

Bound-free transitions in $H + H^-$ collisions

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Abstract. The processes of photo-detachment or ionization of stable molecules are widely investigated in modern atomic physics. But the present work deals with the calculation of the photo-detachment cross-sections in the case of negative quasi-molecules formed during collisions. The reaction $H + H^- + \hbar\omega \rightarrow H + H + e$ has been taken as an example of bound-free transitions in single-active-electron quasi-molecules. For simplicity, we discuss the one-dimensional case in the frame of the zero-range potential model.

1. Introduction

The study of radiative transitions in collisional quasi-molecules, that is temporary molecules formed during atom or ion collisions, is one of the traditional areas in spectroscopy. Until recently the study has mainly been limited to bound-bound transitions between quasimolecular states. In particular, the spectral profiles produced by the reaction of charge exchange $H + H^- \rightarrow H^- + H + \hbar\omega$ was regarded in [1] as an example of asymptotically forbidden transition in quasi-molecules. The aim of the present work is to highlight the case of the bound-free transitions in quasi-molecules having in mind the recent progress in the study of the photo-effect in atoms and stable molecules, e.g. [2]. The specific reaction $H + H^- + \hbar\omega \rightarrow H + H + e$ has been taken into account as a typical example of quasimolecular photo-detachment or photo-ionization processes.

2. Bound-free transitions

The cross-section of photodetachment is proportional to the density of oscillator strengths which is the main characteristic of the dipole transitions

$$\sigma(\omega) = \frac{2\pi^2}{c} \frac{df_{bc}}{d\omega} = \frac{4\pi^2}{c} \omega_{bc} |X_{bc}|^2. \quad (1)$$

For simplicity, we discuss the one-dimensional case. Then the matrix element is

$$X_{bc} = \int \langle \Psi_b | x | \Psi_c \rangle dx. \quad (2)$$

In the LCAO approximation quasimolecular *gerade* and *ungerade* wave functions in the frame of the zero-range potentials model [3] are written as



$$\Psi_b^{g,u} = \sqrt{\frac{\alpha}{2}} [\exp(-\alpha |x + R/2|) \pm \exp(-\alpha |x - R/2|)]; \quad (3)$$

$$\Psi_c^{g,u} = \frac{1}{\sqrt{2\pi k}} [\sin(k |x + R/2|) \pm \sin(k |x - R/2|)]. \quad (4)$$

Then the matrix element dipole moments can be expressed by the formula:

$$X_{b=g,c=u} = \sqrt{\frac{\alpha k}{\pi}} \frac{4\alpha}{(\alpha^2 + k^2)^2} \cos^2\left(\frac{kR}{2}\right) + \sqrt{\frac{\alpha}{\pi k}} \frac{\alpha R}{2(\alpha^2 + k^2)} \sin(kR); \quad (5)$$

$$X_{b=u,c=g} = \sqrt{\frac{\alpha k}{\pi}} \frac{4\alpha}{(\alpha^2 + k^2)^2} \sin^2\left(\frac{kR}{2}\right) - \sqrt{\frac{\alpha}{\pi k}} \frac{\alpha R}{2(\alpha^2 + k^2)} \sin(kR). \quad (6)$$

Although the quasimolecular matrix elements increase with increasing R it does not lead to difficulties at large R . In this case quasimolecular potential energies of both states involved $U_u = U_g$, and it is obligatory to use the sum of amplitudes of two different ways of detachment [4]. Thus, the quasimolecular oscillator strength reduces to the oscillator strength for a single atomic ion at large distances.

The subsequent calculations of the detachment cross-sections of *gerade* σ_{gu} and *ungerade* σ_{ug} quasimolecular states have been made in the frame of the quasistatic approximation widely used in the theory of spectral line shapes, e.g. [5]. Then the main characteristic of the transition is the Condon point R_c that can be found from:

$$\omega = -U_{g,u}(R_c) + \frac{k^2}{2}. \quad (7)$$

The Figure 1 shows the results for the cross-sections in relative units as a functions of the frequency of light. The main feature is the shift of the detachment threshold in the direction of smaller frequencies compared with the threshold in the case of atomic ions, $2.7 \cdot 10^{-2}$. The reason is that the *ungerade* quasimolecular term U_u is repulsive.

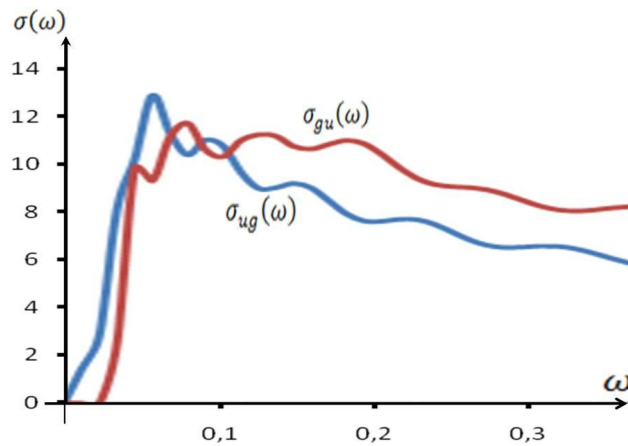


Figure 1. The cross-sections σ_{gu} and σ_{ug} of photo-detachment of *gerade* and *ungerade* quasimolecular states as functions of the frequency of light.

3. Conclusion

The comparisons and simple analytic formulas we have given should make the method presented a useful exploratory tool for the other detachment processes of this type. The main results obtained are as follows. First, collisions result in a lowering of the threshold of the electron detachment compared with the single ion. Second, the cross-sections are oscillating functions of the frequency of light as a consequence of interference under scattering of removed electron on two atoms. The results obtained may contribute to the cold and thermal plasma spectroscopies.

References

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