NUMERICALLY SOLVABLE MODEL OF LOW-ENERGY RESONANT ELECTRON-MOLECULE COLLISIONS WITHOUT BORN-OPPENHEIMER APPROXIMATION

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We suggest a simple model with one nuclear and one electronic degree of freedom that can be solved exactly (without the Born-Oppenheimer approximation) employing the exterior complex scaling method and the finite-element method with discrete variable representation [1]. Using this model it is possible to study basic electron-molecule collisions: the vibrational excitation of a molecule by electron impact

$$\mathrm{e}^- + \mathrm{AB}(\nu_\mathrm{i}) \;\rightarrow\; \mathrm{e}^- + \mathrm{AB}(\nu_\mathrm{f}), \qquad (1)$$

and the dissociative electron attachment to a molecule

$$\mathrm{e}^- + \mathrm{AB}(\nu_\mathrm{i}) \;\rightarrow\; \mathrm{A} + \mathrm{B}^-. \qquad (2)$$

The full Hamiltonian of our model is

$$H = -\frac{1}{2\mu}\frac{d^2}{dR^2} - \frac{1}{2}\frac{d^2}{dr^2} + V(R,r) \qquad (3)$$

where μ is the reduced mass of a molecule, R is the distance between atoms and r is the distance of the electron from the molecule. The potential $V(R,r)$ is written in the form

$$V(R,r) = V_0(R) - \lambda(R)e^{-\alpha r^2} + \frac{J_\mathrm{e}(J_\mathrm{e}+1)}{2r^2} \qquad (4)$$

where $V_0(R)$ is a Morse potential for the vibrational motion of the neutral molecule, the second term describes the interaction between the molecule and the electron and the centrifugal term with $J_\mathrm{e} \neq 0$ is added to provide a resonant behavior in our system.

The interaction of the electron with the molecule was chosen to possess one bound state for large R (dissociative attachment channel) that becomes a resonance state for a given $R = R_c$ (crossing point of the potential energy curves of AB and $(\mathrm{AB})^-$). Choosing $\lambda(R)$ appropriately we can get different types of resonance curves, with or without potential wells, to simulate various real systems.

The suggested model is used to compare various approaches to low-energy resonant electron-molecule collisions, for example the boomerang model [2] or the nonlocal resonance model [3].

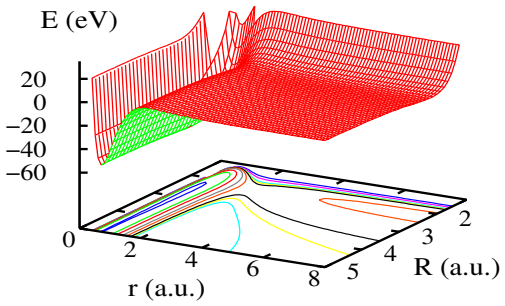

Fig. 1. Potential $V(R,r)$ of the NO-like model adjusted to data of [4].

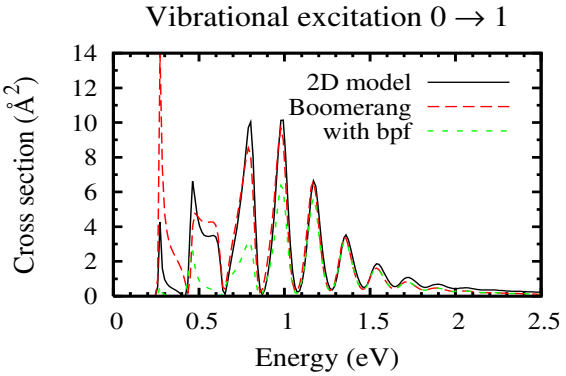

Fig. 2. Comparison of vibrational excitation cross sections for NO-like model obtained using the full 2D model (solid line) and the boomerang model without (long dashed line) and with (short dashed line) barrier penetration factor.

References

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