Electric-field-modified Feshbach resonances in ultracold atom–molecule collision*

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We present a detailed analysis of near zero-energy Feshbach resonances in ultracold collisions of atom and molecule, taking the He–PH system as an example, subject to superimposed electric and magnetic static fields. We find that the electric field can induce Feshbach resonance which cannot occur when only a magnetic field is applied, through couplings of the adjacent rotational states of different parities. We show that the electric field can shift the position of the magnetic Feshbach resonance, and change the amplitude of resonance significantly. Finally, we demonstrate that, for narrow magnetic Feshbach resonance as in most cases of ultracold atom–molecule collision, the electric field may be used to modulate the resonance, because the width of resonance in electric field scale is relatively larger than that in magnetic field scale.

Keywords: Feshbach resonance, ultracold atom–molecule collision

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1. Introduction

Cold atomic and molecular species are extremely versatile systems to investigate a wealth of fascinating phenomena, ranging from precision measurement[1] and quantum-controlled chemistry,[2] to condensed-matter physics.[3] Ultracold atoms and molecules are usually confined in electromagnetic or magneto–optical traps, and collision cross sections of ultracold species change dramatically as the external field varies through a resonance. Tunable Feshbach resonances (FR) thus are powerful tools to control the interaction and scattering properties of ultracold species.[4] Magnetic FRs have been used to realize Bose–Einstein condensates of alkali metal atoms and create associated ultracold molecular species by coherently linking ultracold atoms.[5] In addition, FRs provide experimental access to interesting three-body Efimov states,[6] loosely bound molecules,[7] and strongly correlated many-body states of matter.[8]

The coupling between different internal states of the two-body collision system can cause interaction between different scattering channels. A Feshbach resonance[4,7] occurs when a bound state in a closed-channel exists at the same energy as the dissociation energy threshold of collision pairs. Because the bound states and collision pairs have, in general, different electric or magnetic moments, an external field can be used to tune both their energies and corresponding energy differences, and thus tune the FRs. Magnetic FR has been the major tool in various experiments of ultracold atomic and molecular gases.[9,10] A second way of tuning the FR is to apply a dc-electric field.[11–13] The electric field induces an electric dipole–dipole interaction between heteronuclear colliding atoms. This anisotropic interaction couples the states of different orbital angular momenta, and changes the width of FR resonance to some degree. A recent theoretical work[14] has demonstrated the possibility of inducing and modifying the position and width of narrow FRs by intense nonresonant radiation. The authors show that the resonance widths can be increased by three orders of magnitude up to a few Gauss. The use of combined electric and magnetic fields to control interatomic and intermolecular interactions has also been suggested. It has been demonstrated that dynamics of molecules in a regime of ultracold temperature may be sensitive to the magnitude of an applied field,[15–19] and the combination of electric and magnetic fields may be used to control both the position and width of FRs independently, leading to total control over the character of ultracold collisions.[20] In addition, the magnetic control of collision dynamics is limited to paramagnetic molecules; therefore, the application of electric fields may expand the scope of studies of correlative phenomena in ultracold polar gas.

Recently, we investigated the collisional dynamics of ^{3}He atom and PH($^3\Sigma$) molecule in the presence of a magnetic field.[21] The work has its background of Helium buffer-gas cooling and magnetic trapping experiments, which was first performed successfully for CaH molecule and later for other molecules NH, CaF, and MnH, etc.[30] Our work shows that the PH molecule is a promising candidate for this type of experiment. In the present paper, we will explore the effects of an external electric field on magnetically induced FRs in the ^{3}He–PH collision system. In Section 2 we briefly describe the methods we use to perform the bound state and scattering calculations. In Section 3, we discuss the tuning of magnetic FRs by a dc-electric field and shall conclude in Section 4.

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2. Theoretical approach

To precisely estimate the position of a near zero-energy Feshbach resonance, we first compute the bound state energies of the collision complex as functions of external fields. The method used in this work is analogous to that described in our previous papers.[21–24] Here, we extend it to include the electric and magnetic field effect. The Hamiltonian for the atom–diatom complex has the following form:

$$\hat{H} = -\frac{\hbar^2}{2\mu}R^{-1}\frac{\mathrm{d}^2}{\mathrm{d}R^2}R + \frac{\hat{L}^2}{2\mu R^2} + \hat{H}_{\mathrm{mol}} + V(R,r,\theta), \quad (1)$$

