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Theoretical analysis of the coupling between Feshbach states and hyperfine excited states in the creation of $^{23}Na^{40}K$ molecule*

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We present an intensive study of the coupling between different Feshbach states and the hyperfine levels of the excited states in the adiabatic creation of $^{23}Na^{40}K$ ground-state molecules. We use coupled-channel method to calculate the wave function of the Feshbach molecules, and give the short-range wave function of triplet component. The energies of the hyperfine excited states and the coupling strength between the Feshbach states and the hyperfine excited states are calculated. Our results can be used to prepare a specific hyperfine level of the rovibrational ground state to study the ultracold collisions involving molecules.

Keywords: Feshbach resonance, stimulated Raman adiabatic passage, ultracold molecule

PACS: 31.15.–p, 31.15.aj, 33.15.Pw, 67.85.–d **DOI:** 10.1088/1674-1056/ab6314

1. Introduction

Stimulated Raman adiabatic passage (STIRAP) is a coherent manipulation technique that allows robust population transfer between discrete quantum states.[1,2] The principle of STIRAP can be understood using a three-level system involving two ground states and one excited state. By coupling the two ground states with the excited state using a pump light and a Stokes light, respectively, and adiabatically controlling the Rabi frequencies in a counterintuitive way, the system can be transferred from one ground state to the other one without any losses. Recently, the STIRAP technique has been employed to prepare ultracold alkali-metal diatomic molecules in the rovibrational ground state.[3–10] To prepare the ultracold ground-state molecules, weakly bound Feshbach molecules are first created in an ultracold atomic gas in the vicinity of an atomic Feshbach resonance, and then are transferred to the ground state via a molecule excited state by the STIRAP. An illustration of the STIRAP in the $^{23}Na^{40}K$ system is shown in Fig. 1.

The Feshbach molecule is a kind of long-range molecule, and the long-range wave function is simply determined by the large magnetically-tunable scattering length.[11] This kind of universal property has been employed to study the BEC–BCS crossover in degenerate fermion gases,[12] the dynamics of solitons and votices in Bose-Einstein condensates (BEC),[13,14] and the universal few-body physics.[15,16] However, to prepare the ground-state molecule, we need to understand the short-range wave function of the Feshbach molecule, since the excited state is a conventional rovibrational state of the excited electronic state, and thus the coupling between the Feshbach state and the excited state occurs at the short range.

In the $^{23}Na^{40}K$ system, there are various atomic Feshbach resonances that can be used to create Feshbach molecules.[17,18] The projection of the total angular momentum along the magnetic field and the short-range wave function of these Feshbach molecules are different. The electronic excited state is a combination of the singlet and triplet electronic states, and it has many hyperfine levels due to the coupling between the electron spin and the nuclear spins.[19,20] These rich energy level structures offer the opportunity to create different hyperfine levels of the ground state by choosing the proper hyperfine excited states, the polarization of the pump and Stokes lasers, and the different Feshbach states. In our recent work, we have prepared the molecules in several different hyperfine levels of the rovibrational ground state to study the atom–molecule Feshbach resonances.[10] Besides, it has been demonstrated that in the $^{23}Na^{40}K$ system, the interference between a desired resonant STIRAP via resonantly coupled hyperfine level of the excited state and an unexpected detuned STIRAP via other off-resonantly coupled hyperfine levels can induce the oscillation of the round-trip STIRAP efficiency and affect the purity of the hyperfine ground states.[21] Therefore, it is important to understand the coupling between the Feshbach states and different hyperfine levels of the excited states.

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In this paper, we present a detailed theoretical study of the coupling between the Feshbach states and different hyperfine levels of the excited states in the ^{23}Na^{40}K system. We will consider the broad Feshbach resonances between $|f_{\rm Na}, m_{f_{\rm Na}}\rangle = |1,1\rangle$ and $|f_{\rm K}, m_{f_{\rm K}}\rangle = |9/2, m_{f_{\rm K}}\rangle$ states with $m_{f_{\rm K}} = -9/2, -7/2, -5/2$. For each spin combination, there are two broad atomic Feshbach resonances. We will calculate the short-range wave function of the Feshbach state, and calculate the coupling between these Feshbach states and the hyperfine levels of the excited state, which is a mixture of the electronic excited states $\mathrm{B}^1\Pi\ |v=12, J=1\rangle$ and $c^3\Sigma\ |v=35, J=1\rangle$. Our results can be used to prepare the molecules in various hyperfine levels of the rovibrational ground states.

