Narrow resonances in electron collisions with H_2

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Introduction

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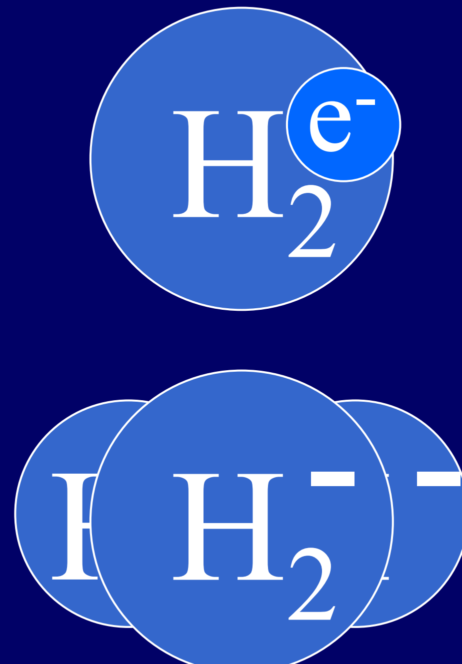
Final notes



$$T = 10^{-15} - 10^{-13}\ \mathrm{s}$$

10^{-6}

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$$e^- + H_2 \rightarrow H_2^- \rightarrow e^- + H_2$$

$$H^- + H \rightarrow H_2^- \rightarrow H^- + H$$

$$e^- + H_2(v) \rightarrow H_2^- \rightarrow e^- + H_2(v') \qquad \text{(VE)}$$

$$e^- + H_2 \rightarrow H_2^- \rightarrow H^- + H \qquad \text{(DA)}$$

$$H^- + H \rightarrow H_2^- \rightarrow e^- + H_2 \qquad \text{(AD)}$$

Coauthors

M. Čížek, J. Horáček, W. Domcke, *J. Phys.* B **31** (1998) 2571

R. Golser, H. Gnaser, W. Kutschera, A. Priller, P. Steier, A. Wallner,
M. Čížek, J. Horáček and W. Domcke: *Phys. Rev. Lett.* **94** (2005) 223003

M. Čížek, J. Horáček, W. Domcke, *to be published*

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I. Introduction

- Resonances in AD cross sections
- Interpretation in terms of potential energy curves
- Long lived states not accessible in AD/DA process

M. Čížek, J. Horáček, W. Domcke, *J. Phys.* B **31** (1998) 2571

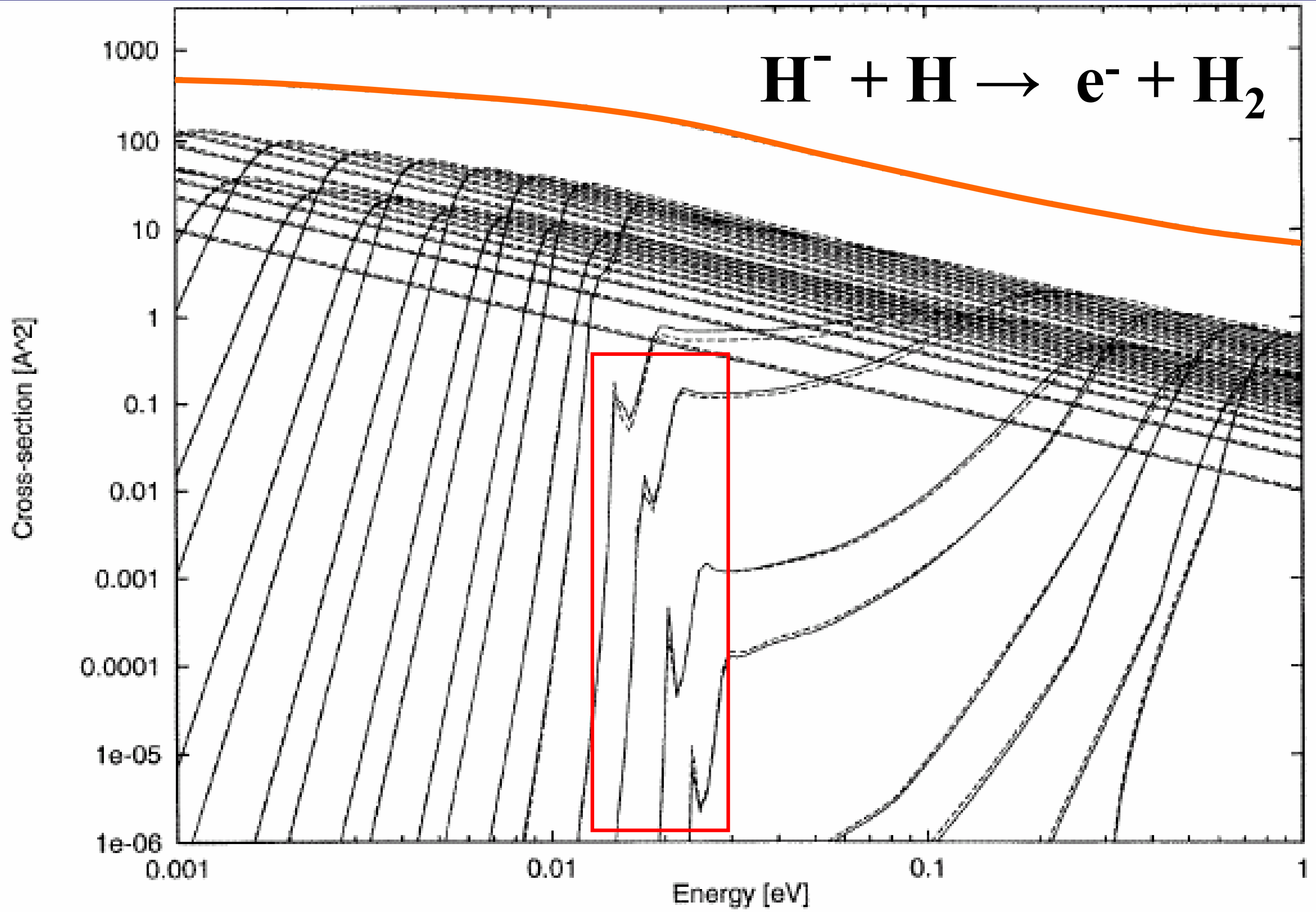

Figure 2. The total H + H⁻ associative-detachment cross section (chain curve) and its partial-wave components (full curves), l = 30, 29, . . . (from the right). Results of the local approximation are given by broken curves.

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Resonances in AD cross section

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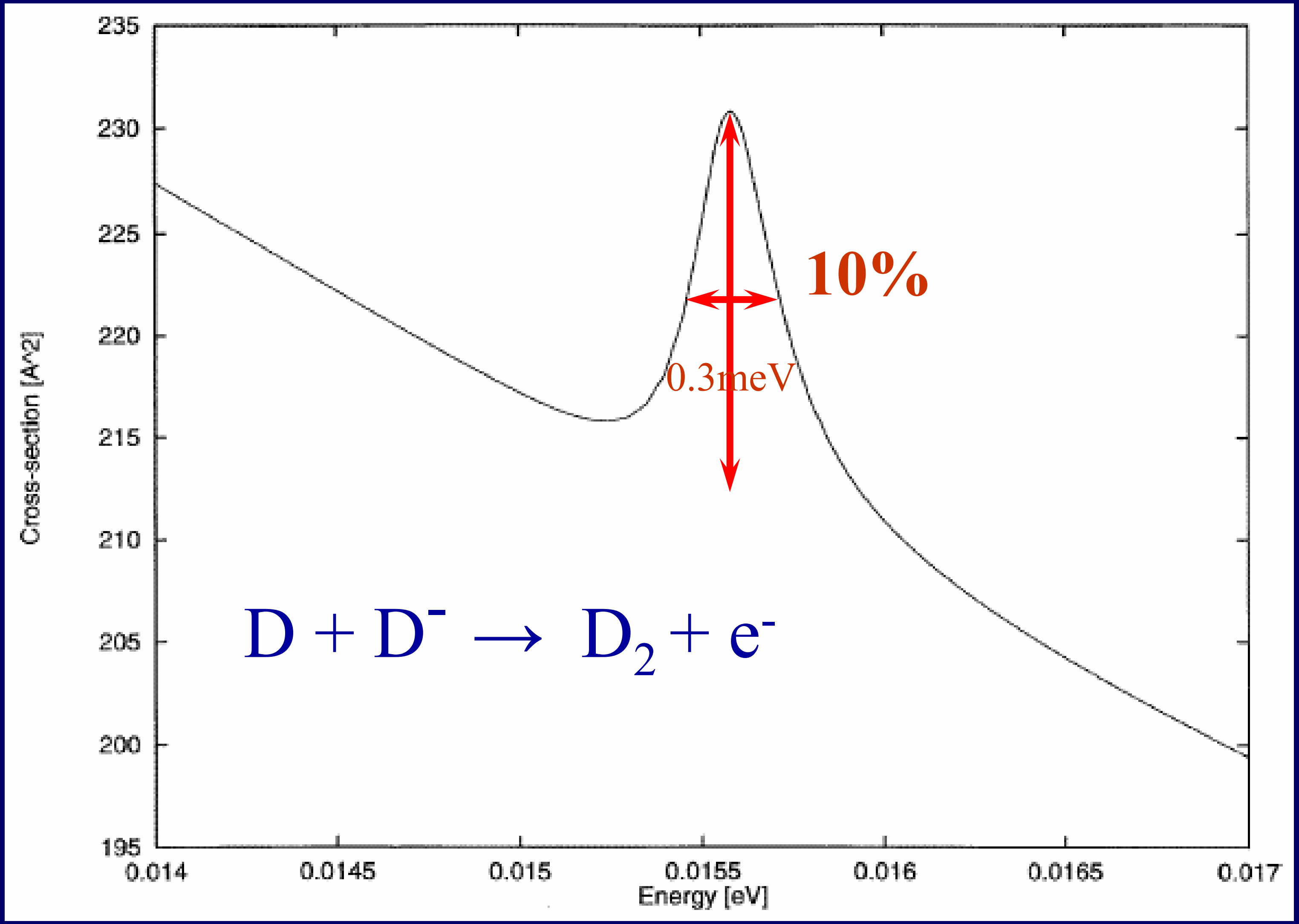

