

# Resonance contributions to low-energy electron collisions with molecular hydrogen

Jiří Horáček,  
Martin Čížek,  
Karel Houfek,  
Přemysl Koloreň,  
Lukáš Pichl

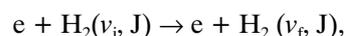
**Abstract** Calculations of electron dissociative attachment and vibrational excitation of molecular hydrogen by low-energy electrons based on an improved nonlocal resonance model are reported. The role of the rotational excitation of the target molecules is discussed.

**Key words** electron scattering • molecules • attachment • vibrational excitation

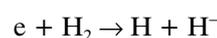
## Introduction

Three resonance inelastic processes in electron–molecular hydrogen system, namely:

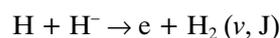
vibrational excitation (VE)



dissociative attachment (DA)



and associative detachment (AD)



can be described in the framework of a single nonlocal resonance model [3, 4]. Understanding of these processes is important for a number of practical applications. AD and DA determine the thermal equilibrium densities of  $H^-$  ions and  $H_2$  molecules in many astrophysical plasmas. Neutral molecules produced in AD are vibrationally excited and the emission spectra of such molecules are quite different from those of molecules excited by ultraviolet pumping or shock excitation. DA of electrons to molecular hydrogen is thought to be the primary source of the  $H^-$  ions produced in hydrogen plasmas. These ions may serve for the generation of neutral particle beams, the injection of ions into controlled thermonuclear devices, or for electromagnetic propulsion of space vehicles.

The main purpose of this contribution is to discuss the role of the rovibrational excitation of the target on the rate of all processes listed above. It is shown that the rotational heating of molecular hydrogen strongly enhances the process of dissociative attachment as well as the process of vibrational excitation. Oscillatory structures, sometimes known as “boomerang oscillations”, were observed in vibrational excitation cross sections of hydrogen by

J. Horáček✉, M. Čížek, K. Houfek, P. Koloreň  
Faculty of Mathematics and Physics,  
Institute of Theoretical Physics,  
Charles University Prague,  
V Holešovičkách 2, 180 00 Praha 8, Czech Republic,  
Tel.: 00420/ 2 2191 2497, Fax: 00420/ 2 2191 2496,  
e-mail: horacek@mbox.troja.mff.cuni.cz

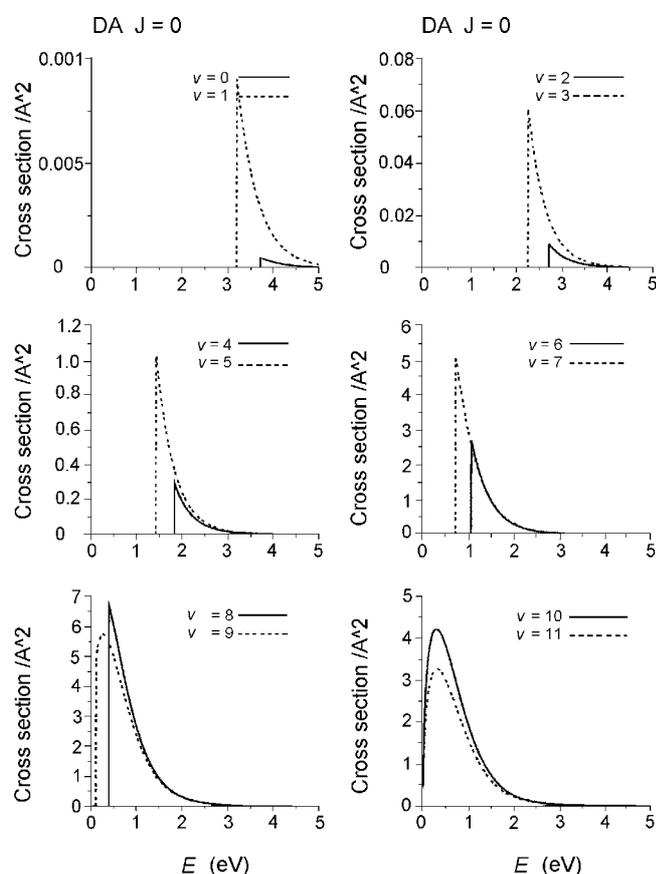
L. Pichl  
The University of Aizu,  
Tsuruga, Ikki, Aizu-Wakamatsu, 965-8580 Japan