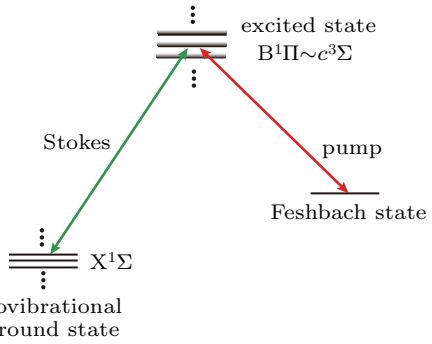


Fig. 1. Illustration of the stimulated Raman adiabatic passage in the ^{23}Na^{40}K system. By choosing the different Feshbach states, the proper hyperfine levels of the excited states, and the laser polarizations, the various hyperfine level of the ground-state molecule can be populated.

2. Feshbach molecules

We first consider the s-wave Feshbach molecule in the vicinity of the Feshbach resonance between the $|f_{\rm Na}, m_{f_{\rm Na}}\rangle = |1,1\rangle$ and $|f_{\rm K}, m_{f_{\rm K}}\rangle = |9/2, m_{f_{\rm K}}\rangle$ states. The Feshbach state is labelled by $|1,1;9/2, m_{f_{\rm K}}\rangle$. The binding energy and the wave function of the Feshbach molecule can be calculated using the Hamiltonian

$$H = T + \sum_{S=0,1} V_S(r) P_S + H_{\rm hf} + H_z. \tag{1}$$

The first term is the kinetic energy $T = -(\hbar^2/2\mu)(\mathrm{d}^2/\mathrm{d}r^2)$ with $\mu = m_{\rm Na} m_{\rm K}/(m_{\rm Na} + m_{\rm K})$ the reduced mass. The second term is the spin-exchanging interaction, where $P_0 = 1/4 - \boldsymbol{s}_{\rm Na} \cdot \boldsymbol{s}_{\rm K}$ and $P_1 = 3/4 + \boldsymbol{s}_{\rm Na} \cdot \boldsymbol{s}_{\rm K}$ are the singlet and triplet projection operators respectively with $\boldsymbol{s}$ being the electron spin. The Born–Oppenheimer potential $V_0(r)$ and $V_1(r)$ represent the interaction potentials of the singlet $X^1\Sigma$ and triplet $a^3\Sigma$ molecule states, respectively. The Born–Oppenheimer potentials can be approximately described by power expansions of r, and the analytic formula can be found in Refs. [18,22]. The hyperfine interaction $H_{\rm hf}$ can be described by

$$H_{\rm hf} = a_{\rm Na} \boldsymbol{s}_{\rm Na} \cdot \boldsymbol{i}_{\rm Na} + a_{\rm K} \boldsymbol{s}_{\rm K} \cdot \boldsymbol{i}_{\rm K}, \tag{2}$$

where $a_{\rm Na} = 885.813$ MHz and $a_{\rm K} = -285.7308$ MHz are the atomic hyperfine constants of the ground states and $\boldsymbol{i}$ denotes the nuclear spin. The last term is the Zeeman term

$$H_z = [(g_s s_{z\rm Na} - g_{i_{\rm Na}} i_{z\rm Na}) + (g_s s_{z\rm K} - g_{i_{\rm K}} i_{z\rm K})]\mu_{\rm B} B, \tag{3}$$

where $g_s = 2.0023$ is the electron g-factor, $g_{i_{\rm Na}} = -0.0008$ and $g_{i_{\rm K}} = 0.000176$ are the nuclear g-factor of ^{23}Na and ^{40}K, respectively, and B is the magnetic field along the z direction.

The internal states can be expressed in terms of the uncoupled basis $|m_{s_{\rm Na}}, m_{s_{\rm K}}, m_{i_{\rm Na}}, m_{i_{\rm K}}\rangle$. The Hamiltonian couples all the internal states with the same projection along the magnetic field $M_F = m_{f_{\rm Na}} + m_{f_{\rm K}} = m_{s_{\rm Na}} + m_{s_{\rm K}} + m_{i_{\rm Na}} + m_{i_{\rm K}}$. For a given M_F and B, we first diagonalize the hyperfine and Zeeman Hamiltonian $H_{\rm hf} + H_z$ to obtain the internal eigenstate $|\chi_i\rangle$ and the threshold energy $E_i^{\rm th}$ of these channels. Expanding the wave function in terms of the new bases $|\psi_F(r)\rangle = \sum_i \psi_i(r)|\chi_i\rangle$, we obtain the coupled-channel Schrödinger equation

$$\sum_j [T\delta_{ij} + \sum_{S=0,1} V_S(r)\langle\chi_i|P_S|\chi_j\rangle]\psi_j(r) = (E - E_i^{\rm th})\psi_i(r). \tag{4}$$

