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Potassium scattering lengths and prospects for Bose-Einstein condensation and sympathetic cooling

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We have determined the scattering lengths for collisions between the different isotopes of two potassium atoms in singlet and triplet molecular states of K_2. We show that for the two bosonic species ^{39}K and ^{41}K the scattering lengths are positive, hence, leading to stable condensates. The fermionic isotope ^{40}K also has positive scattering lengths, but the triplet value is nearly zero, hence, a quasi-non-interacting fermionic gas. We also give results for the interspecies collisions. We conclude that double condensates of ^{39}K and ^{41}K are possible for purely spin-polarized atoms, and sympathetic cooling between the bosonic ^{39}K and the fermionic ^{40}K will be efficient due to low spin-flip rates and a sizable interspecies scattering length.
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The recent observation of Bose-Einstein condensation (BEC) in weakly interacting systems of dilute atomic gases of alkali-metal atoms of rubidium [1], lithium [2], and sodium [3] has generated significant interest in the area of ultracold physics. In these experiments, the BEC is tightly confined by a trap. It may be described by a nonlinear Schrödinger equation (also known as the Gross-Pitaevskii equation). Many properties of the condensate can be determined by a single quantity, the scattering length a. The stability of the condensate depends on the sign of the scattering length, $a>0$, leading to a stable condensate, and $a<0$, leading to an unstable one [4,5]. The value of a is also of prime importance for the evaporative cooling mechanism used to get to the temperature regime where BEC occurs [6]. The creation of double condensates of rubidium [7] was achieved by sympathetic cooling, where the role of the scattering lengths is crucial [7–9]. In the same spirit, the cooling of fermions by a condensate and probing the superfluidity character of the condensate [10] will be dependent on the values of the various scattering lengths of the systems. Finally, the phase separation of multiple condensates and their stability can be shown to be directly described by the ratios of the scattering lengths [11].

In this paper, we investigate the collisional properties of the different isotopes of potassium. This element is attractive in many aspects: there exist two stable bosonic isotopes ^{39}K and ^{41}K and a long-lived metastable fermion ^{40}K with a lifetime of 1.25×10^9 years. We construct improved accurate potentials for the singlet $X\ ^1\Sigma_g^+$ and triplet $a\ ^3\Sigma_u^+$ states of $^{39}K_2$, and utilize them to compute the singlet and triplet scattering lengths a_S and a_T. We use a simple mass scaling to evaluate the different collisions among the various isotopes ^{39}K, ^{40}K, and ^{41}K, and utilize the elastic approximation [12,13] to comment on the possibility of creating double condensates and sympathetically cooling fermions.

In order to determine the long-range form of the potentials, we interpolated the Rydberg-Klein-Rees (RKR) data from Amiot [14] and Zhao *et al.* [15] for the singlet $X\ ^1\Sigma_g^+$ state, and those from Li *et al.* [16] and Zemke *et al.* [17] for the triplet $a\ ^3\Sigma_u^+$ state, with a cubic spline fit. We computed the Coulomb energy ΔE_C and the exchange energy $\Delta E_{\rm ex}$ given by

$$\Delta E_C(R) = -\tfrac{1}{2}[V_X(R)+V_a(R)], \tag{1}$$

$$\Delta E_{\rm ex}(R) = -\tfrac{1}{2}[V_X(R)-V_a(R)], \tag{2}$$

where $V_X(R)$ and $V_a(R)$ correspond to the $X\ ^1\Sigma_g^+$ and $a\ ^3\Sigma_u^+$ states, respectively, and the potentials are taken to be zero at infinite R. The large distance behavior of these two functions are illustrated in Figs. 1 and 2. The Coulomb en-

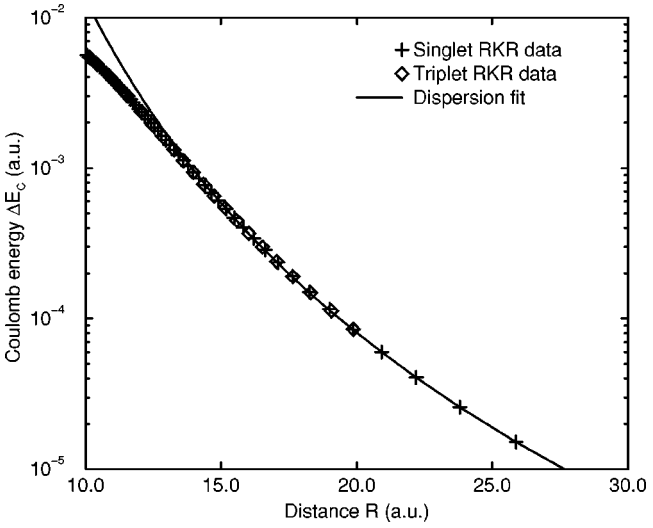

FIG. 1. Coulomb energy ΔE_C as a function of the distance. All of the quantities are in atomic units (a.u.).