Received: 14 November 2002, Accepted: 14 February 2003

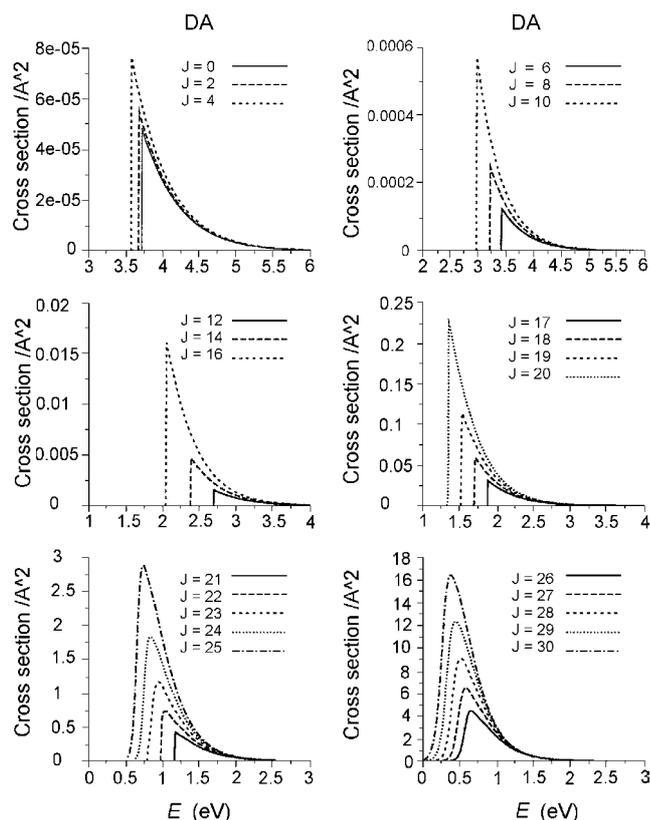
M. Allan [1]. The present model reproduces these structures in excellent agreement with the experimental data. The calculation shows that these structures appear also in the elastic cross section for vibrationally excited target states. It is found that the boomerang structures get more pronounced as the rotational quantum number  $J$  increases and that these structures dominate the cross sections at higher vibrational target states. The processes of VE and DA for molecular hydrogen were studied by several authors, for recent work see [2, 4–6, 8–11] in various degrees of approximation ranging from simple local approximation to elaborated nonlocal calculations. To the best of our knowledge the present approach represents the most elaborated and the most accurate method for treating resonance process in the system electron–diatomic molecule.

### Nonlocal resonance model

The calculation of VE and DA cross sections reported here is based on the use of an improved nonlocal model [3]. This model uses *ab initio* e-H<sub>2</sub> scattering data at short internuclear distances, *ab initio* data for the bound  $^2\Sigma_u^+$  state of H<sub>2</sub> at intermediate distances and exhibits the correct polarization at large internuclear distances. This model also takes full account of the nonlocality of the process. For detailed description of the nonlocal resonance and its application to other molecules see [4].



**Fig. 1.** Dissociative electron attachment cross sections for nonrotating hydrogen molecules and various vibrational initial states  $v$ .



**Fig. 2.** Dissociative electron attachment cross sections for hydrogen molecules in their ground vibrational state  $v = 0$  and various rotational states  $J$ .

