Anisotropy induced Feshbach resonances in mixture of $^6$Li($^2$S) + $^{171}$Yb($^3$P$_2$)

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Abstract

We theoretically explore the scattering properties in collisions between $^6$Li in the ground state and fermionic $^{171}$Yb in the metastable $^3$P$_2$ state. Unlike the role of the electronic spin degree of freedom in collisions of two alkali-metal atoms, the orbital degrees of freedom from the $p$ electron of the metastable atoms, which induce not only mixings between different partial waves but also couplings between channels in different fine-structure manifolds, introduce the anisotropic interactions for producing broad-enough Feshbach resonances. Our closed-coupling calculation shows that this mechanism is similar to that in highly magnetic atoms, but the resonances also suffer from a large inelastic rate at the magnitude of $10^{-10}$ cm$^3$ s$^{-1}$ to lower-lying fine-structure states or Zeeman sublevels, which will be an obstacle for associating ultracold polar molecules with both electron spin and electric dipole momentum. However, such a rich mixture of inelastic processes, and the experimental advantage of immunity from intraspecies inelastic collisions for metastable fermionic $^{171}$Yb, allow for precise investigations on the interspecies scattering properties for systems with excited-state atoms included.

1. Introduction

By allowing the tuning of interaction strength by simply varying the strength of the external magnetic field, magnetic Feshbach resonances (FRs) have not only provided new access to molecular formation [1] and ultracold chemistry [3], but also have been applied in fields of precision measurement [4] and quantum simulation of many-body systems [5–7]. However, until now ultracold molecules formed by magnetic FRs experimentally have been restricted to those dimers, either heteronuclear or homonuclear, comprised of ground-state alkali-metal atoms only [2]. As open-shell alkali-alkaline(rare)-earth dimers have manifested potential application in quantum information due to the electronic spin [8], there is great interest in extending the magnetic FRs to the formation of such molecules, which have already been created by two-color photoassociation [9].

In fact, unlike the broad and observable magnetic FRs that result from the hyperfine interaction between the electron and nucleus in collisions of alkali-metal atoms, FRs for ground-state alkali-alkaline(rare)-earth dimers are difficult to observed, since such interaction does not exist in bosonic ground-state alkaline(rare)-earth-metal atoms. Although the hyperfine interaction exists in fermionic ground-state alkaline(rare)-earth-metal atoms that have nonzero nuclear spin, it has been proven to be less important, since the electron of the alkali-metal atoms strongly couples to its own nucleus [10]. Nevertheless, Żuchowski et al [11] have firstly shown that the RbSr molecule could be produced by magnetic FR induced by the weak, modified space-dependent hyperfine coupling constant of the rubidium atom due to the presence of strontium, and systems made of alkali and Yb have also been checked to have the same mechanism by Brue and Hutson [10, 12]. However, these resonances are predicted to be too narrow, not exceeding several milli-Gauss, and usually posited at a large magnetic field strength. To overcome these difficulties for experiment and observe the resonances, Tomza et al [13] have
proposed an approach with nonresonant light to induce FRs and modify their position and width, which is similar to previous proposals of using the dc-electric field to control the interactions [14, 15].

Another promising approach to observe the magnetic FRs in alkali-earth-ground-(like) systems is to investigate the interaction between the alkali-earth atom in the ground state and the alkali-earth-ground-(like) atom in the metastable excited-state. Alkaline-earth-ground-(like)-atoms in the metastable state have orbital angular momentum and thus are anisotropic, which would introduce some other couplings and induce broader resonances [16]. Several groups have realized the trapping of alkaline-earth-ground-(like) atoms in the metastable state [17, 18]. Particularly, a heteronuclear mixture of ground-state $^4\text{Li}$ atoms and metastable excited-state $^{177}\text{Yb}$ atoms have been produced at arbitrary external magnetic field strength [19], and recently both theoretical and experimental investigations on the magnetic FRs of this system have been reported [20, 21]. They claimed that a resonance at about 450 G was observed in the collision of $^4\text{Li} + ^{177}\text{Yb}(^2\text{P}_j)$, but the resonance also shows a large inelastic loss rate (at the magnitude of $10^{-10}$ cm$^3$ s$^{-1}$ [21]) due to the spin exchange process, which is consistent with the previous calculation of this system [22].

