Collisional properties of ultracold potassium: Consequences for degenerate Bose and Fermi gases

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The hyperfine-state-selected scattering properties of potassium atoms at ultralow temperatures are calculated using interaction potentials gleaned from an analysis of recent photoassociation data. We predict that the small, probably negative value of the ^{39}K triplet scattering length will hamper efforts to produce a Bose-Einstein condensate, unless experiments utilize a broad, accessible magnetic Feshbach resonance. The large positive value calculated for the ^{41}K triplet scattering length makes it a better candidate for condensation at zero magnetic field. The fermionic isotope ^{40}K is also predicted to have a large, positive scattering length for elastic collisions between spin states of experimental interest, implying that it can be efficiently evaporatively cooled to the quantum degenerate regime. In addition, certain spin states possess Feshbach resonances that may enable tuning of its interatomic interactions, possibly leading to the formation of Cooper pairs.
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A number of laboratories have now clearly established that a dilute gas of neutral atoms with integral net spin will undergo Bose-Einstein condensation (BEC) provided they are trapped and cooled to a sufficiently low temperature. Bose condensates have now been successfully produced in the alkali-metal atoms rubidium [1], sodium [2], and lithium [3] , and most recently in hydrogen [4]. Conspicuously absent from this list are potassium and cesium, both of which are hindered by incomplete knowledge of threshold scattering parameters such as scattering lengths and spin-exchange rate coefficients. For cesium, this information is beginning to emerge from comprehensive analyses of the available data [5]. This paper does the same for potassium, based on recent photoassociation (PA) spectra of ^{39}K [6].

Beyond BEC, another intriguing issue in ultracold potassium is the existence of its long-lived fermionic isotope, ^{40}K. Cooling a gas of this atom to the quantum degenerate regime would provide an opportunity to probe a weakly interacting Fermi sea, in contrast to the highly correlated Fermi sea often encountered in condensed matter, nuclear, and atomic physics [7]. Indeed, identical fermionic neutral atoms, when trapped in a unique spin state, hardly interact at all at the microkelvin temperatures encountered in contemporary magnetic traps. This follows because Pauli antisymmetrization excludes *s*-wave elastic collisions, which would otherwise (i.e., for bosons or for nonidentical particles) yield the dominant interactions at these energies.

The desire to probe appreciable interaction effects therefore hinges on the production of mixtures of different fermions in a single trap. If the interaction is effectively repulsive (described by a positive *s*-wave scattering length a), we can anticipate the formation of domains, identified by distinct regions of magnetization [8]. For effectively attractive interactions (negative a), we will find overlapping degenerate Fermi gases, possibly even a mechanism for a BCS-type pairing of fermions [9]. In support of ongoing experiments that are beginning to trap and cool ^{40}K [10,11], we also present calculations for this isotope.

Previous estimates of the potassium threshold scattering properties have appeared in the literature [12,13], but they relied on incomplete information concerning potassium interaction potentials. Our present results are based on our own recent analysis of photoassociation line shapes measured by the Connecticut group [6]. Specifically, we have fitted the intensities of a number of spectral lines corresponding to rovibrational levels of the 0_g^- purely long-range state of K_2 dimers, as populated by a laser from the $f=1$ hyperfine states of a pair of ultracold ^{39}K atoms. Details of this analysis are presented in a separate report [14]. Here we will expand on this basic result, detailing its consequences for the collisional properties of hyperfine-state-selected collision processes, which are not probed directly in the experiment.