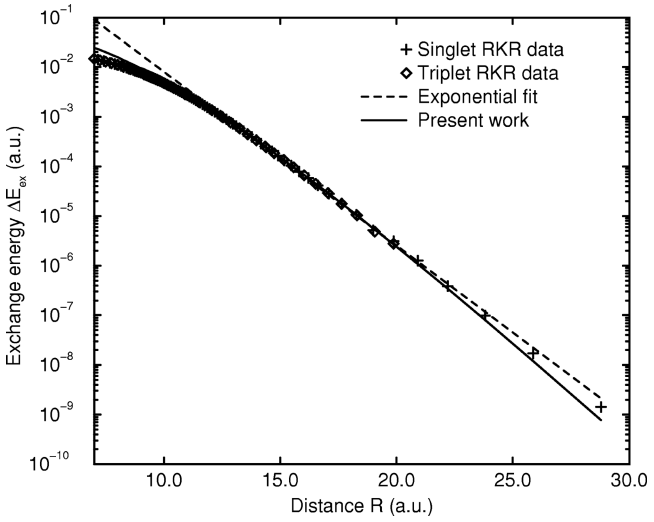

FIG. 2. Exchange energy $\Delta E_{\rm ex}$ as a function of the distance. The data for $R>18a_0$ are uncertain.

ergy can be represented by a dispersion expansion of the form

$$\Delta E_C(R)=\frac{C_6}{R^6}+\frac{C_8}{R^8}+\frac{C_{10}}{R^{10}}, \tag{3}$$

where the dispersion coefficients are taken from Marinescu *et al.* [18]. Figure 1 shows that the agreement of Eq. (3) with the RKR data is extremely good at large distances beyond $R\sim 14a_0$. The exchange term was fitted to the form [19]

$$\Delta E_{\rm ex}(R)=AR^{\alpha}\exp(-\beta R). \tag{4}$$

In atomic units, the values of α and β are 5.195 and 1.130, respectively, and we determined A to be 2.725×10^{-3} by fitting the data. In Fig. 2 we compare Eq. (4) to the usual exponential fit $B\exp(-bR)$ from Zemke *et al.* [17]. Our analytical expression (4) reproduces the RKR data down to distances $R\sim 10a_0$, and is considerably more accurate than the simple exponential fit. From Figs. 1 and 2, we conclude that the RKR points, at distances larger than $R\sim 18a_0$, can be replaced by the analytical expression

$$V(R)=-\frac{C_6}{R^6}-\frac{C_8}{R^8}-\frac{C_{10}}{R^{10}}\mp AR^{\alpha}\exp(-\beta R), \tag{5}$$

where $\mp$ refers to the singlet and triplet states, respectively. This yields more reliable potentials, since the RKR data have appreciable uncertainty at large distances (e.g., in Refs. [15] and [17], these last points were shifted to better create a smooth inner wall).

The complete potential curves were constructed from three distinct regions: a long-range tail, a RKR midsection, and an inner wall. For both the singlet $X\ ^1\Sigma_g^+$ and triplet $a\ ^3\Sigma_u^+$ states, the long-range tail is given by Eq. (5). The RKR midsection was formed from different data sources. We used the RKR data of Amiot [14] for $X\ ^1\Sigma_g^+$ from vibrational levels $v=0$ to 73, and supplemented them by the level $v=74$ from Zhao *et al.* [15]. We kept only the outer turning point $R_+=18.271a_0$, the inner turning point (as well as those for levels $v=75$ to 81) being too uncertain [15]. Oscillations occur in the inner wall from these extra points, and the outer turning points give rise to an inaccurate dissociation energy D_e. We took the value $4450.674\pm 0.072\ \ {\rm cm}^{-1}$ from Zhao *et al.* [15] for D_e. Finally, we added one *ab initio* point at $R=5.00a_0$ from Magnier [20] to complete the inner repulsive wall. We smoothly joined the three regions by a cubic spline fit, and for $R<R_{\rm min}=5.00a_0$, we extended the repulsive wall by an exponential wall of the form

$$C\exp(-cR), \tag{6}$$

where the coefficient $C=V(R)\exp(cR)|_{R_{\rm min}}$ and the argument of the exponential $c=-(d/dR)\ln V(R)|_{R_{\rm min}}$. We chose this inner wall instead of that of Amiot *et al.* [21] or Zemke *et al.* [17] because it incorporates more physical information than a simple exponential fit of RKR data.

