# Quasi-Classical Trajectory Study of Atom-Diatomic Molecule Collisions in Symmetric Hyperspherical Coordinates

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We investigate the reactive dynamics of triatomic systems of the heavy + light-heavy type (e.g., F + HCl and F + HI reactions) for total angular momentum equal zero and for different low-lying rovibrational states of the diatomic molecule. For each of the initial vibrational quantum numbers, the time evolution of the atom-diatom collision process is investigated for a wide range of impact angles and collision energies. To this purpose, the Quasi-Classical Trajectories (QCT) method was implemented in a hyperspherical configuration space. The Hamilton equations of motion are solved numerically in an intermediate effective Cartesian space to exploit the relative simplicity of this intermediate representation. Interatomic interactions are described by London-Eyring-Polanyi-Sato potential energy surfaces specifically developed for the target reactions, and the results of the QCT simulations are discussed in terms of the time-evolution of the hyperangles. The analysis of the collision dynamics using symmetric hyperspherical coordinates provides, in addition to the description in terms of a natural reaction coordinate (the hyperradius), a more striking representation of the exchange dynamics, in terms of the time-dependent probability distribution along the kinematic rotation hyperangle, and a precise distinction between direct and indirect mechanisms of the reaction. The extension of the present study to incorporate quantum effects within the framework of the Quantum Trajectory Method is described.