Assuming the threshold of the lowest channel is $E_o^{\rm th}$, the eigenvalues of the Feshbach state can be expressed as $E = E_o^{\rm th} - E^{\rm b}$, where $E^{\rm b} > 0$ represents the binding energy of the Feshbach molecule. We numerically solve Eq. (4) by means of the renormalized Numerov method[23] to calculate the binding energy and the wave function of the Feshbach state.

The calculated wave function can be expanded in terms of the spin-coupled basis $|\sigma\rangle = |S, M_S, m_{i_{\rm Na}}, m_{i_{\rm K}}\rangle$ by a unitary transformation

$$|\psi_F(r)\rangle = \sum_j \psi_j^F(r)|\sigma_j\rangle, \tag{5}$$

where $|\sigma_j\rangle$ represents the state that conserves the total projection of angular momentum $M_F = M_S + m_{i_{\rm Na}} + m_{i_{\rm K}}$. The wave function includes the singlet component with $S = 0$ and the triplet component with $S = 1$. In Fig. 2, we plot the spatial wave function $\psi_j^F(r)$ of the Feshbach molecule at 104 Gs (1 Gs = 10^{-4} T) in the vicinity of the Feshbach resonance between $|1,1\rangle$ and $|9/2,-7/2\rangle$ at about 110 Gs. The calculated binding energy is about 63 kHz. The Feshbach molecule has a long range component and thus is open channel dominated.

It can be easily seen that only several channels have the long-range components. For these channels, the long-range wave function can be expressed as

$$\psi_j^F(r > r_c^l) \approx c_j^L \psi^L(r), \tag{6}$$

where r_c^l is a cut-off length, and $\psi^L(r)$ represents the common long-range wave function, and the coefficient is

$$|c_j^L| = \sqrt{\int_{r_c^l}^{\infty} \psi_j^F(r)^2}. \tag{7}$$

Therefore, we may express the long-range part of the wave function as

$$|\psi_F(r > r_c^l)\rangle = \psi^L(r)\sum_j c_j^L|\sigma_j\rangle. \quad (8)$$

As shown in Fig. 2(a), for the Feshbhach molecule $|1,1;9/2,-7/2\rangle$, the long-range wave functions exist in 6 channels.

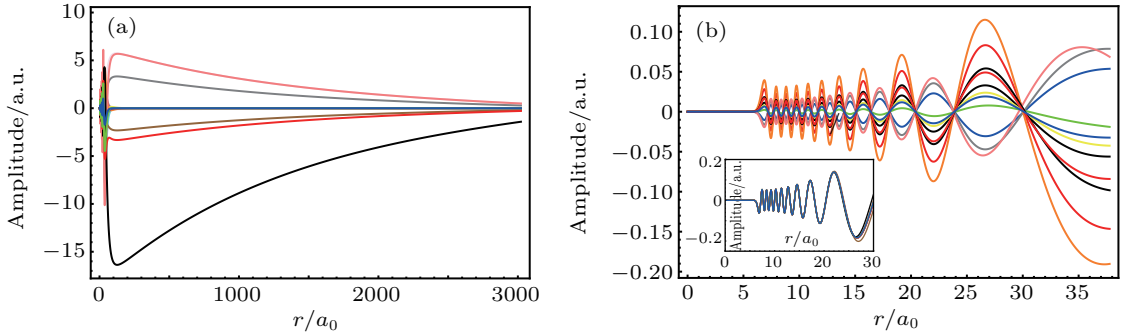


Fig. 2. (a) The spatial wave function of the Feshbach state $|1,1;9/2,-7/2\rangle$ at $B = 104$ Gs (1 Gs = 10^{-4} T). Each color curve represents the wave function $\psi_j^F(r)$ in a certain basis $|\sigma_j\rangle$. (b) The triplet component of the spatial wave function $\psi_j^F(r)$ at the short range. The inset is the normalized short-range wave function $\psi_j^F(r)/c_j^T$, with the cut off length $r_c^s = 23\ a_0$.

Table 1. The coefficients c_j^T of the short-range wave function for different Feshbach molecules $|1,1;9/2,m_f\rangle$ with $m_f = -9/2, -7/2, -5/2$.