where μ is the reduced mass of the collisional system, R is the distance between the center of mass of the diatomic molecule and the atom, and $\hat{L}$ is the orbital angular momentum for the collision. The $V(R,r,\theta)$ is the interaction potential which vanishes as $R \to \infty$. The $\hat{H}_{\mathrm{mol}}$ denotes the Hamiltonian for a $^3\Sigma$ molecule interacting with electric and magnetic fields and is expressed as

$$\hat{H}_{\mathrm{mol}} = b_{\mathrm{e}}\hat{n} + \hat{H}_{ns} + \hat{H}_{ss} + g\mu_0\hat{B}\cdot\hat{s} - \hat{E}\cdot\hat{d}, \quad (2)$$

where b_{e} is the rotational constant of the molecule in the ground vibration state, $\hat{n}$ and $\hat{s}$ are the rotational and spin angular momenta, $\hat{H}_{ns}$ and $\hat{H}_{ss}$ are the spin–rotation and spin–spin interaction terms, $\hat{E}$ and $\hat{B}$ are the electric and magnetic fields, and $\hat{d}$ is the electric dipole moment of the molecule. We assume that the electric and magnetic field vectors are both oriented along the Z space fixed axis.

In the presence of parallel electric and magnetic fields, the total angular momentum J and the total parity which is given by $p = (-1)^{n+L+1}$ are not the good quantum numbers, the only rigorously good quantum number is the total angular momentum projection $M_J = m_n + m_s + M_L$, where m_n, m_s, and M_L are the projections of $\hat{N}$, $\hat{S}$, and $\hat{L}$ individually. There are several basis sets that could be used to expand the eigenfunctions of Eq. (1). We use an uncoupled basis set $|\chi_q(R)\rangle\,|NM_N\rangle\,|SM_S\rangle\,|LM_L\rangle$.[25] The radial basis $|\chi_q(R)\rangle$ are determined as numerical eigensolutions to a vibrational Schrödinger equation using the one-dimensional potential $V(R,r_e,\theta_e)$ cut at steady structure (r_e,θ_e).[21] The matrix elements of the interaction with an electric field can be calculated as follows:[18]

$$\begin{aligned}&\langle nm_n|\langle sm_s|\langle LM_L| - \hat{E}\cdot\hat{d}\,|n'm_n'\rangle\,|sm_s'\rangle\,|L'M_L'\rangle \\ &= -\delta_{nn'}\delta_{m_nm_n'}\delta_{m_sm_s'}\delta_{LL'}\delta_{M_LM_L'}Ed(-1)^{m_n} \\ &\quad\times\sqrt{(2n+1)(2n'+1)}\begin{pmatrix} n & 1 & n' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} n & 1 & n' \\ -m_n & 0 & m_n'\end{pmatrix}. \quad (3)\end{aligned}$$

The other angular matrix elements of operators in Eqs. (1) and (2) can be found in Ref. [25] and the radial matrix elements are calculated by numerical integration. The energies of bound states and corresponding eigenfunctions of the complex are determined from solution of the corresponding secular Eq. (1). The calculations are performed for each of given M_J and electric and magnetic fields.

As for the scattering calculations, we adopt the method for atom–molecule collisions in combined electric and magnetic fields developed by Tscherbul and Krems.[17,26,27] Because the asymptotical Hamiltonian in Eq. (2) is not diagonal in the uncoupled angular basis set $\phi_i = |NM_N\rangle\,|SM_S\rangle\,|LM_L\rangle$, ϕ_i then cannot be used to describe the asymptotic states of the dressed molecule in the presence of the field. We use instead a transformative basis set $\chi_\alpha = \sum_i C_{\alpha i}\,|NM_N\rangle\,|SM_S\rangle$,[28] which diagonalizes the monomer Hamiltonian (2) as

$$[CH_{\mathrm{mol}}C^{-1}]_{\alpha\beta} = \varepsilon_\alpha\delta_{\alpha\beta}, \quad (4)$$

where ε_α is the energy level of the dressed diatomic molecule in the external field. The field removes the degeneracy in $m_j = m_n + m_s$ and each energy level ε_α correlating with a unique value of m_j labeled by $m_j(\alpha)$, where j is the total angular momentum of diatomic molecule, $\hat{j} = \hat{n} + \hat{s}$. For given values of M_J and m_j, $M_L = M_J - m_j(\alpha)$. The basis set describing the collision process is obtained by including the possible values of the quantum number L for each value of α. With the basis set, the close-coupling equations are

$$\begin{aligned}&\left(\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \frac{L(L+1)}{R^2} + 2\mu[E-\varepsilon_\alpha]\right)F_{\alpha,M_L,L}(R) \\ &= 2\mu\sum_{\alpha',M_L',L'}[C^{\mathrm{T}}VC]_{\alpha,M_L,L}^{\alpha',M_L',L'}F_{\alpha',M_L',L'}(R). \quad (5)\end{aligned}$$