M. Čížek, J. Horáček, W. Domcke, *J. Phys.* B **31** (1998) 2571

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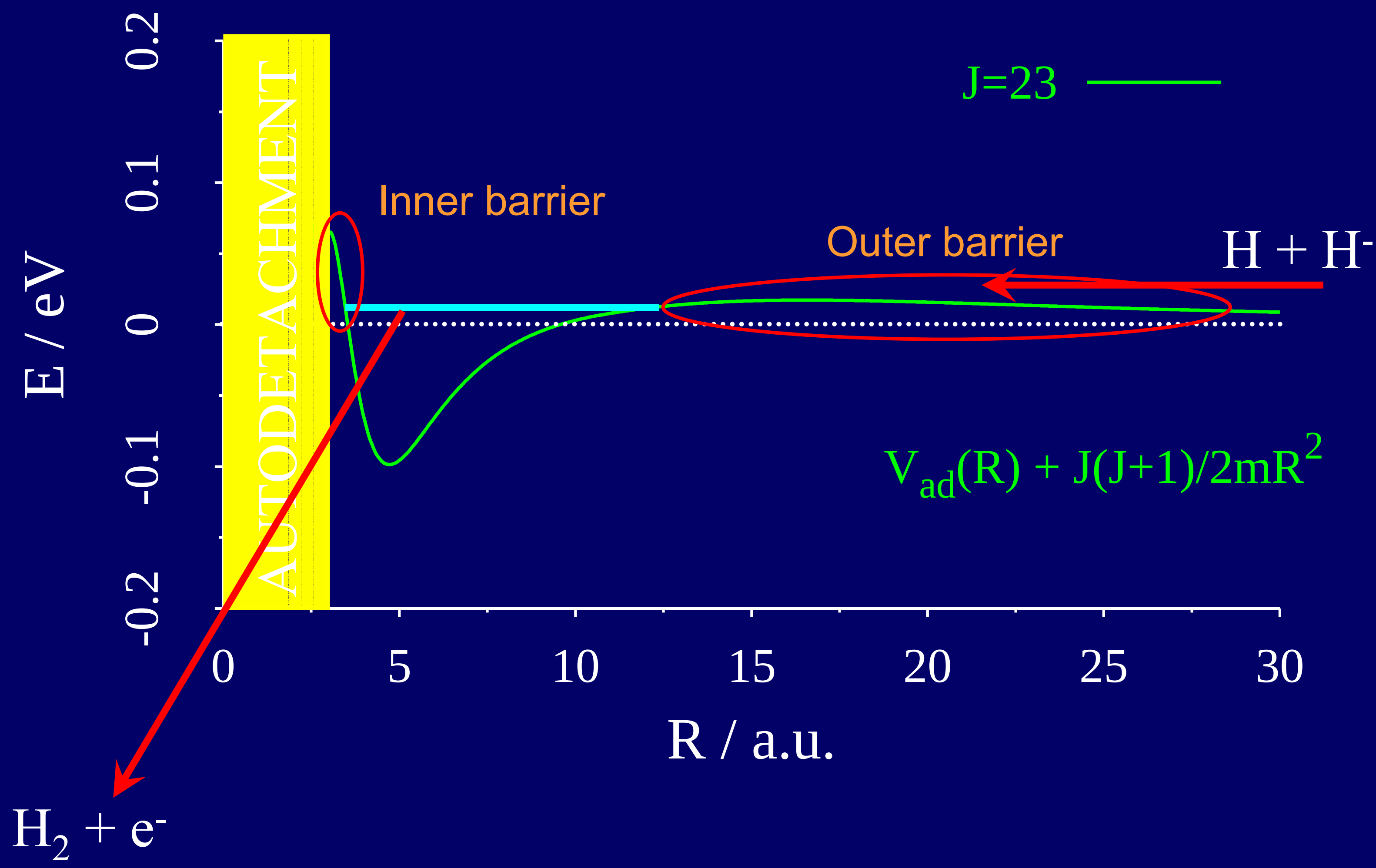
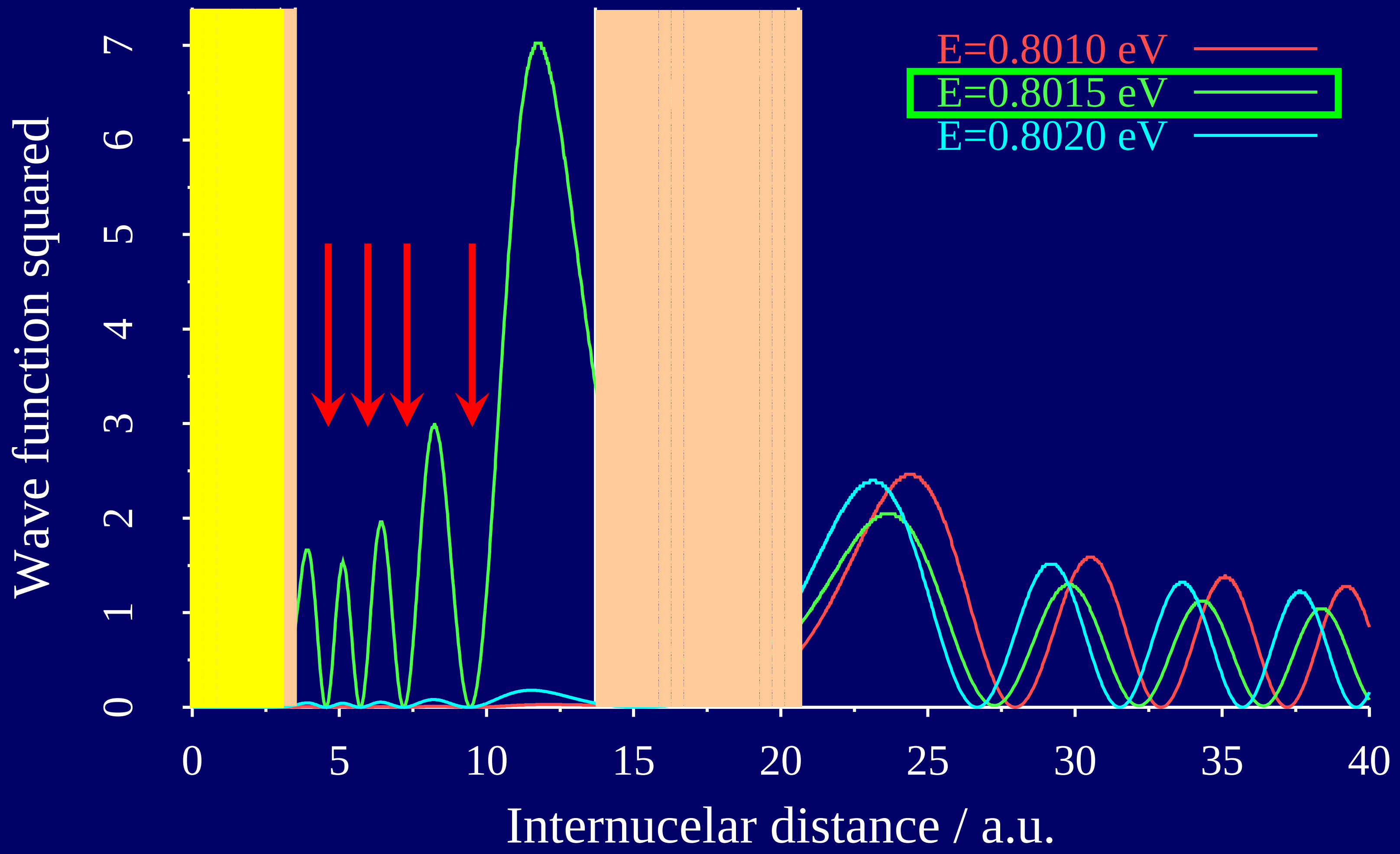
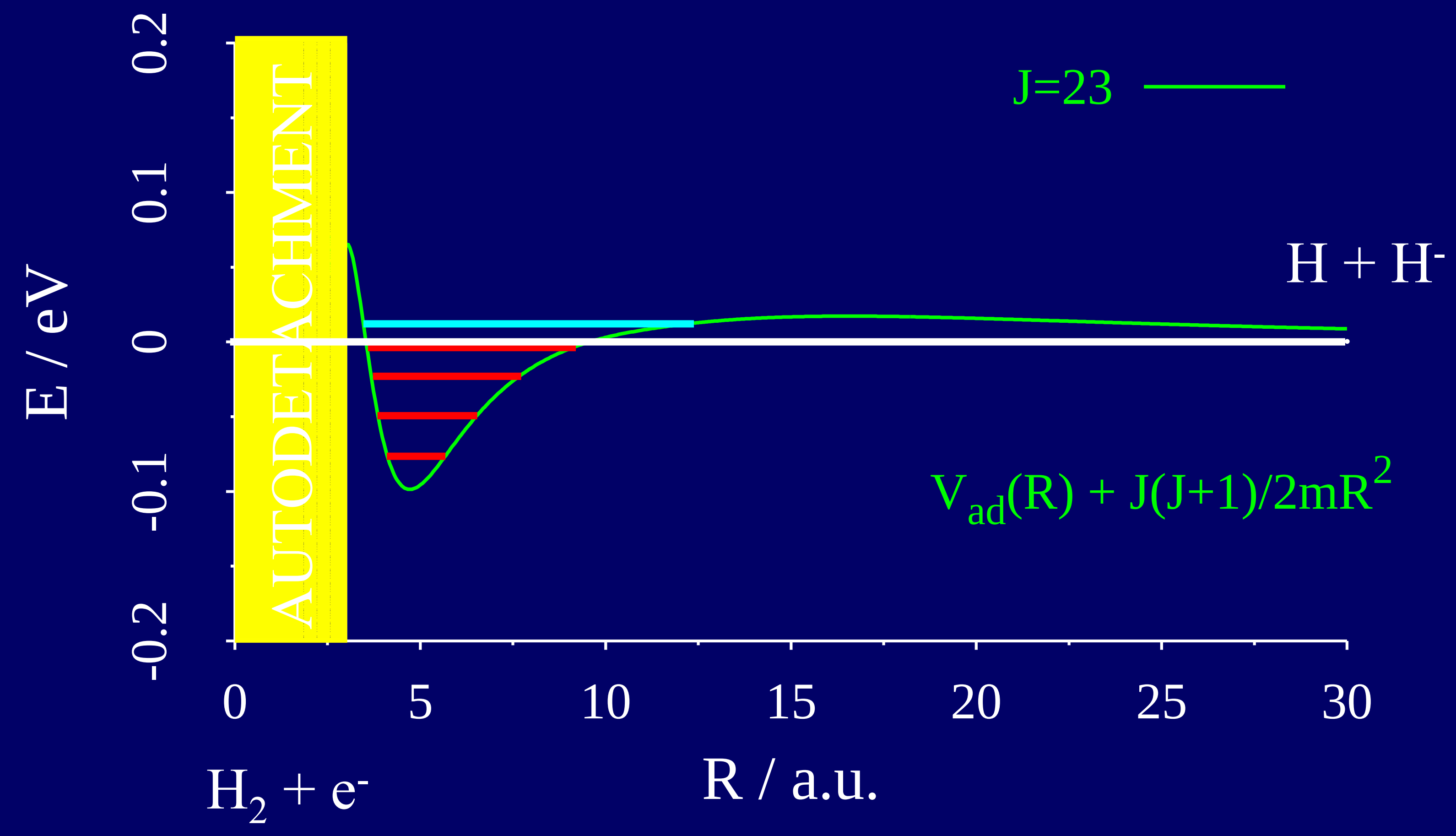
Interpretation in terms of adiabatic $H+H^-$ potential curve