$\|1,1;9/2,-9/2\rangle$ at $B = 85.7$ Gs					$\|1,1;9/2,-9/2\rangle$ at $B = 78$ Gs				
J	M_J	$m_{i_{\rm Na}}$	$m_{i_{\rm K}}$	c_j^T	J	M_J	$m_{i_{\rm Na}}$	$m_{i_{\rm K}}$	c_j^T
1	–1	–3/2	–1	–0.092	1	–1	–3/2	–1	0.113
1	–1	–1/2	–2	0.198	1	–1	–1/2	–2	–0.378
1	–1	1/2	–3	0.154	1	–1	1/2	–3	0.345
1	–1	3/2	–4	0.128	1	–1	3/2	–4	0.035
1	0	–3/2	–2	–0.098	1	0	–3/2	–2	0.126
1	0	–1/2	–3	–0.214	1	0	–1/2	–3	0.287
1	0	1/2	–4	–0.712	1	0	1/2	–4	–0.344
1	1	–3/2	–3	0.345	1	1	–3/2	–3	–0.604
1	1	–1/2	–4	0.481	1	1	–1/2	–4	0.378
$\|1,1;9/2,-7/2\rangle$ at $B = 104$ Gs					$\|1,1;9/2,-7/2\rangle$ at $B = 89.9$ Gs				
J	M_J	$m_{i_{\rm Na}}$	$m_{i_{\rm K}}$	c_j^T	J	M_J	$m_{i_{\rm Na}}$	$m_{i_{\rm K}}$	c_j^T
1	–1	–3/2	0	0.103	1	–1	–3/2	0	–0.150
1	–1	–1/2	–1	–0.168	1	–1	–1/2	–1	0.449
1	–1	1/2	–2	–0.254	1	–1	1/2	–2	–0.288
1	–1	3/2	–3	–0.289	1	–1	3/2	–3	–0.156
1	0	–3/2	–1	0.132	1	0	–3/2	–1	–0.195
1	0	–1/2	–2	0.180	1	0	–1/2	–2	–0.238
1	0	1/2	–3	0.625	1	0	1/2	–3	0.149
1	0	3/2	–4	0.298	1	0	3/2	–4	0.266
1	1	–3/2	–2	–0.268	1	1	–3/2	–2	0.634
1	1	–1/2	–3	–0.459	1	1	–1/2	–3	–0.261
1	1	1/2	–4	–0.048	1	1	1/2	–4	–0.102
$\|1,1;9/2,-5/2\rangle$ at $B = 128$ Gs					$\|1,1;9/2,-5/2\rangle$ at $B = 104$ Gs				
J	M_J	$m_{i_{\rm Na}}$	$m_{i_{\rm K}}$	c_j^T	J	M_J	$m_{i_{\rm Na}}$	$m_{i_{\rm K}}$	c_j^T
1	–1	–3/2	1	–0.108	1	–1	–3/2	1	–0.172
1	–1	–1/2	0	0.147	1	–1	–1/2	0	0.483
1	–1	1/2	–1	0.301	1	–1	1/2	–1	–0.204
1	–1	3/2	–2	0.402	1	–1	3/2	–2	–0.238
1	0	–3/2	0	–0.159	1	0	–3/2	0	–0.263
1	0	–1/2	–1	–0.173	1	0	–1/2	–1	–0.196
1	0	1/2	–2	–0.553	1	0	1/2	–2	0.033
1	0	3/2	–3	–0.346	1	0	3/2	–3	0.284
1	1	–3/2	–1	0.215	1	1	–3/2	–1	0.632
1	1	–1/2	–2	0.423	1	1	–1/2	–2	–0.158
1	1	1/2	–3	0.074	1	1	1/2	–3	–0.152
1	1	3/2	–4	–0.056	1	1	3/2	–4	0.048

For the STIRAP transfer, the short-range wave function is important. The short-range wave function includes the contribution from the the singlet and triplet potentials. In most cases, the contribution from the singlet potential is negligibly small, and thus the wave function of the Feshbach molecule is dominated by the triplet component. That is the reason why we usually need to find an excited state which is a mixture of triplet and singlet electronic excited state to perform the STIRAP.