The cross sections for elastic and inelastic scattering are computed from the S matrix as follows:

$$\sigma_{\alpha\to\alpha'} = \frac{\pi}{k_\alpha^2}\sum_{M_J}\sum_{M_LL}\sum_{M_L'L'}\left|\delta_{\alpha\alpha'}\delta_{M_LM_L'}\delta_{LL'} - S^{M_J}_{\alpha LM_L;\alpha'L'M_L'}\right|^2. \quad (6)$$

The coupled equations are propagated on radial grid points using Johnson's log-derivative algorithm.[29]

3. Applications to the He–PH collisions

We now focus on the electric-field modified Feshbach resonance in ultracold collisions of atom and molecule, taking the ^{3}He–PH collision system as an example. The calculations are performed using the same potential–energy surface and parameters as presented in Ref. [21]. The positions of Feshbach resonances can be identified by the bound state energies of the collision complex as functions of an external field. Figure 1 shows the bound state energies of ^{3}He–PH for $M_J = 0$ and $M_J = -1$ as a function of the magnetic field. The energies are relative to the ground state energy of PH ($^3\Sigma^-$) which is -0.088 cm^{-1}. When an external field is applied, each level at zero field splits into components that can be labeled with the approximate quantum numbers $M_s = 0, \pm1$, and L. As expected, the Zeeman splits are approximately linear for He–PH in the range of fields studied. This is because for a rotational

$n = 0$ state, the coupling arise from the off-diagonal term of $V(R, \theta)$ and spin–spin interaction that mix the rotational excited levels, but the spacing ($\sim 16.8\ \mathrm{cm}^{-1}$) between $n = 0$ and $n = 1$ levels for PH is larger than the Zeeman split tuned by a magnetic field. While an electric field is further added, the energies of bound states will shift slightly, but no new energy level emerges.

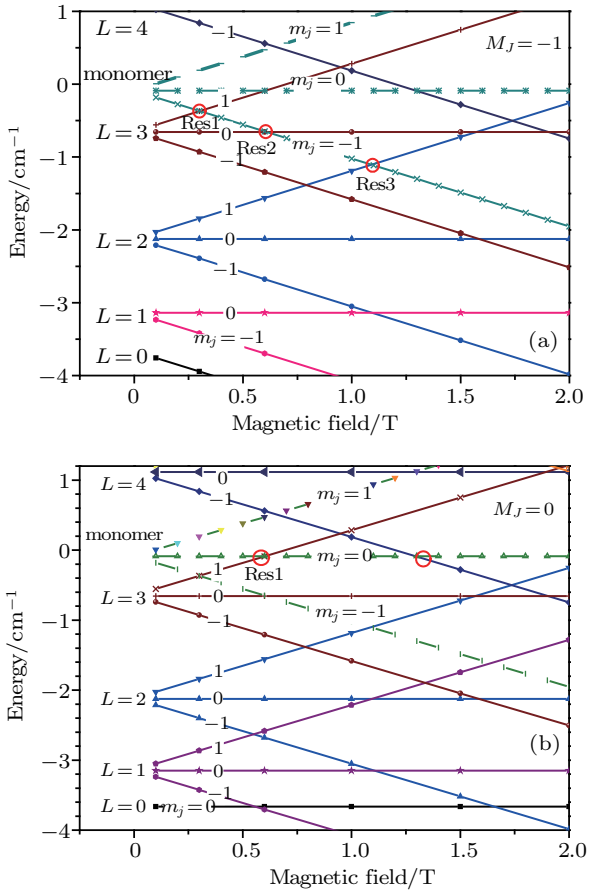


Fig. 1. (color online) Bound-state energy levels of He–PH for $M_J = -1$ (a) and $M_J = 0$ (b) as a function of magnetic field.