However, the intraspecies inelastic loss rate for trapped $^{177}\text{Yb}(^2\text{P}_j)$ measured by Yamaguchi et al [23] is at the magnitude of $10^{-11}$ cm$^3$ s$^{-1}$. A comparison of the two loss rates indicates that not only intraspecies collision of metastable atoms [23–27] but also the interspecies interaction would likely cause the three kinds of widely investigated inelastic processes, including Zeeman-sublevel-changing, fine-structure-changing, and principle-quantum-number-changing relaxations. Thus, it is necessary to take the lower-lying fine-structure states into account in investigations on the collision properties of such systems. On the other hand, studies on the time evolution of the atom numbers of the trapped atomic mixture in [19] suggest that working in an optical lattice [28] or using fermionic isotopes benefitting from the Pauli exclusion principle (that is, inelastic collisions between two fermionic $\text{Yb}(^2\text{P}_j)$ atoms are avoided) could efficiently suppress the intraspecies inelastic effect and consequently allow for precise investigations on the interspecies collision properties. Inspired by the latter suggestion, we focus on the collision properties in the mixture of $^4\text{Li}$ (labeled by $a$) in the $^2\text{S}$ ground-state and $^{177}\text{Yb}$ (labeled by $b$) in the metastable $^2\text{P}$ state.

2. Close-coupling calculation

The Hamiltonian reads,

$$\hat{H} = \frac{\hbar^2}{2\mu} \left( -\frac{1}{r} \frac{d^2}{dr^2} + \frac{\hat{\ell}^2}{r} \right) + \hat{H}_a + \hat{H}_b + \hat{V}_{\text{int}}(r),$$

(1)

where $\mu$ is the reduced mass, $r$ the internuclear separation, and $\hat{\ell}$ the rotational angular momentum operator for the diatomic molecule. The free atomic Hamiltonians $\hat{H}_a$ and $\hat{H}_b$, which contain Zeeman and hyperfine interactions, as well as the spin–orbit coupling-induced interaction term for atom $b$, are taken to be

$$\hat{H}_a = A_{\text{dip}} a^\dagger a + \left( g_e \hat{\mathbf{S}}_{a,z} + g_{\text{iso}} \hat{I}_{a,z} \right) \mu_B B,$$

$$\hat{H}_b = \Delta_e b^\dagger b + A_{\text{dip}} b^\dagger b + \left( g_e \hat{\mathbf{S}}_{b,z} + g_{\text{iso}} \hat{I}_{b,z} \right) \mu_B B,$$

(2)

with $\hat{I}$ the orbital angular momentum operator; $\hat{S}$ and $\hat{s}$ the electron and nuclear spin operators; $\hat{L}$ the total angular momentum coupled by $\hat{l}$ and $\hat{z}$; $\hat{I}_z$, $\hat{s}_z$, and $\hat{\ell}_z$ the z-components of $\hat{I}$, $\hat{s}$, and $\hat{l}$ along the space-fixed z-axis, defined by the direction of the external magnetic field; $g_{e/\text{iso}}$ the electron and nuclear $g$-factors; $\mu_B$ the Bohr magneton; $A_{\text{dip}}$ the magnetic dipole constant; and $\Delta_e$ the fine splitting constant for atom $b$. However, for some atomic species, like $^{179}\text{Yb}(^2\text{P})$, the hyperfine interaction operators should be modified with the electric quadrupole couplings. The interaction operator is given as

$$\hat{V}_{\text{int}}(r) = \sum_{\Lambda, \Sigma} |\Lambda, \Sigma \rangle V_{\Sigma}(r) \langle \Lambda, \Sigma | + \hat{V}_{\text{dip}}(r),$$

(3)

where $\Lambda$ indicates the body-fixed projection of the total electronic orbital angular momentum $\hat{\mathbf{l}} = \hat{\mathbf{l}}_a + \hat{\mathbf{l}}_b$, and $\Sigma$ the total electronic spin. $\hat{V}_{\text{dip}}(r)$ represents the magnetic dipolar interaction induced by the unpaired electrons.