Matching these PA data required flexible ground-state potential curves for the K-K interaction. Essential ingredients for this analysis are singlet [15] and triplet [16,17] potentials garnered from previous spectroscopic literature, and matched at large R to the long-range dispersion potentials of Marinescu *et al.* [18],

$$V_{\mathrm{disp}}(R)=-\frac{C_6}{R^6}-\frac{C_8}{R^8}-\frac{C_{10}}{R^{10}}. \tag{1}$$

In addition, we allowed for a small change of the inner walls of each potential, of the form [19]

$$\begin{aligned} &C_S \tan^{-1}\left[\frac{(R-R_e)^2}{\Delta R^2}\right], \quad R<R_e, \\ &0, \quad R>R_e. \end{aligned} \tag{2}$$

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TABLE I. Singlet and triplet scattering lengths a (in a.u.) and quantum defects μ (dimensionless) for collisions among different pairs of potassium isotopes, assuming a constant $\overline{C}_6=3800$ a.u. The scattering length is related to the quantum defect through the following formula [22]: $a=-C^2\tan(\pi\mu)/[1+\mathcal{G}(0)\tan(\pi\mu)]$, where $C^2=0.9579(2mC_6)^{1/4}$, m is the reduced mass of the atom pair, and $\mathcal{G}(0)=-1.0039$. The quantum defect uncertainties are ± 0.01 for the singlet, independent of C_6. The uncertainty in each triplet quantum defect is given in terms of C_6 by $\mu_t=\overline{\mu}_t+8.0(10^{-15})(C_6-\overline{C}_6)^{+0.04}_{-0.06}$.

Isotopes	a_s	$\overline{\mu}_s$	a_t	$\overline{\mu}_t$
39+39	140^{+3}_{-6}	0.460	-17 ± 25	0.039
40+40	105^{+2}_{-3}	-0.445	194^{+114}_{-35}	0.388
41+41	85 ± 2	-0.366	65^{+13}_{-8}	-0.268
39+40	-1^{+2}_{-5}	0.002	$-460^{+330}_{-\infty}$	0.212
39+41	113 ± 3	-0.474	205^{+140}_{-40}	0.379
40+41	-50^{+4}_{-10}	0.089	104^{+20}_{-11}	-0.441

Here $S=0$ or 1 denotes the total electronic spin, R_e is the minimum of the relevant potential, and ΔR is a width parameter, which we took to be $\Delta R=2$ bohr. This change enabled us to vary the model singlet and triplet scattering lengths to find a best fit with the PA data, without distorting the large R behavior of the potentials. We also accounted for the variation in the leading dispersion coefficient C_6, whose nominal value of 3813 a.u. is uncertain by $\pm 5\%$ [18].

Nuclear spin and hyperfine structure were included in our full Hamiltonian for ground-state K-K collisions, but not in the excited 0_g^- state, as this structure was not resolved experimentally. Fitting to the PA data consisted of matching the relative peak heights for rotational levels of the 0_g^- state, in vibrational levels $v=0$ through $v=6$; details will be reported separately [14]. Tell-tale features, such as broad even-J resonance peaks and nearly vanishing odd-J peaks, allow us to determine the following bounds on scattering lengths: the singlet is bounded by $134<a_s(39)<143$ bohr, whereas the triplet, due to its sensitivity on the C_6 coefficient, is conveniently parametrized by

$$a_t(39)=-17-0.045(C_6-\overline{C}_6)\pm 25 \text{ bohr},$$

$$\overline{C}_6=3800 \text{ a.u.} \tag{3}$$

Uncertainties quoted below for the scattering parameters reflect these uncertainties in $a_s(39)$, $a_t(39)$, and C_6. We regard these error bounds as representing a 2-σ confidence interval, in the sense that the fit to the PA data deteriorates rapidly outside the stated ranges. However, a rigorous error analysis is prohibited by undetermined uncertainties in the PA spectra. Also note that the ranges of scattering lengths are often asymmetric with respect to their nominal values, reflecting the nonlinear dependence of a (via the tangent function) on scattering phase shifts.

TABLE II. Scattering lengths in Bohr and spin-exchange rates in cm^3/sec for the weak-field-seeking spin states of ^{39}K, computed at a collision energy of 1 μK and in zero magnetic field. Uncertainties include a ± 200 a.u. variation in C_6.