In Fig. 1, we also show the rotational $n = 0$ energies of a monomer PH molecule as functions of the magnetic field as dotted lines. When the collision pairs approach each other with near-zero kinetic collision energy, the total collision energy will be approximately equal to the bound state energy of complex, which is the energy constraint for the presentation of a Feshbach resonance. Another constraint is the same conserved quantity of collision channels as the relative bound states.[25] In the case of parallel electric and magnetic fields, M_J is the only conserved quantity. At low collision energies, the cross sections are dominated by incoming s-wave, $L = 0$, and $M_L = 0$. It means that the m_j of a monomer molecule should be equal to the M_J of the bound state of complex. Based on this analysis, we can estimate the positions of FR shown in Fig. 1 by circles and labels of "Res". A detailed scan across a small range of fields in the vicinity of crossings and careful extrapolation of the bound state energies with external fields will give more precise positions of FRs. The scattering calculations are then performed at surrounding values of electric and magnetic fields corresponding to these positions respectively.

3.1. $M_J = -1$, Res3

The FR at $M_J = -1$, Res3 has been reported in our previous work[21] with only the magnetic field applied. In the ultracold collision, we want s-wave resonance, with $L = 0$ in the incoming channel. For ^{3}He colliding with PH ($m_j = -1$) at ultralow kinetic energy, only elastic scattering can occur. Scattering into the $L > 0$ channels is strongly suppressed by the centrifugal barriers. Fitting the scattering length, we obtain the resonance position $B_0 = 10917.111$ G, width $\Delta B = 2 \times 10^{-4}$ G and background scattering length $a_{\mathrm{bg}} = 8.6$ Å.

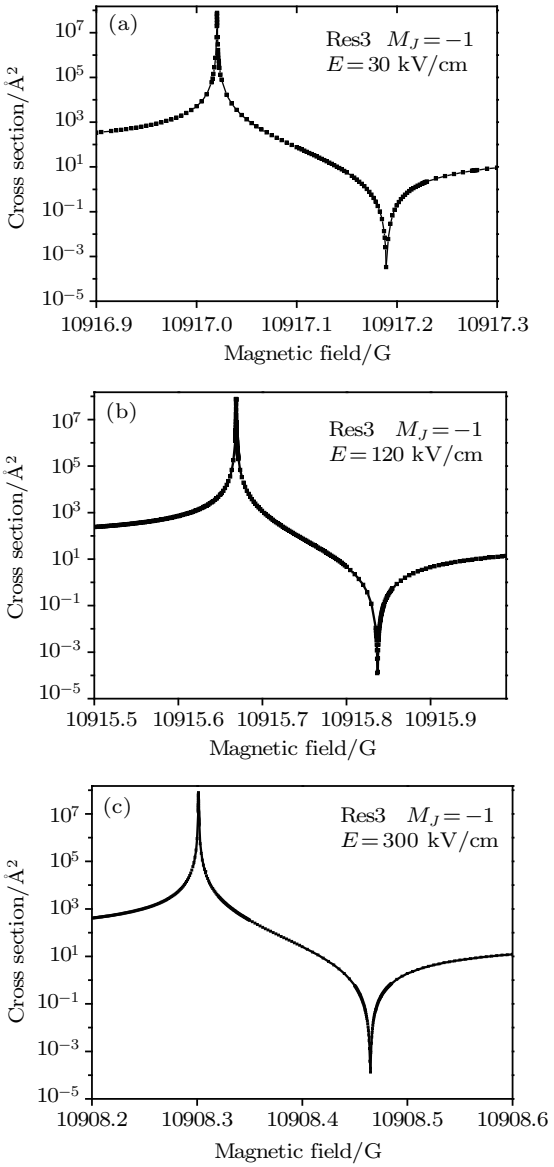


Fig. 2. The effect of the electric field on the magnetically tuned resonance at Res3 in Fig. 1(a). (a) $M_J = -1$, $E = 30$ kV/cm; (b) $M_J = -1$, $E = 120$ kV/cm; (c) $M_J = -1$, $E = 300$ kV/cm.