### Dissociative attachment

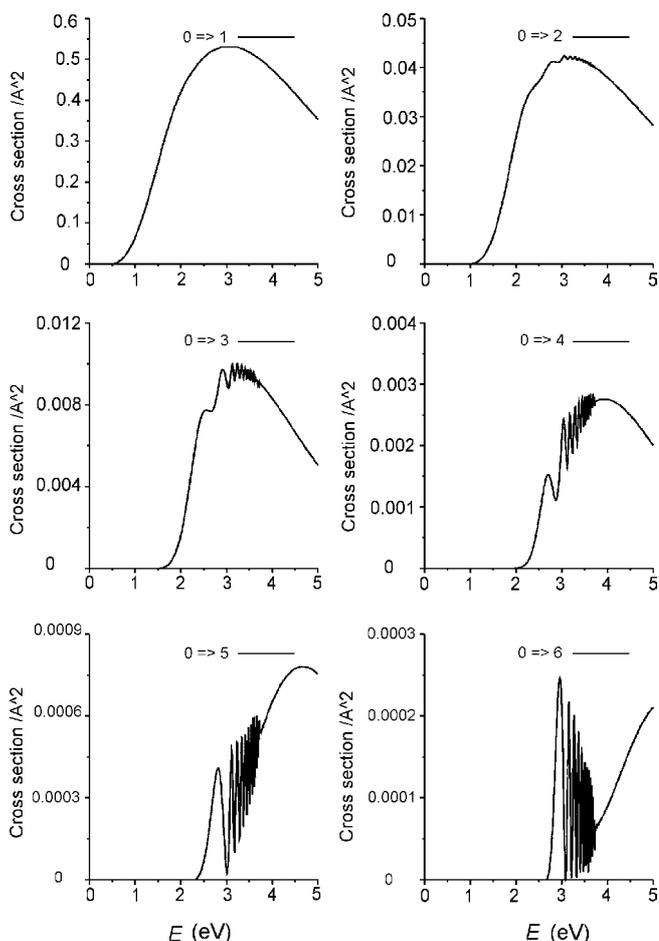
The calculated DA cross sections for nonrotating hydrogen molecules in various vibrational target states are shown in Fig. 1. In each panel two cross sections are plotted: the solid line corresponds to lower vibrational state, the dotted line to a higher vibrational state of the target molecule as denoted in each panel. This calculation confirms the well known fact that the DA cross section for molecules in ground vibrational state is very small but the cross section increases very rapidly with increasing vibrational quantum number  $v$ . In our calculation the highest DA cross section is obtained for  $v = 8$ . At  $v = 10$  the DA process gets exothermic and the cross section decreases with increasing  $v$ . The role of rotational excitation of the target molecules is much less studied than the role of vibrational excitation mainly for highly rotationally excited states. In Fig. 2 the calculated DA cross sections for hydrogen molecules in their ground vibrational state are plotted for a range of rotational quantum numbers  $J$ ,  $J = 0$ –30. It is seen that the DA cross section increases with increasing  $J$  and that at high values of  $J$  the shape of the DA cross section changes. The sharp onset of the DA cross section typical for low lying states gradually disappears and gets smooth even for endothermic processes. This is caused by the build-up of a centrifugal barrier. This calculation shows that huge DA cross sections are obtained even for vibrationally unexcited molecules provided the rotational excitation is high enough. This fact is of importance in astrophysics

where highly excited hydrogen molecules,  $J \cong 30$ , were observed.