$\lvert f_a m_a\rangle+\lvert f_b m_b\rangle$	a (Bohr)	K (cm^3/sec)
$\lvert 22\rangle+\lvert 22\rangle$	-17^{+32}_{-35}	forbidden
$\lvert 22\rangle+\lvert 21\rangle$	-15^{+32}_{-35}	forbidden
$\lvert 21\rangle+\lvert 21\rangle$	5^{+23}_{-17}	$(0.5-1.2)\times 10^{-10}$
$\lvert 22\rangle+\lvert 1,-1\rangle$	-18^{+38}_{-34}	$<3.9\times 10^{-12}$
$\lvert 21\rangle+\lvert 1,-1\rangle$	-19^{+42}_{-54}	$<5.4\times 10^{-12}$
$\lvert 1,-1\rangle+\lvert 1,-1\rangle$	-20^{+42}_{-64}	forbidden

The singlet scattering length is very tightly constrained, primarily by the location of a d-wave shape resonance. Its value is very nearly in agreement with previous estimates of $a_s(39)$ [12,13]. The present triplet value is, however, quite different, lying between the estimates of Refs. [12] and [13]. In both of these previous works, the estimate of $a_t(39)$ was based on an extrapolation of known singlet and triplet bound levels to an uncertain dissociation threshold. Our analysis suggests that this kind of extrapolation is difficult to carry out, at least to the accuracy needed to predict extremely sensitive quantities such as threshold scattering lengths. Nevertheless, we find that the improved dissociation threshold reported in [17] is adequate to determine the number of bound states in the triplet potential. In particular, our singlet and triplet potentials hold 86 and 27 vibrational levels, respectively.

We thus predict $a_t(39)$ will be small in magnitude, and likely negative. This conclusion is consistent with results from a similar analysis of the PA spectra to the 1_u excited state [20]. By adjusting to the appropriate reduced mass, we can derive from these same potentials the singlet and triplet scattering lengths for various combinations of potassium iso-

TABLE III. Scattering lengths in Bohr and spin-exchange rates in cm^3/sec for the weak-field-seeking spin states of ^{41}K, computed at a collision energy of 1 μK and zero magnetic field. Uncertainties include a ± 200 a.u. variation in C_6.

$\lvert f_a m_a\rangle+\lvert f_b m_b\rangle$	a (Bohr)	K (cm^3/sec)
$\lvert 22\rangle+\lvert 22\rangle$	65^{+16}_{-10}	forbidden
$\lvert 22\rangle+\lvert 21\rangle$	65^{+16}_{-10}	forbidden
$\lvert 21\rangle+\lvert 21\rangle$	69^{+13}_{-8}	$(0.06-3.1)\times 10^{-12}$
$\lvert 22\rangle+\lvert 1,-1\rangle$	68^{+15}_{-9}	$(0.1-3.0)\times 10^{-13}$
$\lvert 21\rangle+\lvert 1,-1\rangle$	69^{+14}_{-9}	$(0.2-4.5)\times 10^{-13}$
$\lvert 1,-1\rangle+\lvert 1,-1\rangle$	69^{+14}_{-9}	forbidden

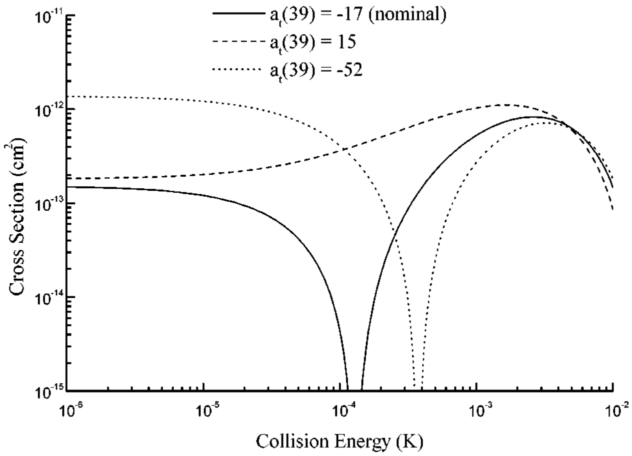

FIG. 1. Energy-dependent *s*-wave partial cross sections for $|22\rangle+|22\rangle$ scattering in ^{39}K, for various values of the triplet scattering length $a_t(39)$. For $a_t(39)<0$, this cross section vanishes at small energies, diminishing its suitability for evaporative cooling.

