

Dissociative Recombination *via* Nonlocal Resonance Model for a Discrete State in Coulomb Continuum

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Synopsis: The nonlocal resonance model based on the projection-operator formalism [1,2] is extended to dissociative recombination and vibrational excitation in electron collisions with molecular cations. Preliminary results for a two-dimensional H_2^+ -like model are benchmarked against an exact two-dimensional solution, demonstrating a quantitatively accurate alternative to existing R -matrix and multichannel quantum defect methods [3,4].

The nonlocal discrete-state-in-continuum model based on the projection-operator (PO) formalism [1,2] provides a natural framework for the description of resonance-mediated processes in low-energy electron collisions. We present an extension of this approach to dissociative recombination (DR) and vibrational excitation (VE) in electron collisions with diatomic molecular cations. Treating cationic targets requires an explicit treatment of the long-range Coulomb interaction and the associated infinite series of Rydberg bound states, which qualitatively alters the structure of the nonlocal level-shift operator compared to the neutral case and gives rise to pronounced vibrational Feshbach resonances (VFRs) in the cross sections.

As a first application, we present preliminary results for a two-dimensional H_2^+ -like model, computing VE and DR cross sections mediated by a p -wave shape resonance. An example of computed cross sections is shown in Figure 1. The results are compared with an exact two-dimensional solution, demonstrating that the projection-operator approach provides a physically transparent and quantitatively accurate alternative to methods currently employed for DR, such as the multichannel quantum defect theory in combination with the frame-transformation approach [3] and the R -matrix approach [4]. The majority of the VFR structures are correctly reproduced across both DR and VE channels, particularly at low collision energies.

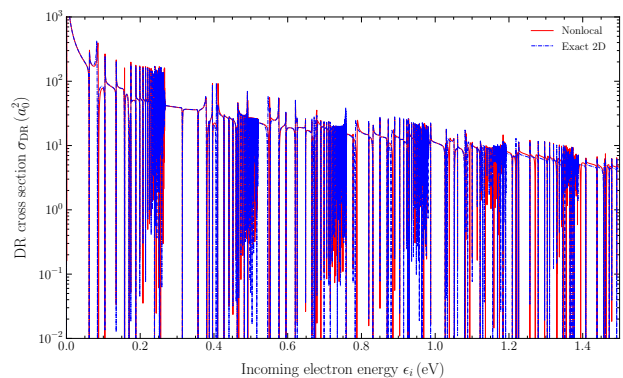


Figure 1: Dissociative recombination (DR) cross section for an H_2^+ -like model as a function of electron collision energy. The nonlocal resonance model results (red) are compared with the exact two-dimensional solution (blue). Individual peaks correspond to vibrational Feshbach resonances associated with Rydberg states of the neutral molecule

References

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