H+H⁻ scattering wavefunction



Interpretation in terms of adiabatic $H+H^-$ potential curve



II. Brief Outline of Theory

- Nonlocal resonance model
- Diabatic /Adiabatic state potential
- Details of calculation of metastable-state-parameters

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Nonlocal resonance model

- Theory as reviewed by

  W. Domcke 1991, *Phys. Rep.* **208**, 97.

- Model obtained from ab initio calculation using projection-operator techniques:

  Berman, Mündel, Domcke 1985, *Phys. Rev. A* **31**, 641.

- Long range $H+H^-$ interaction adjusted in

  Čížek, Horáček, Domcke 1998, J. Phys. B **31**, 2571.

→ Model applicable to all low-energy resonant processes: AD, DA, VE and elastic e^-+H_2, $H+H^-$

Nonlocal resonance model – basic idea

- Electronic basis at fixed R is defined

discrete state $\phi_d(R,r)$ continuum $\phi_\varepsilon(R,r)$

- Complete wavefunction is expanded

$$\Psi(\mathrm{R},\mathrm{r}) = \psi(\mathrm{R})\phi_d(R,r) + \int \mathrm{d}\varepsilon\, \psi_\varepsilon(R)\phi_\varepsilon(R,r)$$

- Continuum part is eliminated (+BO approx.)

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{J(J+1)}{2\mu R^2} + V_d(R) + \hat{F}(E) - E\right]\psi_d(R) = 0$$

$$\langle R|\hat{F}(E)|R'\rangle = \int \mathrm{d}\varepsilon\, V_{d\varepsilon}(R)\left[E - \varepsilon - T_N - V_0(R) + i0\right]^{-1} V^*_{d\varepsilon}(R')$$