The short-range wave function of the triplet component can be written as

$$\psi_j^F(r<r_c^s)\approx c_j^T\psi^T(r), \tag{9}$$

where r_c^s is a cut-off length, and $\psi^T(r)$ represents the common short-range wave function. The coefficient can be calculated by

$$|c_j^T|=\sqrt{\int_0^{r_c^s}\psi_j^F(r)^2}. \tag{10}$$

Therefore, the short-range wave function of the Feshbach molecule can be expressed as

$$|\psi_F(r<r_c^s)\rangle\approx\psi^T(r)\sum_j c_j^T|\sigma_j^T\rangle. \tag{11}$$

For the Feshbach state $|1,1;9/2,-7/2\rangle$ at $B=104$ Gs, we have plotted the short-range wave function $\psi_j^F(r)$ and the normalized wave function $\psi_j^F(r)/c_j^T$ in Fig. 2(b). The normalized wave function $\psi_j^F(r)/c_j^T$ can be approximated by the highest vibrational state of the triplet potential. We have calculated the short-range coefficients c_j^T for the Feshbach molecules in the vicinity of different Feshbach resonances. The results are shown in Table 1. The coefficients c_j^T will be used to calculate the coupling between the Feshbach states and the hyperfine levels of the excited states. Since the triplet s-wave bound state has good quantum numbers $N=0$, $S=1$, and $J=1$, in the following discussions, we use the molecule quantum numbers to represent the basis $|\sigma_j^T\rangle=|N,S,J,M_J,m_{i_{\rm Na}},m_{i_{\rm K}}\rangle$, and the short-range wave function of the Feshbach state can be described by

$$\begin{aligned}&|\psi_F(r<r_c^s)\rangle\\ \propto&\sum_{M_J m_{i_{\rm Na}} m_{i_{\rm K}}} c^T_{NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}}|N,S,J,M_J,m_{i_{\rm Na}},m_{i_{\rm K}}\rangle.\end{aligned} \tag{12}$$

3. Excited states

The excited state used in the STIRAP transfer is a mixture of the singlet electronic excited state $B^1\Pi|v=12,J=1\rangle$ and the triplet electronic excited state $c^3\Sigma\,|v=35,J=1\rangle$, and thus the excited state can be written as a superposition state $|\psi_e\rangle=|\psi_{B^1\Pi}\rangle+|\psi_{c^3\Sigma}\rangle$, where $|\psi_{B^1\Pi}\rangle$ and $|\psi_{c^3\Sigma}\rangle$ represent the singlet and triplet excited states, respectively. The hyperfine level structures of the excited states have been discussed in Refs. [19,20].

The triplet component $|\psi_{c^3\Sigma}\rangle$ accounts for the coupling between the Feshbach state and the electronic excited state, since the short-range wave function of the Feshbach molecule is dominated by the triplet component. The state $|\psi_{c^3\Sigma}\rangle$ can be expanded in the basis $|NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}\rangle$ with $N=1$, $S=1$, and $J=1$. The hyperfine and Zeeman interactions for the $c^3\Sigma$ state are described by

$$H^c=a^{\rm e}_{\rm Na}\boldsymbol{i}_{\rm Na}\cdot\boldsymbol{S}+a^{\rm e}_{\rm K}\boldsymbol{i}_{\rm K}\cdot\boldsymbol{S}+g_s\mu_{\rm B}S_zB, \tag{13}$$

where $a^{\rm e}_{\rm Na}=334$ MHz and $a^{\rm e}_{\rm K}=-28$ MHz are the hyperfine constants of the molecular excited states.

The singlet component $|\psi_{B^1\Pi}\rangle$ is responsible for the coupling between the excited state and the ground state, since the ground molecule state is a singlet state. The $|\psi_{B^1\Pi}\rangle$ state can be expanded in the basis $|J\Omega M_J m_{i_{\rm Na}} m_{i_{\rm K}}\rangle$ with $J=1$ and $\Omega=1$. The $B^1\Pi$ state has negligible hyperfine interaction and the Zeeman interaction is diagonal. The diagonal matrix element is given by $\langle J\Omega M_J m_{i_{\rm Na}} m_{i_{\rm K}}|H^B|J\Omega M_J m_{i_{\rm Na}} m_{i_{\rm K}}\rangle=\mu_B M_J B/(J(J+1))$. The $|NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}\rangle$ state of $c^3\Sigma$ and the $|J\Omega M_J m_{i_{\rm Na}} m_{i_{\rm K}}\rangle$ state of $B^1\Pi$ are mixed by the spin–orbit coupling with a coupling coefficient $\xi_{Bc}=0.54899$ cm^{-1}. Therefore, the energy and the wave function of the hyperfine levels of the excited states are obtained by diagonalizing the coupled Hamiltonian

