

**EIKONAL METHODS**  
**IN CONFIGURATION AND PHASE SPACE**  
**FOR QUANTUM MOLECULAR DYNAMICS <sup>†</sup>**

**David A. Micha <sup>\*</sup>**

*Departments of Chemistry and of Physics,  
University of Florida, Gainesville FL 32611, USA*

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Collision-induced and photoinduced electronic excitation of molecular systems are described in terms of eikonal representations of states for coupled classical-like and quantum-like degrees of freedom. Starting with a description for all the electrons and nuclei, a first principles dynamics has been developed, and equations have been solved in an eikonal approximation for the nuclear motions using a "relax-and-drive" propagation method for an electronic density matrix.[1] This treatment has been extended for a many-atom system to include dissipative dynamics, introducing a partial Wigner transform of the density operator, and dissipative rates into its Liouville-von Neumann equation.[2] Examples of applications will be described, with emphasis on the use of atomic pseudopotentials and on the quality of basis set expansions, for collisional cross sections of alkali atoms interacting with noble gas atoms and for their spectra in noble gas clusters. A second example involves photodesorption of diatomics from metal surfaces by femtosecond pulses, including populations and coherence relaxation rates in a density matrix treatment.[3]

1. D. A. Micha, *J. Phys. Chem.* **103**, 7562 (1999)( Feature Article )
2. D. A. Micha and B. Thorndyke "Dissipative Dynamics in Many-Atom Systems: A Density Matrix Treatment", *Intern. J. Quantum Chem.*, to appear (2002)
3. D. A. Micha, A. Santana, and A. Salam, *J. Chem. Phys.* **116**, 10562 (2002).

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