For the $^4\text{Li} + ^{177}\text{Yb}(^2\text{P}_j)$ system, the nuclear spin $i_a = 1$, $i_b = 1/2$, and the corresponding $g$-factors $g_{e/a} = -0.447654 \times 10^{-3}$, $g_{e/b} = -0.5337474 \times 10^{-3}$. The $g_{e/b}$ is evaluated from data for $^{177}\text{Yb}$ in [29] and CODATA 2010 [30]. The hyperfine magnetic dipole constants $A_{\text{dip}}$ are 0.152137 GHz and $A_{\text{dip}}$ is 2.67227 GHz, whereas the electric quadrupole constant is small enough to be neglected for both atoms. Since the $\Delta_e b^\dagger b$ term describes the fine splitting of the $^2\text{P}$ manifold, we use the energy splittings measured experimentally in [31] for channels with different $j$ numbers. The four electronic potential curves labeled by $^2\Sigma$, $^2\Pi$, $^4\Pi$, and $^4\Sigma$ in terms of the interaction operator (3) can be built with the short-range part and the long-range part. The short-range part is taken from calculated $\text{ab initio}$ data by Gopakumar et al [32], which is consistent with the results in [21].
The long-range non-relativistic Van der Waals coefficients $C_a$ are given as $C_a^{17} = 3279.87$, $C_a^{17} = 2402.98$ in units of $E_\text{b}a_0^6$ in [19], and the short- and long-range parts are connected from 6–12 Å by a switch function [33, 34]. The $V_6(r)$ term has not been taken into account yet, since it is several orders of magnitude smaller than the anisotropic interaction induced by the orbital angular momentum coupling [21], and it has also been checked that the results did not take significant changes with the $V_6(r)$ term considered in [22].

To solve the Schrödinger equation with the Hamiltonian (1), we have implemented the multi-channel close-coupling model based on the expansion of the molecular wavefunctions under a basis set in the partly coupled representation $|s_m, m_s \rangle |i_o, m_i \rangle |f_o, m_f \rangle |b_o, m_b \rangle |\ell, m_\ell \rangle$, where $m$ numbers represent angular momentum projections along the space-fixed z-axis. Equivalently, either the fully coupled basis set $|s_m, m_s \rangle |i_o, m_i \rangle |f_o, m_f \rangle |b_o, m_b \rangle |\ell, m_\ell \rangle$ or the fully uncoupled basis set $|s_o, m_o \rangle |i_o, m_i \rangle |b_o, m_b \rangle |\ell, m_\ell \rangle$ could be employed when they span the same Hilbert space. Owing to the fact that the external magnetic field only conserves the total parity $P = (-1)^{\ell + 1}$ and the projection of the total angular momentum $M_{tot} = m_o + m_i + m_b + m_\ell$, the total molecular wave function is constructed with all possible basis sets, which can produce the same $M_{tot}$ and parity $P$ values with those of the incoming channel. The rate constants for elastic and inelastic collisions for the incoming state lying in $|\alpha \rangle = |s_o, m_o \rangle |i_o, m_i \rangle |b_o, m_b \rangle |\ell, m_\ell \rangle$ are obtained by the sum of contributions from the resulting S-matrix elements for all possible partial waves [35] as $K^{el}_\alpha = \frac{\pi a_0^6}{\mu k} \sum_\ell (2\ell + 1) [1 - S_{\alpha,e;\alpha,e}^{-1} F]$ and

$$K^{in}_\alpha = \frac{\pi a_0^6}{\mu k} \sum_\ell (2\ell + 1) (1 - |S_{\alpha,e;\alpha,e}|^2),$$

where $k^2 = 2\mu E/\hbar^2$, with $\epsilon$ the collision energy. Particularly, the s-wave scattering length $a = (ik)^{-1} [1 - S_{0,0;0,0}]^{-1}$ is obtained from the diagonal element of the S matrix for the $\ell = 0$ incoming channels.