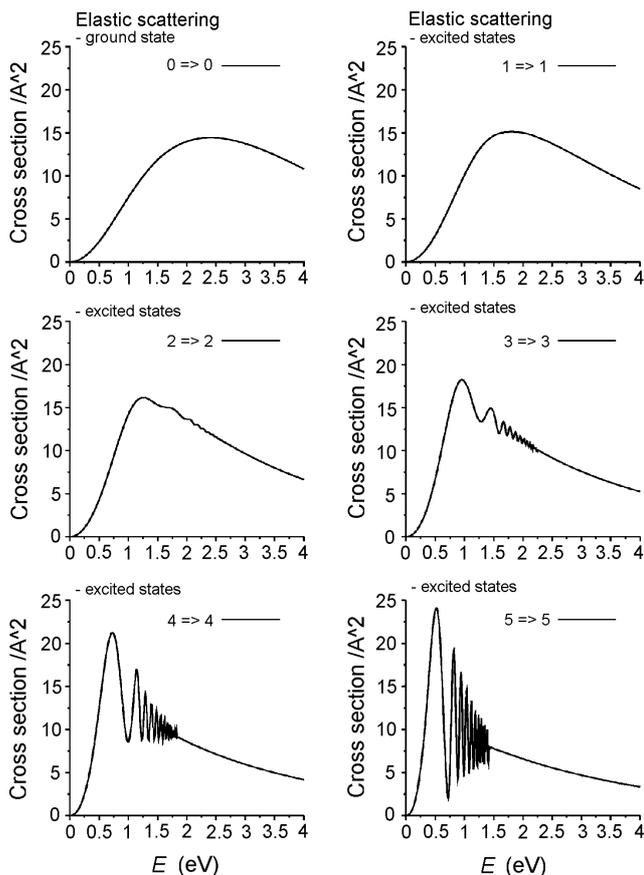
### Vibrational excitation

Calculated vibrational excitation cross sections for non-rotating hydrogen molecules in their ground vibrational state are shown in Fig. 3 for the transitions  $\nu = 0 \rightarrow 1, 2, \dots, 6$ . The cross sections for the transitions  $\nu = 0 \rightarrow 1, 2$  are smooth functions of electron energy but in the higher transitions oscillatory structures appear which eventually dominate the cross sections. Such structures appear for short-living resonances and are sometimes called the boomerang oscillations. Here, however, the origin of the oscillations is different from the boomerang oscillations well known, for example, in the case of  $N_2$ . The oscillations are related to bound states in the  $H + H^-$  system at intermediate internuclear distances.

The present nonlocal resonance model provides only resonance contributions to all cross sections. For inelastic cross sections the direct scattering in the low energy range is usually negligible and the present results represent an excellent approximation. For elastic scattering, however, the direct scattering is generally large even outside the resonance region and cannot be neglected. The direct scattering is usually a smooth function of electron energy



**Fig. 3.** Cross section for vibrational excitation  $\nu = 0 \rightarrow 1, 2, \dots, 6$  of nonrotating molecular hydrogen.



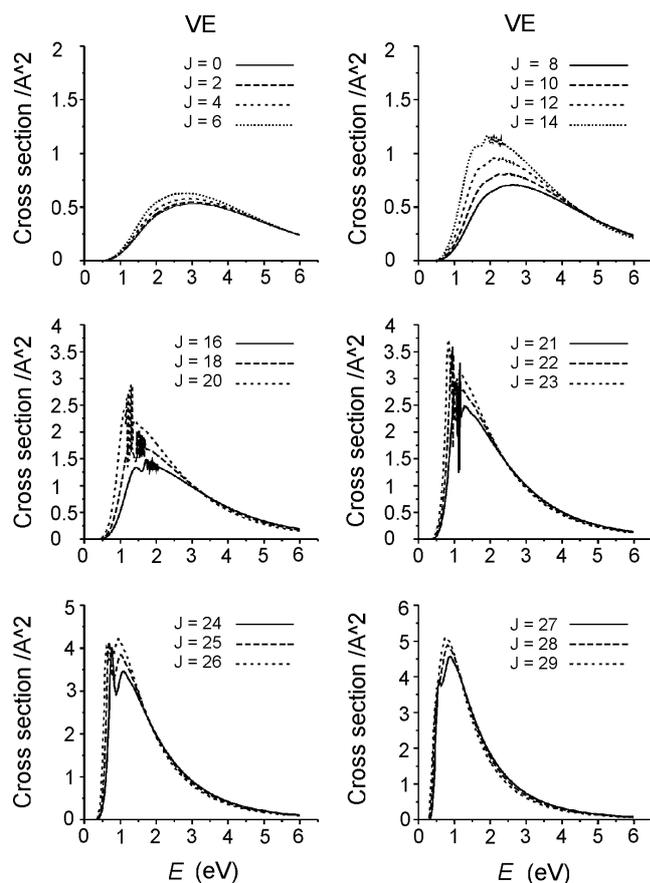
**Fig. 4.** Resonance contribution to the electron elastic scattering with molecular hydrogen at various initial vibrational states,  $\nu = 0, 1, \dots, 5$  of the target.