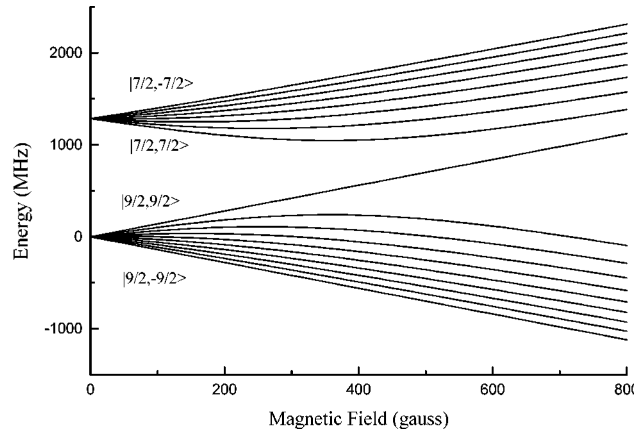

FIG. 3. Variation of the hyperfine energies of ^{40}K versus applied magnetic field, illustrating the nine weak-field-seeking states that can be magnetically trapped.

topes, as presented in Table I. Our triplet scattering length for ^{40}K is in good agreement with a recent collisional measurement [21], further boosting our confidence in the stated limits. This table also lists the quantum defect parameters μ for the various isotopic cases. These quantities, related to scattering phase shifts, are not essential to the present paper, but are included for completeness. They serve as the basic input for a ''frame transformation'' approximation, detailed in Ref. [22], which reproduces remarkably well the results of hyperfine-state-selected scattering calculations. The results of Table I are all quoted for a fixed value of $C_6=3800$ a.u., to bring out explicitly their C_6 dependence, as parametrized in the table caption. Below, in quoting ranges of scattering lengths and rate coefficients, we will include the variation with C_6.

The singlet and triplet potentials are the starting point for construction of the full two-atom Hamiltonian relevant in this low-energy range. We write it in a basis of the total spin of the separated atoms, $|f_a m_a\rangle+|f_b m_b\rangle$. We then add the hyperfine and magnetic field interactions, which are assumed to be independent of the interatomic distance R. For the calculations carried out with a magnetic field present, we further diagonalize the Hamiltonian at large R, implying that our asymptotic scattering channels are actually the atomic states dressed by the magnetic field. The resulting coupled-channel Schrödinger equations are next integrated using a standard log-derivative propagator method [23]. The relevant scattering matrices are computed for an incident energy of 1 μK throughout, and utilized to extract scattering lengths and, where appropriate, inelastic scattering rates arising from spin exchange. Spin-exchange rates are defined by

$$K=\frac{v_i\pi}{k_i^2}\sum_f |S_{fi}|^2, \tag{4}$$

where k_i is the incident wave number, v_i is the incident relative velocity, and the squared off-diagonal scattering matrix elements S_{fi} are added incoherently over all available final channels f.