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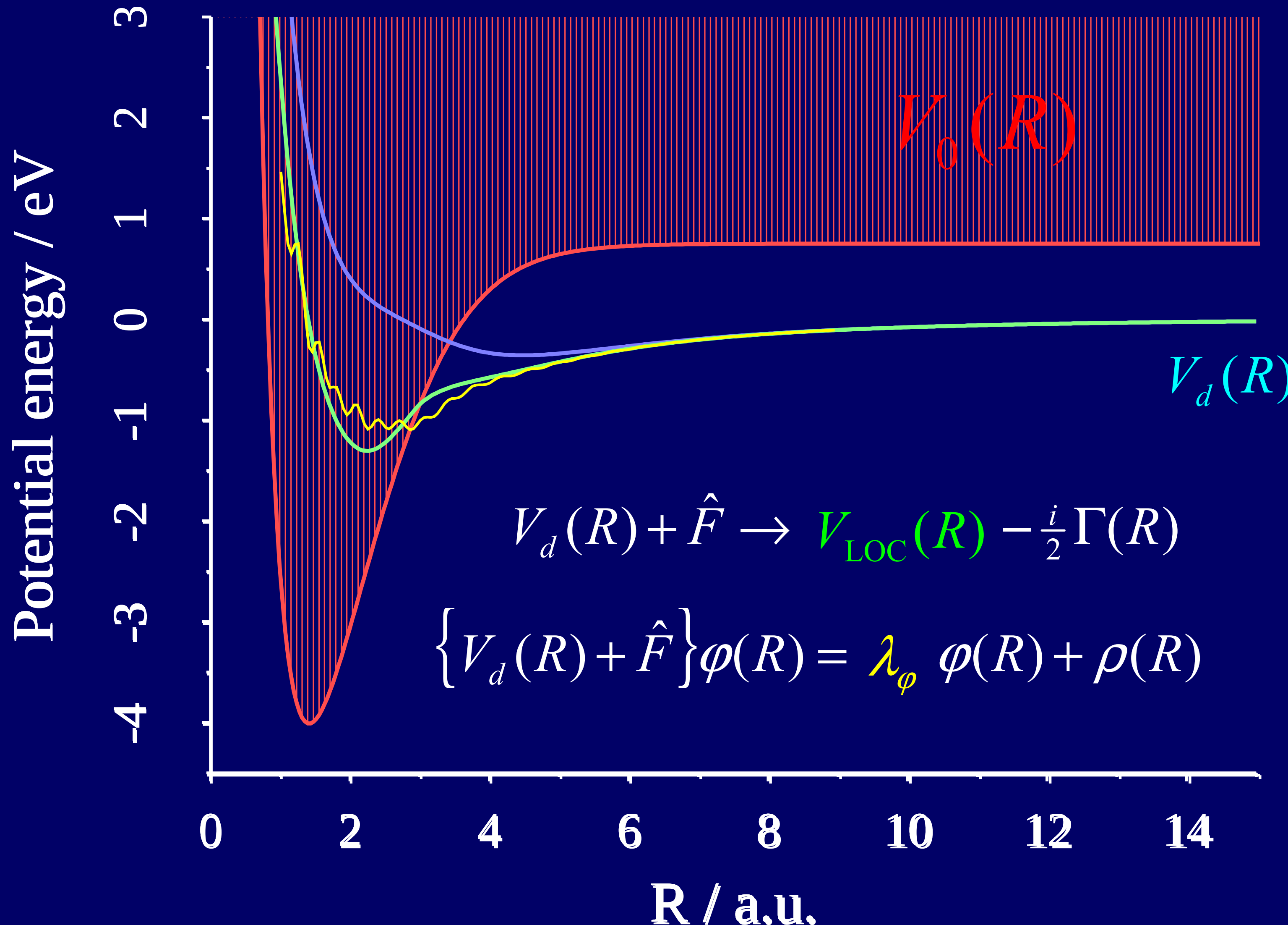
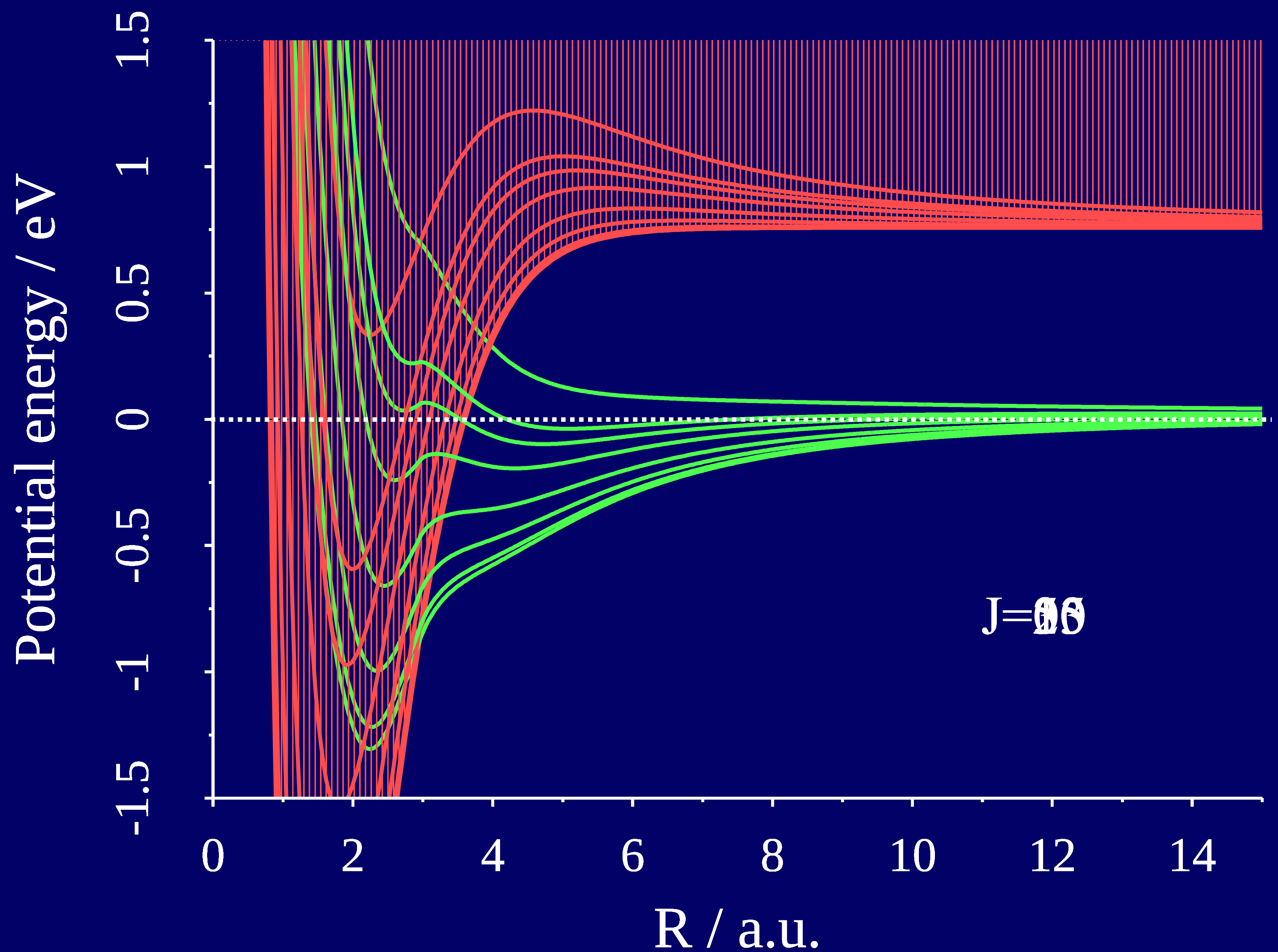
Potential energy curves



Effect of molecular rotation $J(J+1)/2\mu R^2$



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Resonance parameters calculation

1. Calculation of states $|\psi_r\rangle$ and energies E_r in $V_a(R)$
2. Calculation of VE cross section close to E_r
3. Determination of state energy and width using least squares fit to Fano formula:

$$\sigma(E) = \sigma_a \frac{(q+\varepsilon)^2}{1+\varepsilon^2} + \sigma_b, \qquad \varepsilon \equiv \frac{E - E_{res}}{\frac{1}{2}\Gamma_{res}}.$$

