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An Alternative Approach to the Non-local Theory of Low-Energy Electron-Molecule Collisions KAREL HOUFEK, Charles University in Prague — The non-local theory of the nuclear dynamics of the resonant low-energy electron-molecule collisions [W. Domcke, Phys. Rep. 208, 97 (1991)] is reformulated in such a way that the driving equation describing of the nuclear motion in the non-local, complex, and energy-dependent (or time-dependent) potential is replaced by the infinite system of coupled differential equations for nuclear wave functions corresponding to the electronic discrete state and continuum states. This system is then reduced to a finite system using some appropriate discretization of the electronic continuum. For systems with two or more nuclear degrees of freedom like H_20, the resulting system of coupled differential equations with local potentials and couplings could be easier to solve numerically that a single equation with nonlocal potential. We have tested this alternative approach on diatomic molecules. For numerical solution we have applied the FEM and DVR methods together with the exterior complex scaling method [T.N. Rescigno and C.W. McCurdy, Phys. Rev. A 62, 032706 (2000)]. The results have shown that even for relatively small number of the electronic states used for the discretization of the electronic continuum one can get reasonably accurate cross sections for processes of interest.

Karel Houfek
Charles University in Prague

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