$$\begin{pmatrix}E_B\boldsymbol{I}+\boldsymbol{H}^B & \xi_{Bc}\boldsymbol{I}\\ \xi_{Bc}\boldsymbol{I} & E_c\boldsymbol{I}+\boldsymbol{H}^c\end{pmatrix}, \tag{14}$$

where $\boldsymbol{I}$ is the identity matrix of dimension $(2J+1)(2i_{\rm Na}+1)(2i_{\rm K}+1)=108$, and $E_B=17701.427$ cm^{-1} and $E_c=17701.074$ cm^{-1} are the energies of the $B^1\Pi|v=12,J=1\rangle$ and $c^3\Sigma\,|v=35,J=1\rangle$ rovibrational states, respectively. The eigenstates contain two branches and the branch including more triplet components is employed to perform the STIRAP. The typical energy level structure of the hyperfine levels of the excited states is plotted in Fig. 3. Because $a^{\rm e}_{\rm K}$ is much smaller

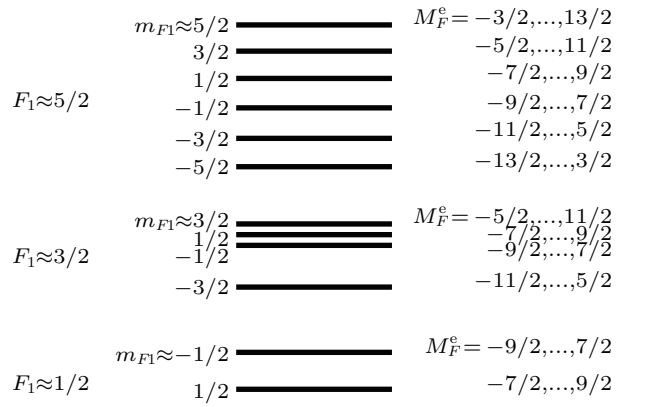


Fig. 3. The energy level structures of the excited states. The quantum numbers $F_1=J+i_{\rm Na}$ and m_{F_1} are approximately good quantum numbers. Each solid line represents 9 nearly degenerate hyperfine states with the same $F_1=J+i_{\rm Na}$ and m_{F_1} but different $m_{i_{\rm K}}$.

than $a^{\rm e}_{\rm Na}$, the quantum numbers $F_1 = J + i_{\rm Na}$, m_{F_1} and $m_{i_{\rm K}}$ can be approximated as good quantum numbers. The hyperfine levels with the same $F_1 = J + i_{\rm Na}$ and m_{F_1} are nearly degenerate. In Fig. 3, the hyperfine levels of the excited states are labelled by these quantum numbers.

The triplet component of the wave function of the hyperfine excited state can be expressed as

$$|\psi_{c^3\Sigma}\rangle \propto \sum_{M_J m_{i_{\rm Na}} m_{i_{\rm K}}} c^{\rm e}_{NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}} |NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}\rangle. \quad (15)$$

Therefore the coupling strength between the hyperfine excited state and the Feshbach state for a q-polarized pump light with $q = 0, \pm 1$ can be calculated by

$$\begin{aligned}\Omega_{\rm ef} &\propto \langle \psi_{c^3\Sigma}|d_q|\psi_F\rangle \propto \sum_{M'_J m'_{i_{\rm Na}} m'_{i_{\rm K}} M_J m_{i_{\rm Na}} m_{i_{\rm K}}} c^{\rm e}_{N'S'J'M'_J m'_{i_{\rm Na}} m'_{i_{\rm K}}} c^{T}_{NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}} \langle N'S'J'M'_J|d_q|NSJM_J\rangle \delta_{m'_{i_{\rm Na}} m_{i_{\rm Na}}} \delta_{m'_{i_{\rm K}} m_{i_{\rm K}}} \\ &\propto \sum_{M_J m_{i_{\rm Na}} m_{i_{\rm K}}} c^{\rm e}_{N'S'J'M_J m_{i_{\rm Na}} m_{i_{\rm K}}} c^{T}_{NSJM_J m_{i_{\rm Na}} m_{i_{\rm K}}} (-1)^{J'-M'_J} \begin{pmatrix} J' & 1 & J \\ -M'_J & q & M_J \end{pmatrix}. \end{aligned} \quad (16)$$

Table 2. The energies of the hyperfine excited states $E^{\rm e}$, relative to a reference frequency of 17700.64 cm^{-1}, and the absolute value of the relative coupling strength $|\Omega_{\rm ef}|$ between different Feshbach states and different hyperfine levels of the excited states. For each Feshbach state with the projection of the total angular momentum M_F, the hyperfine levels of the excited states with $M^{\rm e}_F = M_F, M_F \pm 1$ can be coupled by the pump light.