3. Results and discussions

We firstly consider the collisions between $^6\text{Li}$ ($s = 1/2, m_s = -1/2; i = 1, m_i = 1$) and $^{171}\text{Yb}$ ($j = 2, m_j = -2; i = 1/2, m_i = 1/2$) atoms with a collisional energy of 1 $\mu\text{K}$. Channels with $M_{tot} = -1$ and even $\ell$ are included. To explore the origin of the FRs in this system, close-coupling calculations are firstly implemented under basis sets with $j = 2$ only. Figure 1(a) shows that three extremely narrow resonances, the widths of which are at a magnitude of around 1 mG, exist with only $\ell = 0$ channels included. The resonance positions located by the near-threshold bound-states in the lower panel are consistent with those from the calculation of the s-wave scattering length. Similar with the collisional properties between Li and fermionic Yb, both in the electronic ground-state [10], these FRs are also produced by the mechanism due to hyperfine coupling between the electron spin and the nuclear magnetic moment of Yb, and thus their widths take the same order of magnitude. However, when taking channels with $\ell = 2$ into account, broader resonance begins to

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**Figure 1.** Magnetic field dependence of the s-wave scattering length $a$ for the collision between $^6\text{Li}$ in $|s = 1/2, m_s = -1/2; i = 1, m_i = 1\rangle$ and $^{171}\text{Yb}$ in $|j = 2, m_j = -2; i = 1/2, m_i = 1/2\rangle$ at $1 \mu\text{K}$, including $j = 2$ channels with: only $\ell = 0$ for the upper panel of (a), and $\ell$ up to $\ell_{max} = 2$ for (b) and (c), respectively. Lower panel of (a) shows the near-threshold bound-state energy responsible for the three extremely narrow resonances in the upper panel. $\Delta E$ means the difference between the calculated bound-state energy and the total energy of the two incoming free atoms. In (b) and (c), narrower resonances (the width at the magnitude of mG) are not plotted. $a_0$ is the Bohr radius.
appear, as shown in figure 1(b). Including channels with a higher partial wave number $\ell'$ leads to many more resonances (see figure 1(c) for $\ell'$ up to $\ell_{\text{max}} = 4$), and their widths are more than two orders of magnitude larger than those in figure 1(a). Consequently, it can be confirmed that the broad resonances are induced by strong mixing between channels with different partial waves. According to the derivation of the matrix elements for the interaction operator in appendix, we emphasize that this strong mixing of different $\ell'$ is determined by $k = 2$ and originates from the orbital degree of freedom-induced anisotropic interactions (see the fifth Wigner $3j$ symbol in equation (A.1)) in couplings of the four potential terms.

This phenomenon, that broad FR appears with an increasing number of channels from higher partial waves, is unlike those already observed in ground-state alkali-metal atom collisions [2] or in collisions of the strongly magnetic Cr atom [36]. For these atoms, the resonances do not take significant changes when channels with higher partial waves are added, which is an inevitable consequence, since the Hamiltonian for these systems conserves the partial wave number $\ell$ when the anisotropic spin–spin dipole interaction terms, which would introduce couplings between channels with $\Delta \ell = 2$, are not under consideration. On the other hand, this behaviour of adding higher $\ell'$ channels for metastable fermionic Yb is, to some extent, similar to that in the heavy submerged shell-elements collisions, like Dy and Er. In fact, the resonances for bosonic Dy and Er are chaotically distributed, and their extremely complex Feshbach spectra have been measured experimentally [37, 38]. Theoretical close-coupling investigations for these two atomic species [37, 39] indicate that the complex FRs are induced by larger (compared with the alkali-metal atomic collisions) magnetic dipole–dipole interaction and strongly anisotropic dispersion of the potential energy surface, both of which originate from their complex atomic electronic structures. However, unlike the complex short- and long-range potential surface in $^{164}$Dy (orbital angular momentum $l = 6$) [39], the systems considered in this work have much simpler interatomic potentials, and thus the relationship between the anisotropic couplings and the orbital angular momentum of metastable atoms could be easily analyzed. Neglecting the magnetic dipole–dipole terms, couplings between orbital angular momentum $\hat{l}$, electronic, nuclear spin $\hat{s}$ and molecular rotational angular momentum operator $\hat{I}$ (described by the partial wave number $\ell$) lead to anisotropic potential coupling terms, especially for two channels with $|\ell - \ell'| = 2$, and further induce those broad FRs.