For $a\ ^3\Sigma_u^+$, we used RKR data for $v=0$ to 13 from Li *et al.* [16], extended with data for $v=14$ to 17 from Zemke *et al.* [17]. However, we replaced the two last outer turning points $R_+(v=16)$ and $R_+(v=17)$ by the long-range values of Eq. (5). The dissociation energy was taken to be $D_e=252.74\pm 0.12\ \ {\rm cm}^{-1}$ [15]. We completed the potential with an inner wall using the *ab initio* values of Magnier [20] from $R=5.00a_0$ to $8.75a_0$. These points were smoothly joined by a cubic spline fit to the long-range tail (5), and extended at short distances ($R<5.00a_0$) by an exponential wall of the form (6). Contrary to Zemke *et al.* [17], we did not add $7.504\,25\ \ {\rm cm}^{-1}$ to the *ab initio* points and the highest inner turning point $R_-(v=17)$; as we will see below, this shift has little influence on the value of the scattering lengths.

Using these two potential curves, which we believe are the most accurate available, we evaluated the scattering lengths by computing the elastic phase shift $\delta_l(k)$, where $E=\hbar^2k^2/2\mu$ is the collisional energy for the system of reduced mass μ. At low temperatures, only the $l=0$ partial wave (s wave) contributes to the scattering [22], and the scattering length a is given by

$$\lim_{k\to 0} k\ \cot\ \delta_0(k)=-\frac{1}{a}. \tag{7}$$

It can also be expressed in an integral form [22]. We computed a for two colliding ^{39}K atoms in pure singlet and triplet states, and checked the sensitivity of its values to the different possible inner walls and exchange term, as well as for the uncertainty in D_e. The results are summarized in Table I. The scattering length sensitivity to the potential changes is not severe. Indeed, taking the extreme values, we find a_S varying between $238a_0$ and $292a_0$; our value is $278a_0$. Similarly, a_T takes values between $73.3a_0$ and $84.2a_0$, with our value equal to $81.1a_0$. We conclude that the minor changes in the inner wall or the exchange term do not greatly affect our results, and we adopt this construction from now on.

By scaling the mass appropriately, we computed a for both the singlet and triplet collisions for the different isotopic combinations. They are listed in Table II. A large variety of values occurs, both in magnitude and sign, due to the shifting of bound levels near threshold. Our results are very different

TABLE I. Values and uncertainties of singlet and triplet scattering lengths in a_0 for accurate K_2 potentials, including those improved and recommended here. The different inner walls and long-range tails are described in the text.

Singlet		Triplet	
Potential	a_S	Potential	a_T
Present work	278±14	Present work	81.1±2.4
Zemke inner wall only	254±11	Inner wall shifted up only	75.6±2.3
Exponential tail only	270±13	Exponential tail only	81.8±2.4
Both Zemke wall and tail	248±10	Both inner wall shifted and tail	76.3±2.5

from those of Boesten *et al.* [23], shown in Table III. They predicted a negative value for a_T between -1200 and $-60a_0$ in the case of ^{39}K contrary to our positive value near $80a_0$. This discrepancy may be explained in part by their use of an earlier version of the triplet energy curve $a\ ^3\Sigma_u^+$, for which D_e was shifted by 1.78 cm^{-1} [15,16]. Such a large shift changes the position of the last bound level drastically and, hence, the value of the scattering length. The same effect is translated into their value of a_T for ^{41}K, since they also used a mass scaling to evaluate it. For both isotopes, our singlet values are nearly twice those of Ref. [23]. It is difficult to explore the origin of the differences due to the complex nature of the changes they made to the initially similar $X\ ^1\Sigma_g^+$ curves [23]. However, we agree that a_S is positive.

All BEC experiments, to date (see Note added in proof), have been performed in magnetic traps. The atoms are trapped in specific hyperfine states, namely the low field seekers. For the two bosonic K species, the trapped states are $f=2$, $m_f=+2$ and $f=1$, $m_f=-1$, the first one corresponding to a pure triplet state and the second to a mixture of singlet and triplet states. In the elastic approximation [12,13], the scattering length can be estimated by projecting the hyperfine states onto the molecular singlet and triplet states. We write

$$a \simeq P_S a_S + P_T a_T, \tag{8}$$

where P_S and P_T are the probabilities of being in the singlet and triplet state, respectively. For $f=2$, $m_f=+2$, $P_S=0$, and $P_T=1$ (pure triplet state), and for $f=1$, $m_f=-1$, $P_S=3/16$, and $P_T=13/16$. From Table I, we estimate the scattering lengths a_{f,m_f} for the trapped states to be $a_{2,2}=81.1a_0$ and $a_{1,-1}=118a_0$ for ^{39}K, and $a_{2,2}=286a_0$ and $a_{1,-1}=255a_0$ for ^{41}K. In the case of the fermionic isotope ^{40}K, the trapped states will not scatter (since s-wave scattering is not allowed due to the antisymmetric nature of the wave function), unless different hyperfine states are trapped together.