$\|1,1;9/2,-9/2\rangle$ at $B = 85.7$ Gs						$\|1,1;9/2,-9/2\rangle$ at $B = 78$ Gs					
$M^{\rm e}_F = -5/2$		$M^{\rm e}_F = -7/2$		$M^{\rm e}_F = -9/2$		$M^{\rm e}_F = -5/2$		$M^{\rm e}_F = -7/2$		$M^{\rm e}_F = -9/2$	
$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$
107	0.43					100	0.32				
58	0.18	63	0.24			55	0.33	58	0.31		
8	0.06	9	0.20	11	0.07	7	0.06	9	0.33	10	0.20
–45	0.01	–48	0.07	–50	0.15			–44	0.08	–46	0.22
		–106	0.03	–113	0.06	–90	0.01	–97	0.01	–104	0.05
–224	0.33					–226	0.15				
–231	0.20	–229	0.24			–234	0.05	–232	0.21		
–246	0.14	–243	0.28	–240	0.11	–249	0.12	–246	0.15	–244	0.12
–324	0.07	–328	0.18	–333	0.38	–318	0.07	–323	0.23	–327	0.43
–446	0.11	–450	0.02	–453	0.63	–442	0.21	–445	0.40	–448	0.43
–512	0.04	–517	0.03			–505	0.10	–510	0.06		
$\|1,1;9/2,-7/2\rangle$ at $B = 104$ Gs						$\|1,1;9/2,-7/2\rangle$ at $B = 89.9$ Gs					
$M^{\rm e}_F = -3/2$		$M^{\rm e}_F = -5/2$		$M^{\rm e}_F = -7/2$		$M^{\rm e}_F = -3/2$		$M^{\rm e}_F = -5/2$		$M^{\rm e}_F = -7/2$	
$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$
166	0.19					150	0.2				
117	0.38	123	0.01			105	0.19	110	0.04		
65	0.11	69	0.23	74	0.31	57	0.33	61	0.27	65	0.02
9	0.06	11	0.16	13	0.08	7	0.08	8	0.36	10	0.21
–51	0.03	–53	0.08	–56	0.14	–45	0.01	–47	0.10	–49	0.27
–109	0.01	–118	0.04	–126	0.09	–95	0.01	–103	0.03	–110	0.08
–222	0.39	–220	0.03			–225	0.15	–223	0.01		
–228	0.25	–226	0.26	–224	0.01	–232	0.08	–230	0.20	–228	0.01
–242	0.17	–238	0.28	–235	0.07	–247	0.17	–244	0.17	–241	0.07
–331	0.08	–336	0.19	–341	0.32	–322	0.10	–327	0.29	–331	0.42
–453	0.10	–457	0.13	–462	0.59	–445	0.26	–449	0.40	–452	0.28
–523	0.06	–528	0.14	–534	0.18	–510	0.09	–516	0.04	–521	0.2
$\|1,1;9/2,-5/2\rangle$ at $B = 128$ Gs						$\|1,1;9/2,-5/2\rangle$ at $B = 104$ Gs					
$M^{\rm e}_F = -1/2$		$M^{\rm e}_F = -3/2$		$M^{\rm e}_F = -5/2$		$M^{\rm e}_F = -1/2$		$M^{\rm e}_F = -3/2$		$M^{\rm e}_F = -5/2$	
$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$	$E^{\rm e}$/MHz	$\sqrt{6}\|\Omega_{\rm ef}\|$
186	0.24	193	0.05			162	0.24	169	0.05		
132	0.33	138	0.01	145	0.01	113	0.08	119	0.07	126	0.02
74	0.06	79	0.22	85	0.03	62	0.30	66	0.21	71	0.01
11	0.05	14	0.12	17	0.09	7	0.09	9	0.37	11	0.21
–58	0.05	–61	0.09	–63	0.13	–50	0.04	–52	0.12	–54	0.32
–126	0.02	–135	0.06	–144	0.12	–103	0.01	–112	0.04	–121	0.13
–218	0.44	–217	0.09	–215	0.10	–223	0.16	–221	0.01	–220	0.02
–223	0.28	–222	0.33	–219	0.13	–230	0.10	–228	0.30	–225	0.00
–235	0.17	–232	0.26	–229	0.03	–244	0.23	–241	0.20	–237	0.04
–342	0.07	–348	0.20	–354	0.28	–328	0.14	–333	0.32	–338	0.40
–463	0.06	–469	0.20	–474	0.55	–450	0.28	–455	0.34	–459	0.17
–538	0.06	–545	0.25	–551	0.22	–519	0.07	–525	0.15	–531	0.24