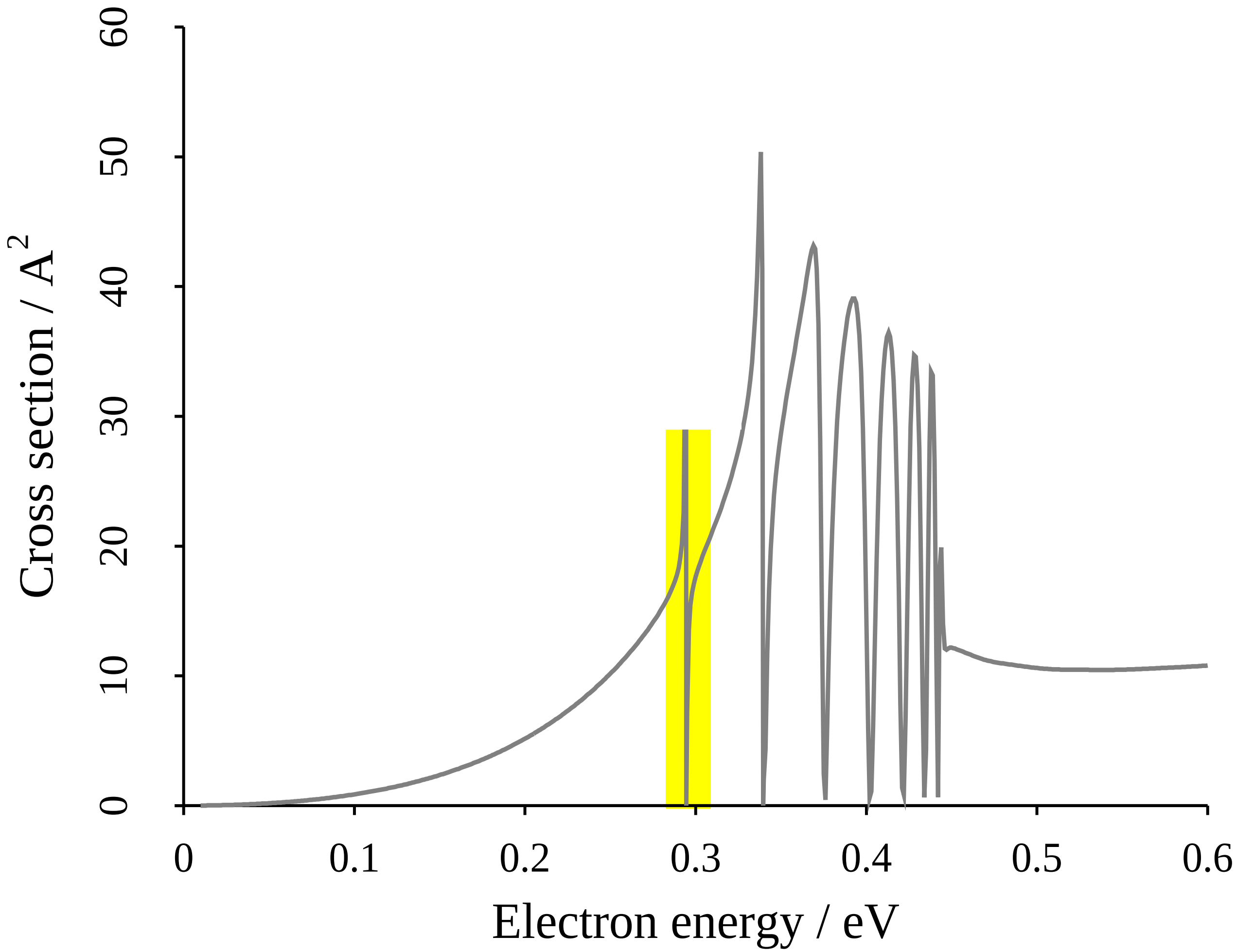
Alternative method

Projection-formulation starting from $|\psi_r\rangle$ as discrete state interacting with $H+H^-$ and H_2+e^- continua

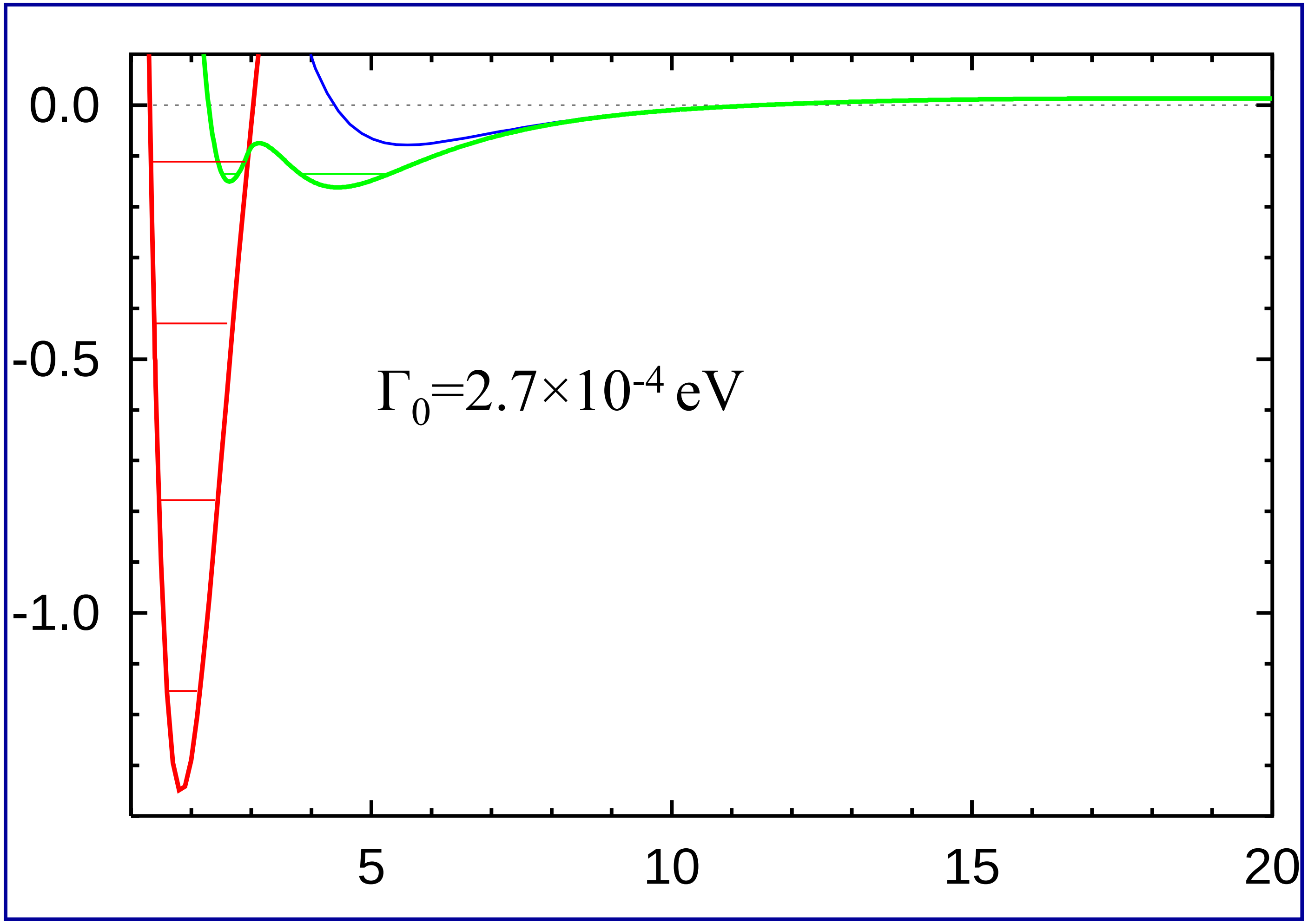
III. Metastable States

- Examples of VE cross sections
- Summary: energies and lifetimes
- Nonlocal character of the decay

Elastic cross section for $e^- + H_2$ (***J*=21**, v=2)



Energy and width for J=21



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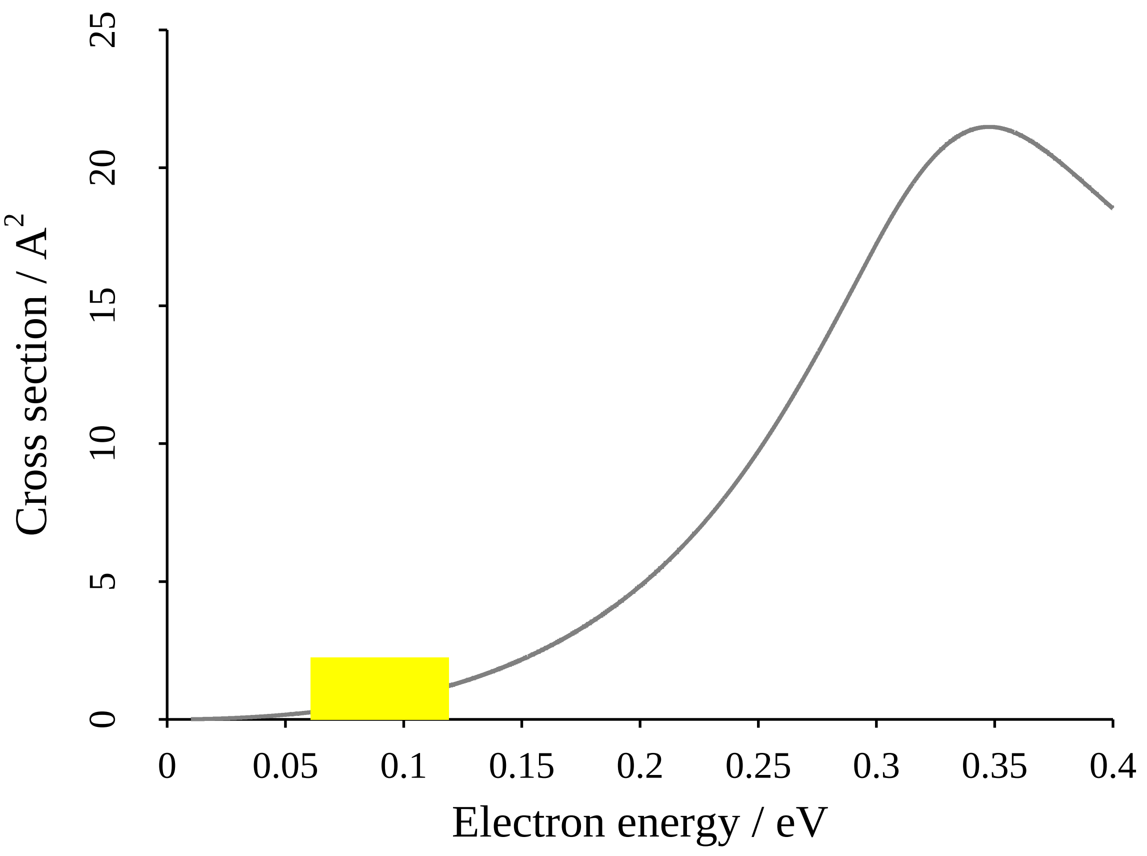
Elastic cross section for $e^- + H_2$ (***J*=25**, v=1)



