Abstract Submitted
for the GEC05 Meeting of
The American Physical Society

Numerically Solvable Model of Low-Energy Resonant Electron-Molecule Collisions without Born-Oppenheimer Approximation K. HOUFEK, LBNL, C.W. MCCURDY, UC Davis, T.N. RESCIGNO, LBNL — 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. Using this model it is possible to study basic electron-molecule collisions: the vibrational excitation of a molecule by electron impact and the dissociative electron attachment to a molecule. The full Hamiltonian of our model is $H = -1/2\mu\, d^2/dR^2 - 1/2\, d^2/dr^2 + V_0(R) - \lambda(R)e^{-\alpha r^2} + l(l+1)/2r^2$ where $V_0(R)$ is a Morse potential for the vibrational motion of the neutral molecule, the forth term describes the interaction between the molecule and the electron and the centrifugal term with $l \neq 0$ is added to provide a resonant behavior in our system. The suggested model enables us to compare various approximations used in low-energy resonant electron-molecule collisions (for example the boomerang model or the nonlocal resonance model) with the exact solution and to investigate when these approximations are valid.

Thomas Rescigno
LBNL

Date submitted: 15 Jun 2005 Electronic form version 1.4