and all rapid changes are caused by the presence of the resonance. The resonance contributions to the elastic scattering for ground and vibrationally excited hydrogen molecules are shown in Fig. 4. In analogy with the vibrational excitation, the oscillatory structures in elastic scattering get more pronounced at higher vibrational states of the molecules. This feature might serve as a diagnostic tool of vibrationally excited molecules. The rotationally resolved elastic scattering cross section was measured by Linder and Schmidt [7]. The calculated resonance contribution to the elastic scattering cross section is quite large. In fact for  $\nu = 0$  the resonance contribution to elastic scattering at 3 eV obtained by the present model represents over 90% of the experimental value [7].

Finally, in Fig. 5 the dependence of the vibrational excitation cross section for the transition  $\nu = 0 \rightarrow 1$  on the rotational state of the target is shown. The oscillatory structures are seen even for the transition  $\nu = 0 \rightarrow 1$  if the rotational quantum number  $J$  is sufficiently large.

### Conclusions

The improved nonlocal resonance model represents the most elaborated method of calculating inelastic resonance cross sections in the system electron–molecule. This model provides accurate cross sections for the processes of vibrational excitation, dissociative attachment and associative detachment. In this paper VE and DA cross sections were reported and the role of rotational excitation



**Fig. 5.** Vibrational excitation cross section  $\nu = 0 \rightarrow 1$  of hydrogen molecules as a function of the rotational state  $J$  of the target.

discussed. A more detailed study will be published in a subsequent paper.

**Acknowledgment** This work was supported by projects ME556 and ME562 of MŠMT CR.

## References

1. Allan M (1985) Experimental observation of structures in the energy dependence of vibrational excitation in  $H_2$  by electron impact in the  $^2\Sigma_u^+$  resonance region. *J Phys B: At Mol Opt Phys* 18:L451–L455
2. Atoms DE, Wadehra J (1993) Resonant contributions to dissociation of  $H_2$  by low-energy electron impact. *J Phys B: At Mol Opt Phys* 26:L759–L765
3. Čížek M, Horáček J, Domcke W (1998) Nuclear dynamics of the  $H_2$  collision complex beyond the local approximation: associative detachment and dissociative attachment to rotationally and vibrationally excited molecules. *J Phys B: At Mol Opt Phys* 31:2571–2583
4. Domcke W (1991) Projector operator approach to the non-local dynamics of molecular complexes. *Phys Rep* 208:97–191
5. Gallup GA, Xu Y, Fabrikant II (1998) Nonlocal theory of dissociative electron attachment to  $H_2$  and HF molecules. *Phys Rev A* 57:2596–2607
6. Gertischke PL, Domcke W (1993) Time-dependent wave-packet description of dissociative electron attachment. *Phys Rev A* 47:1031–1044
7. Linder F, Schmidt H (1971) Rotational and vibrational excitation of  $H_2$  by slow electron impact. *Z Naturforsch A: Phys Sci* 26:1603–1617
8. Orient OJ, Chutjian A (1999) Experimental study of dissociative attachment in  $H_2$ ; effects of vibrational excitation. *Phys Rev A* 59:4374–4378
9. Xu Y, Fabrikant II (2001) Dissociative electron attachment rates for  $H_2$  and its isotopes. *Appl Phys Lett* 78:2598–2600
10. Xu Y, Gallup GA, Fabrikant II (2000) Dissociative electron attachment to vibrationally and rotationally excited  $H_2$  and HF molecules. *Phys Rev A* 61:052705–1–7
11. Xu Y, Kazansky AK, Fabrikant II (2000) Low-energy  $e-H_2$  scattering: Separation of dissociative attachment and dissociation channel. *Phys Rev A* 63:014703–1–4