Energy and width for J=25

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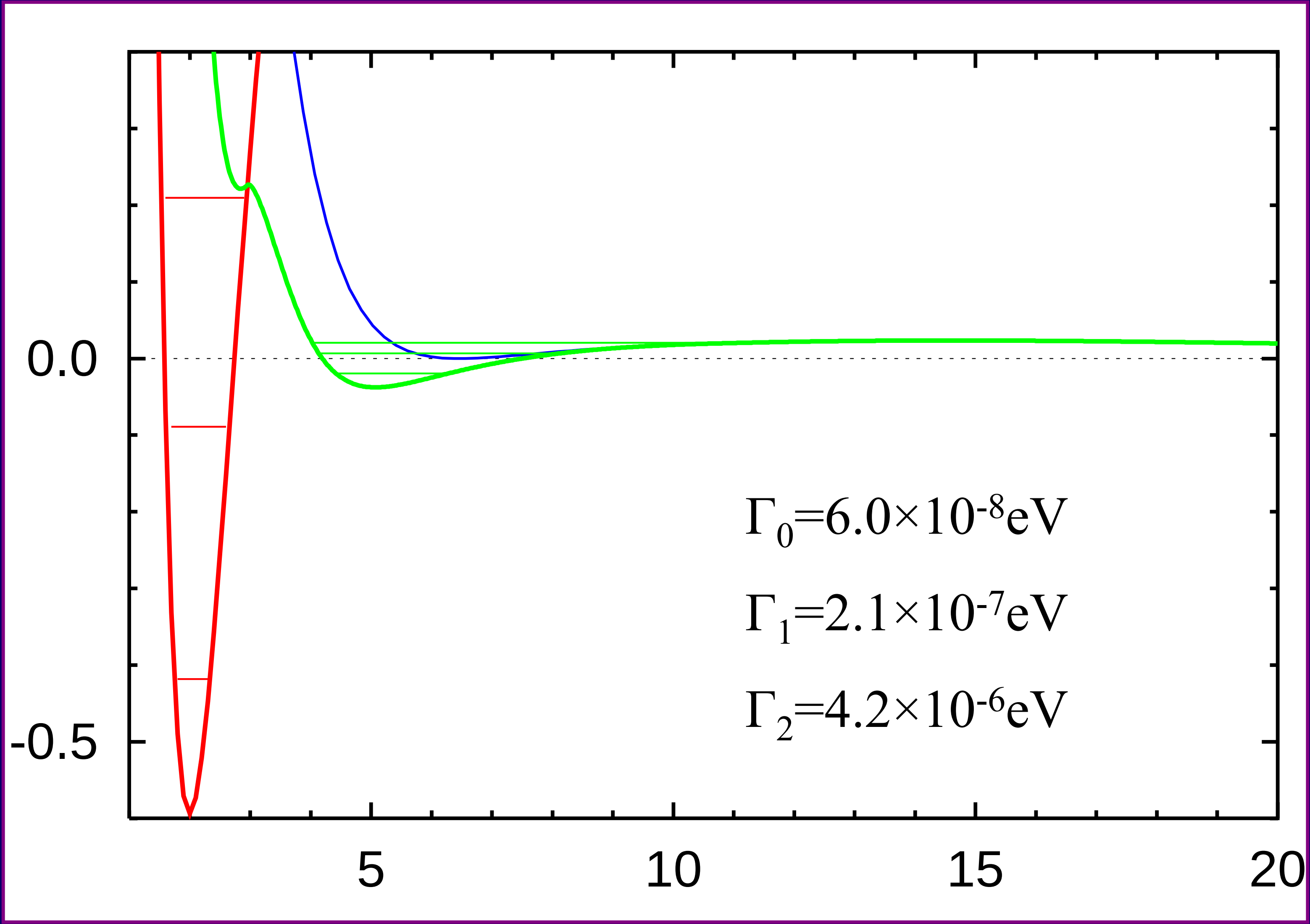
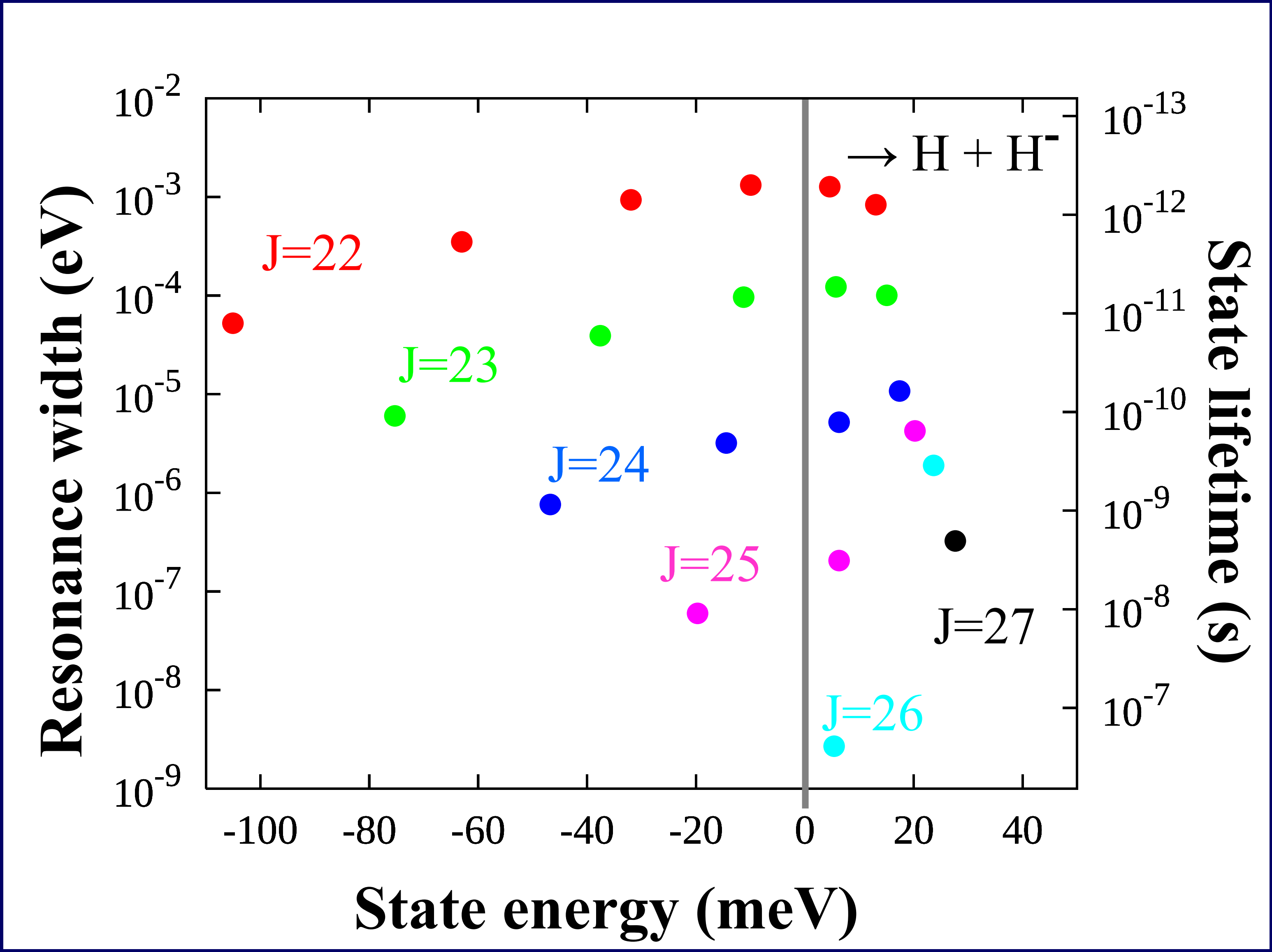
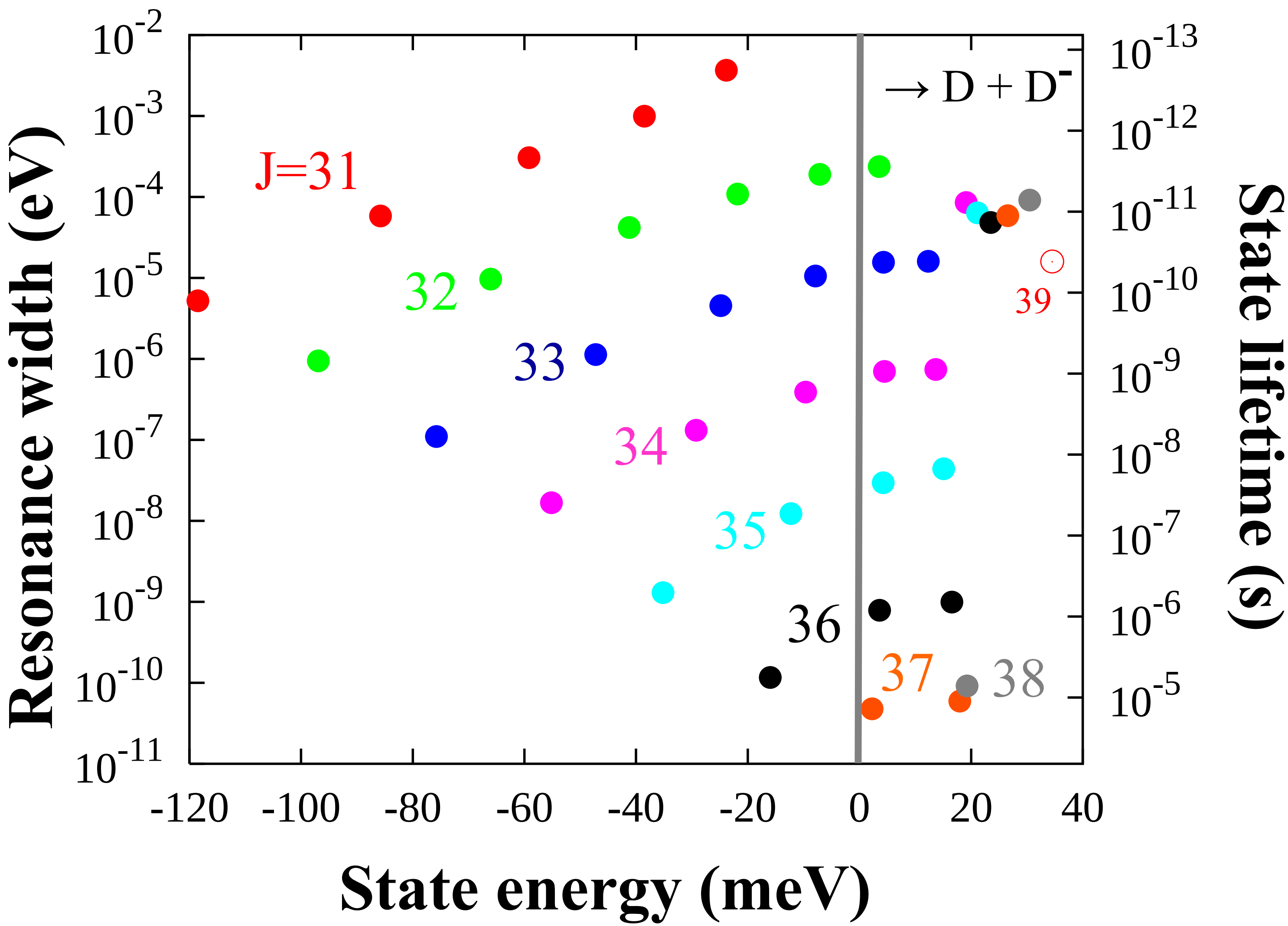