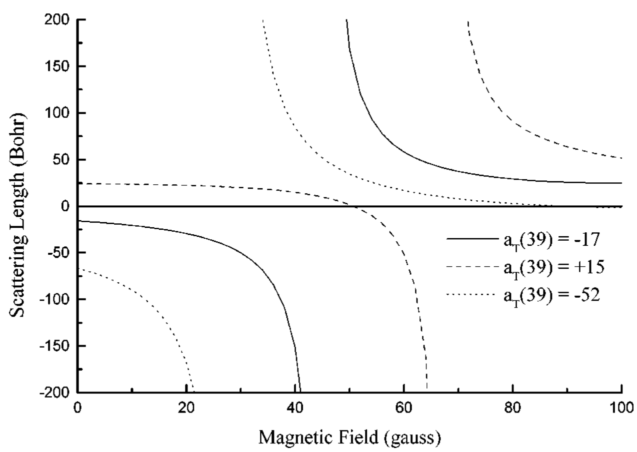

FIG. 2. Magnetic-field-induced resonances in the scattering length for ^{39}K atoms in their $|f,m\rangle=|1,-1\rangle$ state. The three curves show the resonance for our nominal scattering parameters, as well as for their extreme values, as indexed by the ^{39}K triplet scattering length. Note that this state remains magnetically trapped up to magnetic fields of 85 G.

We first present results for the bosonic species ^{39}K and ^{41}K. Each of these possesses a nuclear spin of $I=3/2$, implying total spin states of $f=1$ or $f=2$. Tables II and III present the zero-field scattering lengths and spin-exchange loss rates for various combinations of weak-field-seeking spin states. Spin-polarized ^{41}K should prove a reasonable candidate for BEC, as its positive scattering length is intermediate between ^{23}Na and ^{87}Rb, both of which have been

TABLE IV. *S*-wave scattering properties for several states of the fermionic isotope ^{40}K, computed at a collision energy of 1 μK and zero magnetic field. Uncertainties include a ± 200 a.u. variation in C_6. Note that none of these collisions suffer spin exchange at ultracold temperatures.

$\|f_a m_a\rangle+\|f_b m_b\rangle$	a (Bohr)	Feshbach resonance?
$\|9/2,9/2\rangle+\|9/2,9/2\rangle$	forbidden	N/A
$\|9/2,9/2\rangle+\|9/2,7/2\rangle$	196^{+346}_{-44}	no
$\|9/2,9/2\rangle+\|9/2,5/2\rangle$	196^{+346}_{-44}	yes

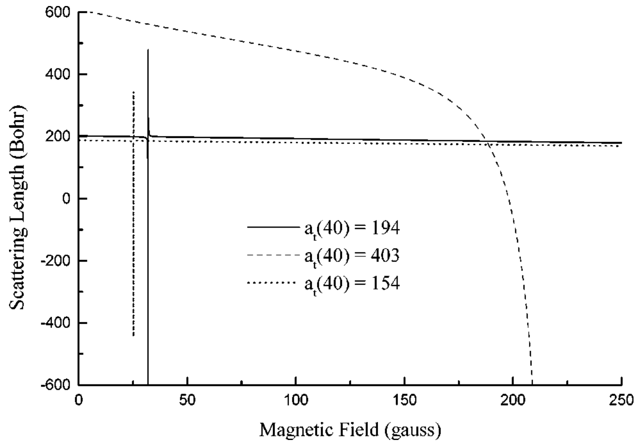

FIG. 4. Magnetic field dependence of the $|9/2,9/2\rangle + |9/2,5/2\rangle$ scattering length in ^{40}K. As in Fig. 2 we show these variations for the nominal and extremal values of the scattering parameters. For the nominal case, an extremely narrow resonance exists at 30 G. Near one extreme of our uncertainty [$a_t(40) = 403$ B], however, a much broader resonance appears accessible.

