Chapter 7

Further studies and outlook
We have developed new theoretical methods for treating electric field effects on two heteronuclear atoms or a polar molecule. So far we have applied our theoretical techniques to the case of Li + Cs system only. However, our methods are more general and be applied to all other polar systems of current interest such as KRb, RbCs, NaCs and so on. The K + Rb system is particularly important for ultracold PA experiments because of its exceptionally strong excited long-range interactions. In addition, both K and Rb atoms have a rich variety of stable isotopes, $^{39}$K, $^{41}$K, $^{40}$K, $^{85}$Rb and $^{87}$Rb. We have chosen bosonic $^{41}$K$^{87}$Rb system for our study since several experimental works have been reported with $^{41}$K$^{87}$Rb [1, 2] for the production of quantum degenerate gas of polar molecules.

Figure 7.1: The interaction potentials and the dipole moment functions (inset) of the KRb molecule in the $^1\Sigma$ (red lines) and $^3\Sigma$ (blue lines) states.

### 7.1 Further studies: KRb system

In this chapter we present results of some further studies on electric field effects on $^{41}$K$^{87}$Rb system. Ultracold heteronuclear polar KRb molecules have attracted tremendous attention in recent times. The presence of a permanent dipole moment in the absolute rovibrational ground state ($^v = 0, ^J = 0$) makes external control very convenient.

Figure 7.1 show the interaction potentials and the dipole moment functions in the $^1\Sigma$ and $^3\Sigma$ states for KRb molecule. The potential energy curves and the dipole moment functions are taken from Ref. [3] and [4], respectively. For both $^{41}$K and $^{87}$Rb, $^i_1 = ^i_2 = 3/2$ and $^s_1 = ^s_2 = 1/2$. Therefore according to the relation $\vec{f}_j = \vec{s}_j + \vec{i}_j$, only four collisional channels are possible as given in table 7.1. These four hyperfine channels
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Table 7.1: Four different hyperfine channels of $^{41}$K and $^{87}$Rb.

<table>
<thead>
<tr>
<th>Channel index</th>
<th>$f_1(^{41}$K)</th>
<th>$f_2(^{87}$Rb)</th>
<th>$f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>b</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>c</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>d</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
</tbody>
</table>

![Diagram showing potentials of KRb](image_url)

Figure 7.2: The long range part of the potentials of KRb in different diabatic hyperfine channels as a function of the internuclear separation $R$ are plotted. $f_1$ and $f_2$ are the hyperfine quantum numbers of the $^{41}$K and $^{87}$Rb, respectively.

are shown in Fig. 7.2. In 2009 Aikawa et. al. [1] have directly converted laser-cooled $^{41}$K and $^{87}$Rb atoms into ultracold $^{41}$K$^{87}$Rb molecules in the ro-vibrational ground state via PA followed by stimulated Raman adiabatic passage. As they have prepared both K and Rb atoms in their lowest hyperfine states i.e. $f_1 = 1$, $f_2 = 1$, we have chosen this channel for our numerical calculation. The hyperfine constant of $^{41}$K = 127.007, and $^{87}$Rb = 3417.341 [5].

Next, we have shown the electric field effects on continuum states of $^{41}$K + $^{87}$Rb collision. We have solved Eq. (3.61) as given in chapter 3, under the approximation of a single hyperfine channel and determine the scattering cross-section $\sigma$ according to Eq. (3.63). Unlike $^7$Li$^{133}$Cs system, convergent results for scattering cross-section as a function of electric field are obtained only for a minimum angular momentum of $\ell = 6$. In fig. 7.3. the scattering cross-section is plotted as a function of electric field for three different collisional energies. Like LiCs a prominent resonant structure appears only in the ultracold regime. The first resonant peak is obtained near 985 kV/cm. Though the cross-section increases by three orders of magnitude at resonant electric field but the amplitude of the wave
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Figure 7.3: Total elastic cross-section $\sigma$ in cm$^2$ as a function of electric field $\mathcal{E}$ in kV/cm is plotted for three different collisional energies $E = 50 \mu K$ (black line), $500 \mu K$ (red line) and $5 \text{ mK}$ (green line).

function at resonant electric field does not increase much as shown in the upper and lower panel of Fig. 7.4.