Decay widths H_2^- - summary



Decay widths D_2^- - summary



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Nonlocal character of the width

Parameters of the states for J=23

v	LCP: E_{res}	Fano: E_{res}	LCP: Γ_{res}	Fano: Γ_{res}
0	-0.075362	-0.075294	1.662×10^{-5}	6.020×10^{-6}
1	-0.037674	-0.037587	9.168×10^{-5}	3.912×10^{-5}
2	-0.011331	-0.011244	2.174×10^{-4}	9.611×10^{-5}
3	0.005578	0.005701	2.861×10^{-4}	1.227×10^{-4}
4	0.015078	0.015055	2.414×10^{-4}	1.007×10^{-4}

IV. Experiments

- Experimental evidence 1970 – 1985
- Xuefeng Jang
- Recent experiments in Wien

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Previous experimental evidence

- Hurley 1974 – observation of H_2^- from low-energy arc source.
- Aberth *et al.* 1975 – observation of HD^-, D_2^- from ($\tau > 10\mu s$).
- Bae *et al.* 1984 – existence of D_2^- not confirmed in two-step experiment designed to produce metastable quartet state ($\tau < 2\times10^{-11}$s).
- Wang et al. 2003 – observed signature of H_2^- in signal from discharge plasma.

Xuefeng Yang

New experiments

R. Golser, H. Gnaser, W. Kutschera, A. Priller, P. Steier, A. Wallner, M. Čížek, J. Horáček and W. Domcke:

Phys. Rev. Lett. **94** (2005) 223003

- Anions are created by sputtering of TiH_2 and TiD_2 targets by Cs^+ ions (impact energy of 5 keV, 0.5 mA)
- Products are mass preselected and stripped of electrons
- Further accelerated (~MeV), mass analyzed and their energy is measured

Unambiguous detection of H_2^- and D_2^- with lifetimes of at least μs order

V. Conclusions

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Conclusions

1. Long lived states have been found in nonlocal resonance model for $H_2 + e^-$. The states can be understood as orbiting $H + H^-$ protected by potential barriers from both autoionisation and dissociation. Energies are all within 0.1eV from DA threshold. Widths vary $10^{-10} – 10^{-2}$ eV

2. LCP model gives accurate positions of the resonances but only order of magnitude estimate for the lifetimes.

Conclusions

3. The long lived states are difficult to create in "two-body" collisions – the cross sections are as high as 100Å^2, but the resonant peak is very narrow. "Three body" collisions like $H^- + H_2$ or sputtering are probably much more efficient also due to high angular momentum needed.
4. Further experimental evidence (lifetimes, energies, …) is needed to establish that the states seen in experiments are really of this nature.

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Acknowledgements

Jiří Horáček, Wolfgang Domcke, Xuefeng Yang

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Suplementary matherial – for potential questions

