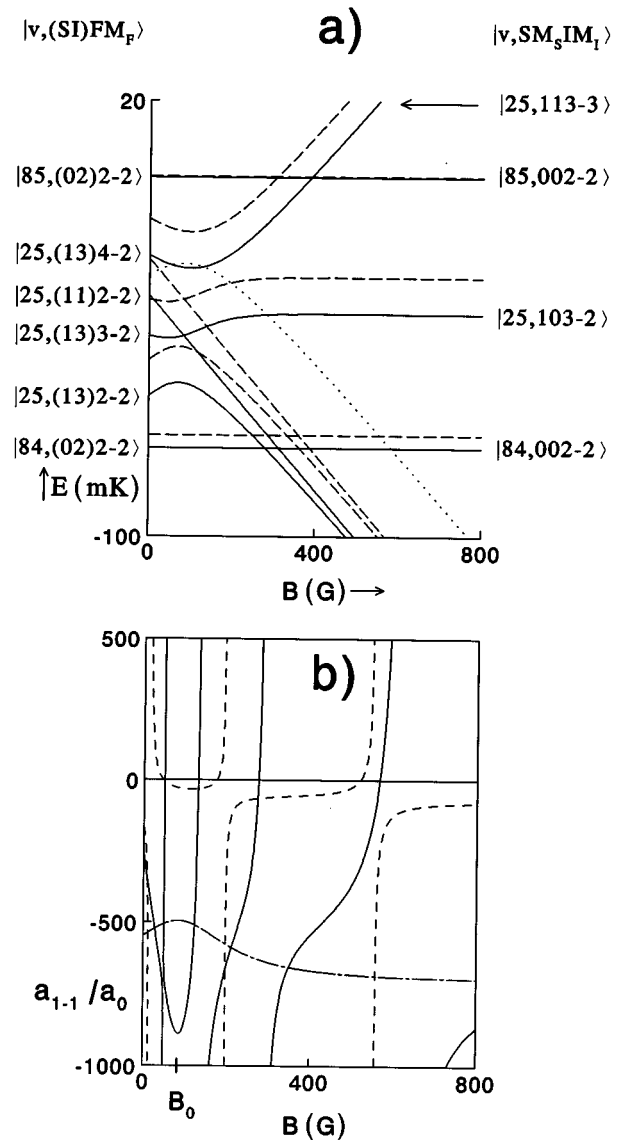


FIG. 3. Same as Fig. 2 for  $^{39}\text{K}$ .

the simple coupled  $|(SI)FM_F\rangle$  and decoupled  $|SM_SIM_I\rangle$  structures valid in the weak and strong field limits, and the  $B$ -dependent threshold of the continuum (dotted line), equal to the sum of the single-atom  $f=1$ ,  $m_f=-1$  energies. Feshbach resonances are expected where a bound-state level crosses the threshold and becomes a quasibound state embedded in the continuum. Figure 2(a) suggests that a Feshbach resonance may exist close to or inside the field range where the atoms can be trapped. Note, however, that we have neglected the contribution  $V_{hf}^- = \frac{1}{4}a_{hf}/\hbar^2\{(\vec{s}_1 - \vec{s}_2) \cdot (\vec{i}_1 - \vec{i}_2)\}$ , antisymmetric in the atomic electron spins, that couples singlet and triplet states. This might be a bad approximation when the energy distance between the latter is comparable to  $a_{hf}$  as is the case for low  $B$ . In fact we expect the  $|v=26,(11)2,-2\rangle$  state to be repelled by the higher  $v=87$  singlet level.

The result of a rigorous coupled-channel calculation of  $a_{1,-1}$  is presented in Fig. 2(b) for the same two extreme sets of potential parameters. Clearly, we predict at least one Feshbach resonance in the field range  $B < B_0$  where the atoms are low-field seeking, for the whole range of possible

potential parameters. Apparently, the  $V_{hf}^-$  coupling does play an important role for weak fields. A gas of  $^{41}\text{K}$  atoms in the  $f=1$ ,  $m_f=-1$  state may therefore very well be an experimental example where the scattering length changes sign due to the existence of a Feshbach resonance in the interesting field range. To illustrate the difference with the flat behavior of the simple DIS prediction, Fig. 2(b) also shows the above-mentioned average of  $a_S$  and  $a_T$  for one of the extreme sets of parameters (dash-dotted line, corresponding to the solid line for coupled channels). Another interesting feature visible in Fig. 2(b) is the interference of two nearby overlapping Feshbach resonances for a range of possible potential parameters. If this actually occurs experimentally, an intriguing time-dependent behavior with two competing time scales might show up in a measurement, especially when the field is varied as a function of time through the field range where the overlap occurs.

Taking into account the uncertainties in the potential parameters, the field ranges where the resonances are predicted to occur at threshold are  $16 < B_{S=1} < 44$  G,  $515 < B_{S=1} < 630$  G, and  $740 < B_{S=0} < 785$  G, where we indicate the resonances by their predominant singlet or triplet character. The interfering resonances are predicted to occur for  $40 < B_{S=1} < 85$  G.

Figure 3 shows analogous results for  $^{39}\text{K}$  atoms. Note that due to the lower atomic mass the resonances are associated with vibrational states having lower  $v$  values. The coupled-channel results lead to the conclusion that the probability of finding a change of sign of  $a$  in the field range  $B < B_0$ , taking into account the uncertainty in the potential, is about 80%. A remarkable feature of the resonances is that they extend over a much wider field range than in  $^{41}\text{K}$ . The field ranges where the resonances are predicted to occur at threshold turn out to be  $0 < B_{S=1} < 16$  G,  $195 < B_{S=1} < 295$  G, and  $550 < B_{S=0} < 630$  G.

In conclusion, we have studied collision properties of cold  $^{39}\text{K}$  and  $^{41}\text{K}$  atoms, relevant for BEC experiments. Despite the small hyperfine splittings we predict at least one Feshbach resonance for  $^{41}\text{K}$  in the field range where the highest state of the lower hyperfine manifold can be trapped and a large probability for at least one in  $^{39}\text{K}$ . The broadness of the resonance features in  $^{39}\text{K}$  should make them more easily observable experimentally.

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