Figure 2 shows the magnetically tuned FR at three values of electric fields. It can be seen that electric fields can shift

the position of FRs significantly. When the electric field increases, the position moves to the low magnetic-field direction (corresponding to a shift of the associated bound state to high energy). The width of resonance changes trivially and is still in order of 10^{-4} G. The magnetic field of this degree of accuracy is difficult to be produced in an experiment. The FR with a width of this order of magnitude is thus unlikely to be tuned by the magnetic field. From the energy point of view, a narrow FR width of magnetic field implies a narrow energy interval. The electric field energy density is customarily smaller than that of the magnetic field, so for a given energy interval, there is a relatively larger field interval in the electric field than the magnetic field. This fact can be used to tune the narrow magnetic FRs by the electric field. Figure 3 displays the cross section as a function of the electric-field. The magnetic field is fixed at 10917.1 G, which is in the vicinity of the magnetic FR. It can be seen that the electric field can also be used to achieve the control of the FR. The resonance width attains 0.14 kV/cm in the electric field scale. It thus is preferable that, for a narrow magnetic FR, we can first adjust the magnetic field to a position near the FR, and then finely tune the electric field to achieve resonance.

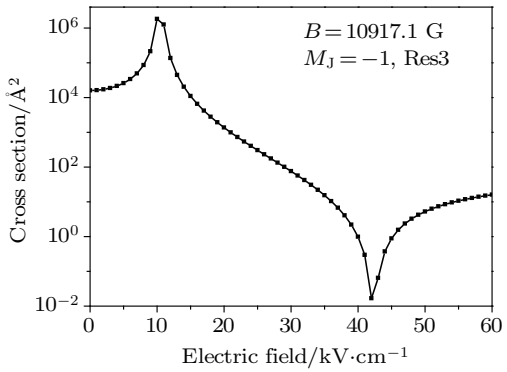


Fig. 3. Variation in the cross section for s-wave collisions as a function of the electric-field strength with fixed magnetic field at 10917.1 G.

3.2. $M_J = -1$, Res1, and Res2

When only a magnetic field is applied, no FRs take place at the intersection points $M_J = -1$, Res1 and $M_J = -1$, Res2. This is because the magnetic field cannot couple the rotational states of the PH monomer molecule with different parities,[25] the incoming s-wave channel ($L = 0$, $n = 0$, $m_j = -1$) has parity of -1, but the bound states of the complex relative to the resonances are ($L = 3$, $m_j = 0, 1$) with parity of $+1$. The lowest Zeeman energy level of the monomer molecule labeled with ($n = 0$, $m_j = -1$) has a main ingredient of ($n = 0$, $m_n = 0$, $m_s = -1$). The electric field can produce coupling of the states of different parities (see Eq. (3) $-3j$ sign) with $\Delta n = n - n' = \pm 1$, and cause the dynamic mixing between ($n = 0$, $m_n = 0$, $m_s = -1$) and ($n = 1$, $m_n = 0$, $m_s = -1$) rotational states. Therefore, the electric field will induce FRs which cannot occur with only the magnetic field applied. Figure 4 shows the scattering length of FRs at $M_J = -1$, Res1, and Res2 induced by an electric field of 30 kV/cm. The position of FR shifts to the high magnetic-field direction as the electric field increases, contrary to that at $M_J = -1$, Res3. The position of the resonance shifted to the high magnetic field or low magnetic field direction, is determined according to whether the discrete bound state crosses resonance from above or below. The electric-induced FRs have first been demonstrated in heteronuclear mixtures of bi-alkali atomic gases.[11,12,15,20] The anisotropic interaction between the instantaneous dipole moment of a heteronuclear collision complex with the external electric field, couples the states of different orbital angular momenta with $\Delta L = L - L' = \pm 1$, and results in multiple resonances. The mechanism is thus different from that described here.

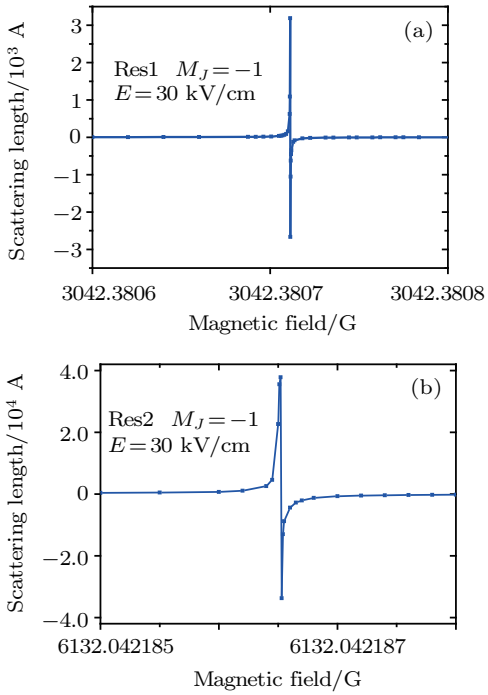


Fig. 4. (color online) Scattering length of FRs at $M_J = -1$, Res1, and Res2 in Fig. 1(a) induced by an electric field of 30 kV/cm.