However, the above results do not give complete insight into the collision properties for systems with an atom in the metastable state, since the couplings to lower-lying fine-structure states $^3P_{1,0}$ of the $^{171}$Yb atom are neglected. It is well known that the scattering length for FRs in the presence of inelastic spin relaxation to lower-lying levels is complex, and the imaginary part is in term with the inelastic loss rate constant [40]. Adding basis sets that conserve $M_{\text{tot}}$ and $P$ in $j = 1, 0$ manifolds leads to close-coupling calculations, including 22 channels with $\ell' = 0$, and the results are shown in figure 2. Comparing the spectra in the upper panel with that in figure 1(a), it can be easily recognized that broad resonances, although along with the inelastic rate constant ranging from $10^{-14}$ cm$^3$ s$^{-1}$ up to $10^{-10}$ cm$^3$ s$^{-1}$, as shown in the lower panel of figure 2, appear, and they are
induced by the added couplings to lower $^3P_1$ and $^3P_0$ states. This is an inevitable consequence due to the three fine-structure states sharing the same four potential curves. In fact, when deriving the matrix elements ($A.1$) for the interaction operator, couplings between different $^3P$ states produce nonzero off-diagonal elements for different either $j$ or $m_j$, so these anisotropic potential couplings should be in charge of the broad resonances in figure 2.

Based on the above discussions, we conclude that anisotropic potential terms, either from couplings between different partial waves or from couplings with lower-lying $j = 1, 0$ states, play dominant roles in producing those broad resonances. To check whether this $^6\text{Li}(^2S) + ^{174}\text{Yb}(^4\text{P}_2)$ system is a promising candidate for forming a molecule, we have performed close-coupling calculations, including 433 channels with $j = 2, 1, 0$ and even $\ell$ up to $\ell_{\text{max}} = 8$, and the converged resulting $s$-wave scattering length and inelastic collision rate constant are illustrated in figure 3. The spectrum contributed by so many Fano shapes at first sight is disorganized, especially for the region of low magnetic field strength, but the resonance positions can be located by the peaks of the inelastic rate in the lower panel [40]. Since $M_{\text{tot}}$ conserves and $m_\ell$ ranges from $-\ell$ to $\ell$, the chosen channels will cover all possible internal spin states for two atoms when larger $\ell$ are included. Consequently, when tuning the strength of the magnetic field, so many bound-states cross the incoming collision energy threshold, that the Fano shapes for those bound-states which have a small energy difference with each other, say, $|i_{\alpha}, m_{j_{\alpha}}\rangle |i_{\beta}, m_{j_{\beta}}\rangle$ and $|i_{\alpha}, m_{j_{\alpha}} + 1\rangle |i_{\beta}, m_{j_{\beta}} - 1\rangle$ channels, that they would likely partly coincide or even mask others. Compared with the case for bosonic $^{174}\text{Yb}(^4\text{P}_2)$ [22], where the Fano shapes could be clearly figured out from each other, such complicated behaviours in figure 3 result from the extra degree of freedom from nuclear spin $i_0 = 1/2$ of fermionic $^{174}\text{Yb}(^4\text{P}_2)$. Nevertheless, three undisturbed resonances at 204 G, 488 G and 713 G can be observed and potentially be used to tune the interactions between two atom species, but their large inelastic loss rate at the magnitude of around $1 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ is still an obstacle for the formation of the LiYb molecule. On the other hand, since both atoms lie in the energetically lowest magnetic sublevel of their Zeeman manifolds, respectively, naturally the inelastic rate shown in the lower panel of figure 3 should be totally contributed by the fine-structure-changing relaxations to the lower-lying $^3P_{1,0}$ states. The magnitude of the inelastic loss rate takes the same order with that for the case of $^{174}\text{Yb}(^4\text{P}_2)$ [20–22]. Another issue is that these resonances still cannot be identified with the dominantly contributed channels, as has been done in [21], since calculations of the bound-state energy with so many channels converge extremely slowly.

