Couplings in the Continuum

J. Royal and A. E. Orel

Department of Applied Science, University of California, Davis, CA

When two or more electronic resonances of the same symmetry are close together in energy, electronic coupling between the resonances can occur. Because the states are chosen to be the adiabatic eigenstates of H_{el}, the resonant states can interact with each other, in second order, via the electron scattering continuum into which the resonances can decay. The process is described as follows: an electron is captured into a resonant state. During dissociation, the electron makes a 'virtual' transition from the original resonance to the continuum, and then makes a second 'virtual' transition from the continuum to a second resonance state, which will dissociate into stable products. These resonant states are coupled by the same potential, which is responsible for the finite auto detachment lifetimes of isolated molecular negative-ion states [1].

This mechanism was first used by Hazi [1] to describe dissociative electron attachment to HBr. In dissociative attachment this is not a common situation since there are usually a small number of resonant states. In contrast, in the case of dissociative recombination, there exist core-excited resonance states which form a Rydberg series converging to excited states of the ion that have the same symmetry. We will present the first application of this mechanism for the case of dissociative recombination specifically to the system HeH^+.

Larson and Orel [2] reported calculated total cross sections and product state distributions for the dissociative recombination of HeH^+ with electrons in the high-energy resonance region. They compared several models for the non-adiabatic coupling, and were able to predict total cross section values that agreed with the experimental values. However, the prediction for the product state distributions did not agree with experiment. The redistribution of flux between the various channels due to this mechanism and its effect will be discussed.

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References

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