3.3. $M_J = 0$, Res1

In Fig. 1(b), the monomer molecule threshold state ($n = 0$, $m_j = 0$) crosses two bound states of complex, one is ($L = 3$, $m_j = 1$) and the other is ($L = 4$, $m_j = -1$). Doing scattering calculations in the vicinity of two crossings, we only find a resonance that is marked with "Res1", and do not find resonance at the other crossing point, possibly due to the suppression by a centrifugal energy barrier. This resonance has not been reported in our previous work.[21]

Figure 5 illustrates the cross section as functions of the magnetic field near the crossing point fixed the electric field at zero and 120 kV/cm, respectively. For He colliding with PH ($m_j = 0$), elastic and inelastic scattering are possible. The in-

coming channel is ($L = 0$, $n = 0$, $m_j = 0$), the outcoming channel may be either elastic scattering channels ($L = 0$–8, $n = 0$, $m_j = 0$), or inelastic channels ($L = 0$–8, $n = 0$, $m_j = -1$). In ultracold collision energy, the elastic channels with $L > 0$ make no significant contribution.

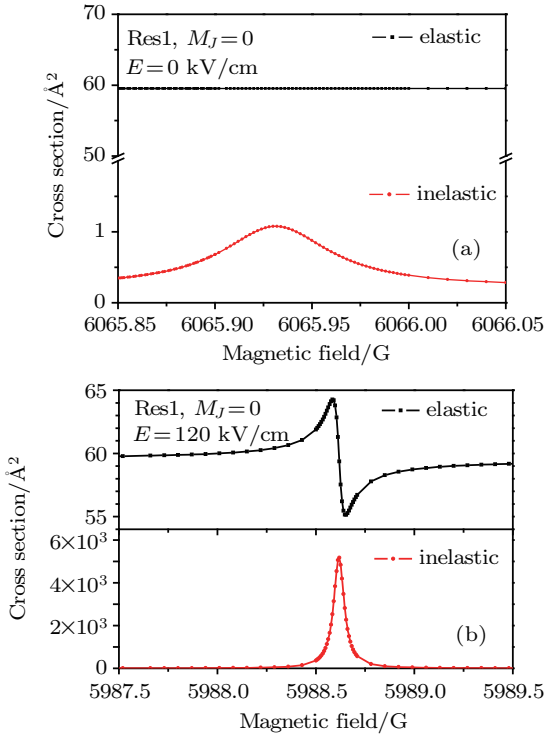


Fig. 5. (color online) Cross section for s-wave collisions as a function of the magnetic field strength with a fixed electric field at 0 kV/cm and 120 kV/cm, respectively.

The following characteristics can be seen. (I) When the electric field is zero, the resonance phenomenon occurs only in the inelastic cross section, while the elastic cross section is essentially the same size of about 59.5 Å^2. (II) The electric field induces the resonance in the elastic cross-section, and the resonance position shifts toward a low magnetic field with the electric field increasing. The resonance peak is antisymmetric. (III) The affect of the electric field on the resonance amplitude of the inelastic cross section is very obvious, for example, from about 1 Å^2 at $E = 0$ to 5×10^4 Å^2 at $E = 120$ kV/cm. (IV) The line shape of the inelastic cross section is symmetrical.

4. Conclusion

When the collision energy of free atom and molecule coincides with that of a bound state of complex, the Feshbach resonance phenomenon occurs. In this work, we study the effect of the electric field on the magnetic Feshbach resonance in atom–molecule ultracold collision taking the He–PH system as an example. We begin with the examination of bound state energies of the collision complex with the variation of the electromagnetic field, and find the energy intersection points of the collision system and the bound state of the complex. This method is especially effective for determining the very narrow resonance position as in the case of most atom–molecule ultracold collisions. The close coupled scattering calculations are then performed by scanning the electromagnetic field around these cross-over points carefully. Results show as follows that: (i) the electric field can induce Feshbach resonance, which cannot occur when only a magnetic field is applied; (ii) the electric field can shift the position of the magnetic Feshbach resonance, and can change the amplitude of resonance significantly; (iii) the width of resonance in electric field scale is relatively larger than that in magnetic field scale. For narrow magnetic FR, the control by an electric field may be preferable.

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