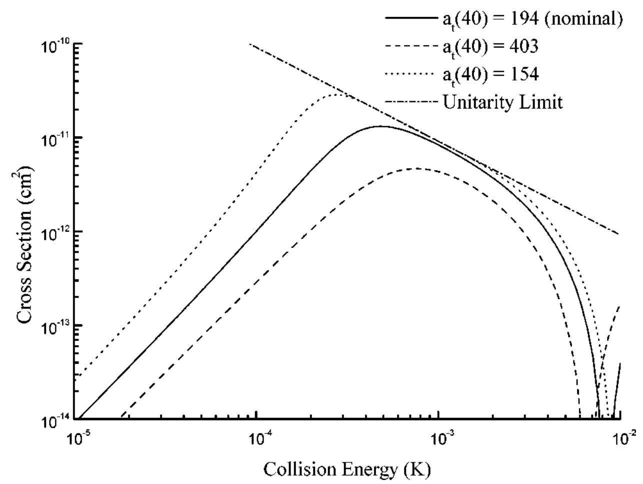

FIG. 5. Energy-dependent *p*-wave partial cross sections for $|9/2,9/2\rangle + |9/2,9/2\rangle$ scattering in ^{40}K, indexed by the value of the ^{40}K triplet scattering length $a_t(40)$. These cross sections exhibit shape resonances at temperatures in the vicinity of several hundred μK.

successfully evaporatively cooled and condensed. ^{41}K may also be useful for sympathetically cooling the fermionic isotope ^{40}K, given their large positive mutual scattering length.

The most abundant potassium isotope, ^{39}K, appears to be a particularly problematic candidate for evaporative cooling, owing to its small scattering length. This problem will be exacerbated if the scattering lengths turn out to be negative. Figure 1 illustrates this point, by showing the energy-dependent *s*-wave cross sections for $|22\rangle + |22\rangle$ collisions. For a small *positive* value of $a_t(39)$, the cross section remains nearly constant over the first several mK of collision energy. In the case of a *negative* $a_t(39)$, however, the cross section exhibits a prominent zero in the 100 μK range; this ''hole'' would diminish the rate of rethermalizing collisions just where they are most needed. The large qualitative difference in cross-section behavior should make it possible to determine the sign of $a_t(39)$, by measuring the temperature-dependent thermalization rates: a strong variation with temperature would point to $a_t(39) < 0$, while an essentially temperature-independent rate would imply $a_t(39) > 0$.

An unfortunately placed zero has already been noted in the cross section of ^{85}Rb, which also has a negative scattering length [24]. This minimum can be understood by examining the energy dependence of the *s*-wave scattering phase shift $\delta_0(E)$. Levinson's theorem [25] guarantees that $\delta_0(0) = N\pi$ at threshold, where N is the number of bound states supported by the potential. In the high energy limit where the scattering is perturbative, the phase shift tends instead to zero, $\lim_{E\to\infty}\delta_0(E) = 0$. The corresponding *s*-wave contribution to the cross section, $\sigma_0(E) \propto \sin^2\delta_0(E)$, will therefore suffer at least $N-1$ zeros. The threshold behavior of the *s*-wave phase shift is given by $\lim_{kr_0 \ll 1}\delta_0 \sim N\pi - ka$, where r_0 defines a cutoff for the potential beyond which any additional accumulated phase shift is negligible. In the case of a negative *s*-wave scattering length *a*, the phase shift therefore *rises* initially implying that the *s*-wave cross section will have at least N minima. An application of quantum defect theory [22] demonstrates that the first zero in cross section tends to occur at a lower energy for a negative scattering length as opposed to a positive scattering length given comparable magnitudes [26]. We note also that exceptions to this rule could occur if there are resonances in the relevant energy range.

Although ^{39}K in its spin-polarized $|22\rangle$ state seems an unlikely candidate for BEC, the $|1,-1\rangle$ state remains an interesting possibility owing to the presence of a magnetically induced Feshbach-type resonance (see Fig. 2). Such resonances have long been predicted [27], and have been observed recently in ^{23}Na [28] and ^{85}Rb [29]. In ^{39}K, this resonance lies at a magnetic field $B = 43^{+22}_{-18}$ G, with the largest uncertainty arising from the uncertainty in $a_t(39)$. For comparison, we note that the $|1,-1\rangle$ state of ^{39}K remains magnetically trapped up to field values of 85 G, meaning that this resonance should be readily observed and exploited. No such resonance appears accessible in ^{41}K.