To investigate the effect of Zeeman-sublevel-changing relaxation, we have repeated the close-coupling calculation for metastable $^{174}\text{Yb}$ in another spin state, for instance, $|j = 2, m_j = -1\rangle = 1/2, m_j = 1/2\rangle$, but with only $j = 2$ channels included. Figure 4 shows the inelastic rate constant $K_{\text{im}}$ as a function of magnetic field, with $^6\text{Li}$ in the lowest Zeeman sublevel. The spectrum exhibits a complicated line shape, and the peaks are generally at the magnitude of $10^{-10} \text{ cm}^3 \text{ s}^{-1}$, which takes the same order with the inelastic rate in figure 3. Consequently, we make a conclusion that both the Zeeman-sublevel-changing and fine-structure-changing relaxations play a significant role in spin-stretched collisions. This behaviour is similar to that in collisions of Li with bosonic metastable $^{174}\text{Yb}(^4\text{P}_2)$ [20–22] since it has been observed that significant loss fractions end up in

![Figure 3](image_url.png)

*Figure 3.* The real part of $s$-wave scattering length $a$ (upper panel) and inelastic scattering rate constant $K_{\text{im}}$ (lower panel) as functions of magnetic field under the same condition as that in figure 2 but including channels with $j = 2, 1, 0$ and even a partial wave up to $\ell_{\text{max}} = 8$. 
Another essential matter is the effect of the quantitative uncertainty of the four potential curves, since it is not possible to calculate perfectly correct ab initio short-range potential terms. Slight changes of tens of cm\(^{-1}\) to the depths of the potential wells will lead to significant tremble for positions of those near-threshold vibrational bound-states and thus change the positions of the FRs. Figure 5 illustrates the magnetic dependence of the inelastic scattering rate constant under different short-range potentials in collisions of \(^6\text{Li}\) with \(^{171}\text{Yb}\) at a collisional energy of 1\(\mu\)K. Only \(j = 2\) channels are included.

Additionally, inclusion of the magnetic dipole–dipole term \(V_\text{D}\) in (3), the effect of which has been checked to be extremely un conspicuous [22], would in some extent lead to some modifications and thus induce a much more complicated spectrum, as observed in collisions of the Dy atom [39]. Another term, first revealed in exploring the possibility of magnetic associating RbSr and alkali-Yb(\(S_0\)) molecules [10–12], is the \(\tau\)-dependence of the hyperfine coupling, which has also been proven to be significantly smaller when compared with the anisotropic couplings for the systems considered in this work.
4. Conclusion

To conclude, we have theoretically investigated the scattering properties for collisions between $^6\text{Li}$ in the $^2S$ ground-state and fermionic $^{171}\text{Yb}$ in the metastable $^3\text{P}_2$ state. Applying fully closed-coupling calculations, we have elucidated that broad FRs are induced by the anisotropy. The anisotropic potential coupling terms originate from two mechanisms: the ability of the interaction operator to strongly mix channels satisfying $\Delta \ell = 2$, even when the magnetic dipole–dipole term is neglected, and the couplings with lower-lying $j = 1, 0$ fine-structure states. A comparison with collisional properties in alkali-metal systems and highly magnetic rare-earth-metal atoms indicates that both the original mechanisms are introduced by the orbital degree of freedom from the outermost electron of the metastable Yb atom. However, with higher partial wave $\ell \geq 2$ and lower-lying $^3\text{P}_{1,0}$ channels included, broad observable resonances appear, but with large inelastic relaxations rates at the magnitude of $10^{-10}$ cm$^3$ s$^{-1}$. Such rapid inelastic relaxations will be obstacles for molecular formation, although the $^6\text{Li} (^2S) + ^{171}\text{Yb} (^3\text{P}_2)$ system, at first sight, can be potentially applied for associating ultracold polar molecules due to the broad resonances and long lifetime of $15\ s$ for metastable Yb atoms. We have also studied the uncertainty effects from the $\text{ab initio}$ calculated short-range potentials, which are not accurate enough yet.