PHYSICAL REVIEW A VOLUME 47, NUMBER 2 FEBRUARY 1993

Time-dependent wave-packet description of dissociative electron attachment

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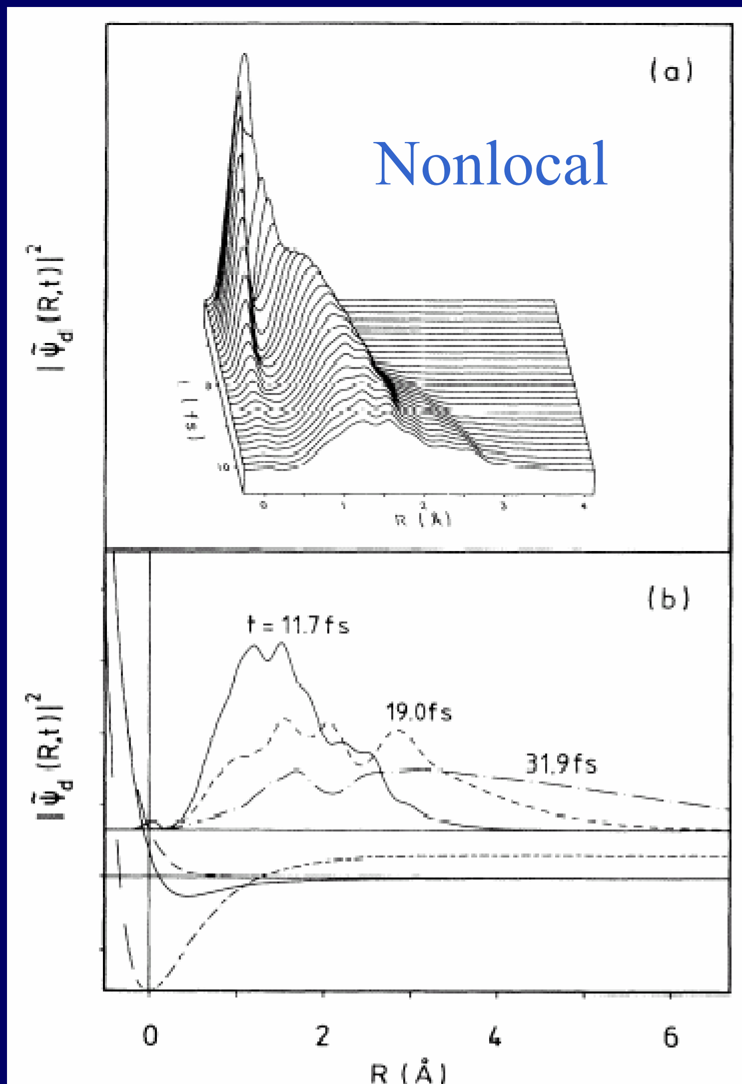
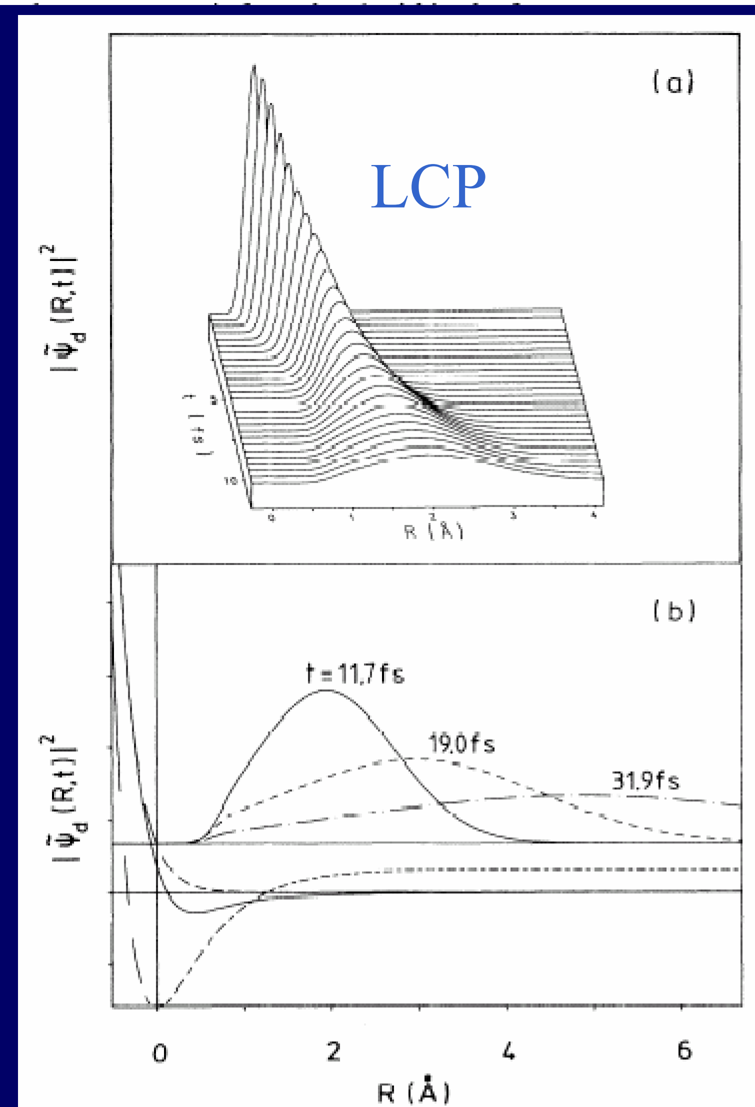
Institute of Physical and Theoretical Chemistry, Technical University of Munich, D-8046 Garching, Germany
(Received 4 August 1992)





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Chemical Physics Letters 285 (1998) 114–120

LETTERS

Potential energy surfaces of excited states of H_2^-

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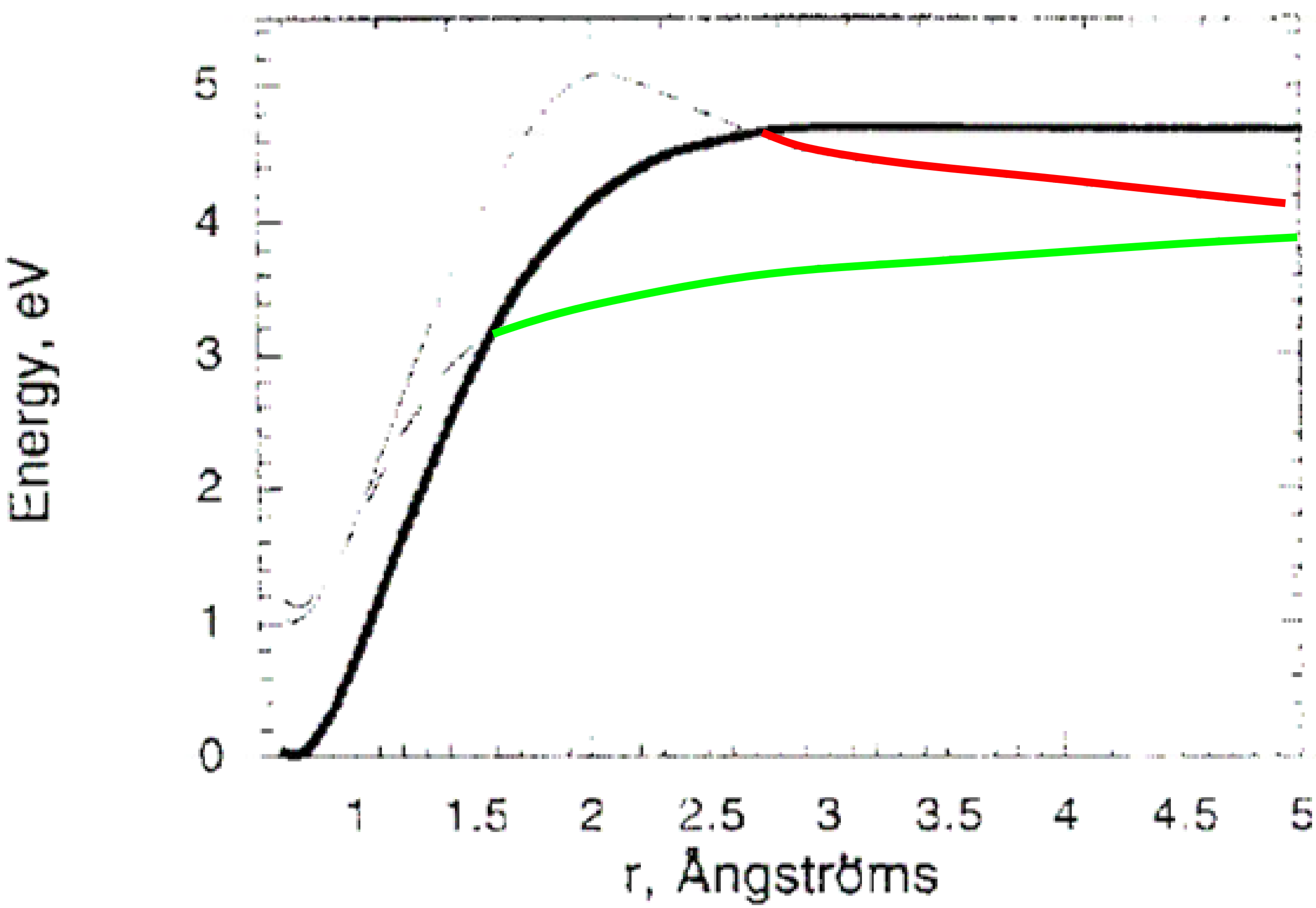

Suplementary matherial – for potential questions

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