We now move on to the fermionic isotope ^{40}K. With nuclear spin $I=4$, its electronic ground state can have a total spin (nuclear plus electronic) of either $f=9/2$ or $f=7/2$. Moreover, the hyperfine energies are ''inverted'' for this isotope, whereby the lower spin state, $f=7/2$, is actually higher in energy by $\Delta_{\rm hf} = 1285.78$ MHz. Figure 3 shows the Zeeman levels of ^{40}K in a magnetic field. Of the 18 spin states $|fm\rangle$, nine rise in energy as the magnetic field grows and are thus magnetically trappable. Consequently, a magnetically trapped, condensed Fermi gas of ^{40}K might have a nine-component order parameter, at least at small magnetic field values, making it a very rich system.

Table IV presents scattering information for several pairs of ^{40}K collision partners. Information on the scattering lengths, etc., for other partners must remain sketchy, since they experience poles as we vary our triplet potential within its range of uncertainty. Collisions between pairs of $|fm\rangle = |9/2,9/2\rangle$ atoms are forbidden by Fermi symmetry in the *s*-wave limit. Of greater interest to degenerate Fermi-gas studies, therefore, are collisions between two ^{40}K atoms in the hyperfine substates $|9/2,9/2\rangle$ and $|9/2,7/2\rangle$. This combination is particularly noteworthy in that such collisions suffer no spin-exchange: the expected process $|9/2,9/2\rangle$

$+|9/2,7/2\rangle \rightarrow |9/2,9/2\rangle + |7/2,7/2\rangle$ is energetically forbidden at low temperatures, owing to the inverted hyperfine structure. Moreover, the large, positive scattering length (≈ 196 bohr) predicted for this pair has two important consequences. First, it guarantees that degenerate mixtures of the two species $|9/2,9/2\rangle$ and $|9/2,7/2\rangle$ will have a substantial interaction (repulsive in this case) so that issues of domain formation can be studied. Second, the relatively strong interaction between the two spin states implies large elastic cross sections, which are crucial for evaporative cooling. This result implies that it should not become necessary to cool ^{40}K sympathetically by immersing it in a gas of bosons, e.g., ^{87}Rb or ^{41}K.

One other pair of collision partners bears discussion here, namely, $|9/2,9/2\rangle + |9/2,5/2\rangle$. Note that it has the same scattering length (at zero magnetic field) as the pair $|9/2,9/2\rangle + |9/2,7/2\rangle$, since both cases project identically onto singlet and triplet states. The pair $|9/2,9/2\rangle + |9/2,5/2\rangle$ is also immune to spin exchange at low temperatures. Unlike the previous example, it has an interesting behavior in a magnetic field, depicted in Fig. 4. Namely, magnetic-field-induced Feshbach resonances may be accessible for this pair, providing control over the interatomic interaction. An effectively attractive interaction would make possible detailed studies of Cooper pairing in the dilute ^{40}K system. For our nominal value of $a_t(40)$, there is a very narrow resonance at 32 G. However, if $a_t(40)$ turns out to lie at the upper end of its range, we expect to find a quite broad resonance at an accessible field strength (the $|9/2,5/2\rangle$ state remains magnetically trappable up to fields of 255 G).

Finally, we draw attention to the probable existence of a *p*-wave shape resonance in ^{40}K, as illustrated by the *p*-wave cross sections in Fig. 5. The presence of such a resonance implies stronger interactions than might originally have been expected in spin-polarized gases. It may even have implications in the quantum degenerate regime, controlled by the *p*-wave analog [30] of the contact potential responsible for interactions in BEC.

Note added in proof. The *p*-wave-shape resonance depicted in Fig. 5 has now been observed in a collisional measurement.

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