Recently, an investigation on FRs in the ground-state Li + Er system [41] has also shown that atoms with a larger orbital angular momentum (for Er in the $^4\text{H}$ ground-state, $l = 5$) would likely produce non-chaotic, complicated Feshbach spectra, while those for metastable alkali-earth-metal(-like) atoms ($l = 1$) exhibit much simpler behaviour. Suffering from the inelastic relaxations, the Li ($^2S$) + $^{171}\text{Yb} (^3\text{P}_2)$ system might not be a good candidate for producing ultracold polar molecules with both electron spin and electric dipole momentum. However, a rich mixture of inelastic processes and the experimental advantage of immunity of intraspecies inelastic collisions for metastable fermionic $^{171}\text{Yb}$ allow more precise investigations on the interspecies scattering properties with the assistance of an optical lattice, just like the experiment on the Yb($^4\text{S}_0$) + Yb($^3\text{P}_2$) mixture [28].

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Appendix. Matrix element for the interaction operator

Since the first term of the interaction operator in equation (3) is expanded in a body-fixed basis $|S, m_S; l, \Lambda\rangle$, transformations are required to obtain the matrix elements in the space-fixed basis represented by $|\Phi\rangle = |s_a, m_{s,a}; i_a, m_{i,a}; j_a, m_{j,a}; k_a, m_{k,a}; l_a, m_{l,a}; \ell_a, m_{\ell,a}; \ell_a, m_{\ell,a}\rangle$. Following the derivation in [16], the matrix elements take the form

$$
\langle \Phi | \sum_{\Lambda, S} (S, \Lambda) V_{\Lambda S} (r) \left( S, \Lambda \right) | \Psi\rangle = \delta_{m_{s,a}, m'_{s,a}} \delta_{m_{i,a}, m'_{i,a}} \delta_{m_{j,a}, m'_{j,a}} \delta_{m_{k,a}, m'_{k,a}} \delta_{m_{l,a}, m'_{l,a}} \delta_{m_{\ell,a}, m'_{\ell,a}} \delta_{m_{\ell,a}, m'_{\ell,a}} 
\times \sum_{k,q} (-1)^{2(s_a - b_a) + m_{s,a} + m'_{s,a}} (2b_a + 1)^{1/2} (2b_a' + 1)^{1/2} 
\times (-1)^{2(s_a - n_a - m_a)} (2S + 1) \times (-1)^{2b_a - m_{s,a} - m_{\ell,a}} (2b_a + 1) 
\times (-1)^{-m_{\ell,a}} (2\ell_a + 1)^{1/2} (2\ell'_a + 1)^{1/2} \times (-1)^{k + q} (2k + 1)^2 
\times \left( \begin{array}{ccc} s_a & l_a & j_a \\ m_{s,a} & m_{l,a} & -m_{j,a} \\ \end{array} \right) 
\times \left( \begin{array}{ccc} b_b & l_b & j_b \\ m_{s,b} & m_{l,b} & -m_{j,b} \\ \end{array} \right) 
\times \left( \begin{array}{ccc} s_b & l_b & j_b \\ m_{s,b} & m_{l,b} & -m_{j,b} \\ \end{array} \right) 
\times \left( \begin{array}{ccc} s_a & s_b & S \\ m_{s,a} & m_{s,b} & -m_S \\ \end{array} \right) 
\times \left( \begin{array}{ccc} l_a & k & l_b \\ -m_{l,a} & q & m_{l,b} \\ \end{array} \right) 
\times \left( \begin{array}{ccc} l_b & k & l_b \\ q & m_{l,b} & -m_{l,b} \\ \end{array} \right) 
\times \left( \begin{array}{ccc} k & 0 & k \\ 0 & q & 0 \\ \end{array} \right) 
\times V_{\Lambda S} (r), \quad (A.1)
$$

where the braces denote the Wigner 9$j$ symbol. In fact, taking advantage of $l_a = 0$, this formula is a reduced form from matrix elements of the interaction operator for systems comprised of two arbitrary (but not including S).
states, say two $P$ states [16]. On the other hand, by simply setting $l_b = 0$, the above form could also be simplified to the form of those for systems of two $S$-state atoms, for example, equation (A.1) in [42] for a diatomic system of two alkali-metal atoms, both in the ground-state.

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