The energies of the hyperfine levels of the excited state, relative to a reference frequency of 17700.64 cm^{-1}, and the relative coupling strength between the hyperfine excited states and the Feshbach states in the vicinity of different Feshbach resonances are listed in Table 2. For each Feshbach state with M_F, three hyperfine levels of the excited states with the total projection $M_F^e = M_F, M_F \pm 1$ can be coupled by choosing the polarization of the lasers. To perform the STIRAP, we can choose a resolvable hyperfine level of the excited state, which should have a strong coupling with the Feshbach state and should be well separated from neighbouring hyperfine excited states. The good candidates are the states with $F_1 \approx 5/2, m_{F_1} \approx 5/2, \ldots, -5/2$, the states with $F_1 \approx 3/2, m_{F_1} \approx -3/2$, and the states with $F_1 \approx 1/2, m_{F_1} \approx \pm 1/2$.

The coupling between the excited state and the ground state can be easily calculated once the singlet component of the excited state is obtained. The ground state can be expressed as $|NSJM_J m_{i_{Na}} m_{i_K}\rangle$ with $N = S = J = M_J = 0$. The singlet component accounts for the coupling between the excited state and the ground state, and it can be expressed as,

$$|\psi_{B^1\Pi}\rangle \propto \sum_{M'_J m'_{i_{Na}} m'_{i_K}} c^e_{J'\Omega' M'_J m'_{i_{Na}} m'_{i_K}} |J'\Omega' M'_J m'_{i_{Na}} m'_{i_K}\rangle. \quad (17)$$

Therefore the coupling strength between the hyperfine level of the excited state and the ground state $|\psi_g\rangle = |NSJM_J m_{i_{Na}} m_{i_K}\rangle$ for the q-polarized Stokes light with $q = 0, \pm 1$ is described by

$$\begin{aligned}\Omega_{eg} &\propto \langle \psi_{B^1\Pi}|d_q|\psi_g\rangle \\ &\propto \sum_{M'_J m'_{i_{Na}} m'_{i_K}} c^e_{J'\Omega' M'_J m'_{i_{Na}} m'_{i_K}} \\ &\quad \times \langle J'\Omega' M'_J|d_q|NSJM_J\rangle \delta_{m'_{i_{Na}} m_{i_{Na}}} \delta_{m'_{i_K} m_{i_K}} \\ &\propto c^e_{J'\Omega' M_J m_{i_{Na}} m_{i_K}} (-1)^{J'-M'_J} \begin{pmatrix} J' & 1 & J \\ -M'_J & q & M_J \end{pmatrix}. \quad (18)\end{aligned}$$

The hyperfine level of the ground state that can be populated in the STIRAP can be understood as follows. For a hyperfine level of the excited state with M_F^e, the quantum number m_{i_K} is approximately a good quantum number. Therefore, for a Stokes light with q polarization, the hyperfine level of the ground state that can be dominantly populated from this hyperfine excited state is the $|NSJM_J, m_{i_{Na}} = M_F^e - q - m_{i_K}, m_{i_K}\rangle$ state.

4. Conclusion

In summary, we have presented an intensive investigation of the coupling between the Feshbach states and the hyperfine levels of the excited states in the adiabatic creation of the $^{23}Na^{40}K$ molecule. The $^{23}Na^{40}K$ ground state molecules have 36 hyperfine levels. By employing the different Feshbach molecules discussed in the present work, in principle we can address 21 hyperfine levels of the ground state by choosing the proper laser polarization and hyperfine levels of the excited states. This is more efficient and convenient than using the microwave pulses to prepare different hyperfine levels of the molecular ground states. This is because a microwave Raman π pulse or two resonant microwave π pulses can only change the projection of the nuclear spin $m_{i_{Na}}$ or m_{i_K} by 1. This means many π pulses may be required if we prepare one hyperfine ground state by the STIRAP and use microwave pulses to transfer it to other hyperfine states. However, by choosing proper hyperfine excited states and laser polarizations, various hyperfine states can be populated by simply preforming the STIRAP. By preparing the different hyperfine levels of the molecule states, we can study the atom-molecule scattering resonances in different spin state combination, precisely change the number of open channels, and investigate the role of nuclear spins in the ultracold molecule collisions.

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