TABLE II. Singlet and triplet scattering lengths in a_0, for isotopically pure and mixed potassium gases, and $\Delta \equiv (a_T - a_S)^2$ in a_0^2. The possible errors in the scattering lengths reflect only the uncertianties in the dissociation energies.

Isotopes	a_S	a_T	Δ
^{39}K+^{39}K	278±14	81.1±2.4	38 770
^{40}K+^{40}K	158±3	1.7±4.4	24 430
^{41}K+^{41}K	121±2	286±36	27 225
^{39}K+^{40}K	35.4±1.1	47.5±2.3	146
^{39}K+^{41}K	180±5	5.1±4.1	30 590
^{40}K+^{41}K	12.8±1.6	−162±36	30 555

TABLE III. Comparison of scattering length values in a_0.

	Scattering length	
Isotope	Present work	Boesten *et al.* [23]
^{39}K	$78.7 < a_T < 83.5$	$-1200 < a_T < -60$
	$264 < a_S < 292$	$+132 < a_S < +144$
^{41}K	$250 < a_T < 322$	$+25 < a_T < +60$
	$119 < a_S < 123$	$+80 < a_S < +88$

In the zero-energy limit, the elastic spin-flip cross section σ_{SF} is given by [12]

$$\sigma_{SF} = M_{SF}\pi(a_T - a_S)^2, \tag{9}$$

where M_{SF} is a constant depending on the exact hyperfine states considered. Although the elastic approximation fails at low energies, studies of spin-flip in ^{87}Rb [7–9] and ^{23}Na [8] show that the approximation is useful in indicating that small cross sections occur when singlet and triplet scattering lengths are equal. We present the square of the triplet and singlet scattering length difference $\Delta \equiv (a_T - a_S)^2$ in Table II.

From the above results, we predict a stable condensate for both bosonic isotopes ^{39}K and ^{41}K if they are in a pure hyperfine state $(fm_f)=(2+2)$ or $(1-1)$. However, the existence of double condensates in a single species (between the two trapped hyperfine states) is limited by large spin-flip rates arising from large values of Δ. A double condensate between ^{39}K and ^{41}K is possible if both isotopes are in the same purely spin-polarized states, i.e., $(2+2)$ or $(1-1)$. The scattering lengths being large, the two condensates would cool rapidly by evaporative cooling. The sympathetic cooling between the two isotopes would not be very efficient for $(2+2)$ states, the mixed triplet scattering length having a small value of $5a_0$. However, for the other possible spin-polarized state $(1-1)$, the scattering length given by Eq. (8) is larger $(38a_0)$, giving rise to a more efficient sympathetic cooling between the isotopes. Sympathetic cooling of the fermionic isotope ^{40}K by either bosonic isotope would be feasible. In the case of purely spin-polarized collisions, corresponding to a pure triplet collision, the scattering lengths have large magnitudes ($47.6a_0$ for ^{39}K+^{40}K and $-162.4a_0$ for ^{41}K+^{40}K), leading to efficient cooling. The negative value for ^{41}K+^{40}K could be of significance to the dynamics of the many-body fermion-boson system. More important is the extremely small spin-flip rate coefficient for collisions between ^{39}K+^{40}K due to almost equal values of the scattering lengths and small Δ. This implies possible sympathetic cooling of other combinations than the purely spin-polarized case, giving more experimental flexibility.

Finally, from Table II, many scattering lengths are near zero. These cases represent good candidates for the study of dilute noninteracting quantum gases [4], as well as for manipulation of the scattering length by external fields (magnetic, electric or photon coupling with the excited-state energy curves).

In conclusion, we have assembled potential-energy curves for collisions between different potassium isotopes, and used them to compute the scattering properties of cold atoms. We have found that BEC should be realizable for both bosonic isotopes, with possible double condensates for the purely spin-polarized combination of ^{39}K and ^{41}K. We also showed that sympathetic cooling of fermions by the condensates may be effective, and a good candidate is ^{39}K with ^{40}K, for which the spin-flip rates appear to be low.

Note added in proof. Recently, condensates have been loaded into optical traps [24], where the constraints on the high field seeker states are lifted, leading to various combinations of hyperfine states.

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