ABSTRACT

Ph.D. Thesis of Ioan Cristian Morari: "Zeitabhängige Untersuchungen zu reaktiven Streuprozessen" ("Time-dependent investigations of reactive scattering processes"), University of Siegen, Germany, 2001.

After a short introduction to the reactive molecule dynamics methods **(Section 1)** in **Section 2** the most important observables that characterize molecular dynamics are discussed. Time-dependent and time-independent approaches to scattering processes are presented in **Section 3**. The specifics for atom-diatom collisions are exposed in **Section 4**. **Section 5** describes the implementation of a FORTRAN-program solving the time dependent Schrödinger equation. This can be summarized as follows: (a) the evolution operator is expanded in a set of Chebychev polynomials; (b) the discrete variable representation is used to represent the wavepacket; (c) the fast Fourier transform algorithm is used to compute the kinetic energy; (d) optical potentials are used to impose appropriate boundary conditions; (e) for the analysis of the propagated wavepacket one can choose between split-functions, autocorrelation or flux methods. With the present implementation the propagation of wavepackets (for total angular momentum $J \geq 0$) on coupled potential energy surfaces can be performed. One version of the code runs efficiently on a parallel architecture. The information extracted from a simulation includes reaction probabilities, cross sections and reaction rate constants. We used the D+$H_2(v = 0; j = 0) \rightarrow$ DH +H reaction as a benchmark test for the code. Accurate and approximate calculations of cross sections and rate constants are presented in **Section 6**. Calculations at different levels of accuracy are discussed. A wavepacket simulation of the charge transfer reaction $H^+ + H_2(v = 0, j = 0) \rightarrow H_3^+ \rightarrow H_2^+ + H$ is presented in the last subsection.