Figure 7.4: Energy normalized scattering wave function is plotted as a function of the internuclear separation $R$ (a.u.) at zero electric field $\mathcal{E} = 0$ (upper panel) and the first resonant electric field $\mathcal{E} = 985 \text{ kV/cm}$ (lower panel).
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Table 7.2: The change $\Delta v,j,M$ in GHz in binding energy of the field-dressed ground bound state $(v,j,M)$ with respect to its field-free binding energy for different electric field strengths in kV/cm.

<table>
<thead>
<tr>
<th>$E$ (kV/cm)</th>
<th>$\Delta_{35,0,0}$</th>
<th>$\Delta_{4,0,0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>-2.35</td>
<td>-3.44</td>
</tr>
<tr>
<td>100</td>
<td>1.72</td>
<td>-4.77</td>
</tr>
<tr>
<td>500</td>
<td>3.71</td>
<td>-21.56</td>
</tr>
<tr>
<td>985</td>
<td>-0.19</td>
<td>-70.52</td>
</tr>
<tr>
<td>1000</td>
<td>0.02</td>
<td>-72.01</td>
</tr>
</tbody>
</table>

The effects of electric field on rovibrational states of the ground potential for the chosen hyperfine channel have been calculated. We have considered $v = 35, J = 0$ and $v = 4, J = 0$ vibrational states to show the effect of electric field on high- and low-lying bound states of the ground potential. In both the cases the magnetic quantum number is fixed at $M = 0$. The shift in binding energy with respect to the field-free part for different electric field strengths are presented in table 7.2. The shift as given by $\Delta v,j,M(E) = -E_{v,j,M}(E) + E_{v,j,M}(0)$ is also defined previously in chapter 4. With increasing electric field strength, binding energy of the low-lying vibrational states increases whereas for high-lying states it shows oscillatory behavior. This is in contrast with the LiCs case where the binding energy of the high-lying states increases and that of the low-lying states shows oscillatory behavior. As the dipole moment function peaks around the equilibrium internuclear separation it will significantly affect the low-lying states than the high-lying states as shown in table 7.2.

7.2 Outlook

In the presence of an external static electric field, a large number of partial waves in the ground continuum of scattering states of heteronuclear atoms becomes strongly coupled giving rise to anisotropic scattering resonances at low energy. Electric field can also non-perturbatively affect the rovibrational states of a heteronuclear molecule. For calculating bound state wave functions in the presence of an external static electric field, we have developed a non-perturbative numerical method based on renormalized Numerov algorithm. We have used field-dressed wave functions to calculate one- and two-color PA spectra and shown that it is possible to enhance both one- and two- color PA rates by several orders of magnitude even at electric field strength on the order of a few hundred kiloVolt per centimeter. Moreover, higher rotational levels in the excited electronic state...
become populated due to electric field-induced rotational anisotropy. This is not possible at ultracold temperature in the absence of a static electric field.

All our calculations of PA spectrum have been carried out for low intensity PA lasers. It would be interesting to investigate coherent PA of heteronuclear atom-pairs in intense laser fields in the presence of a static electric field of moderate strength of experimental relevance for controlling rotation-vibration coupled molecular states with a view to attain efficient state transfer with multiple lasers. Static electric field strength ranging from 100 to 500 kV/cm [6] are of current interest. There are practical difficulties to use an electric field larger than 500 kV/cm in an experiment with cold atoms. There is an alternative way to produce nonperturbative electrical effects in scattering states by controlling a shape resonance with a non-resonant intense laser field as proposed by González-Férez and Koch [7]. To induce an equivalent anisotropic resonance effect between two similar atoms with a laser field, the required intensity of laser is of the order of $10^{13}$ W cm$^{-2}$. For two different atoms there will be combined effects of permanent and induced dipole interactions due to an intense laser field. However, due to dynamical nature of the laser field, the possibility of transitions among different rotational states in ground state manifold can not be ruled out. Nevertheless, it would be an interesting pursuit to device an alternative approach to realize the discussed effects with an intense laser field.
Bibliography


