# Abstract

In the first part of the summary of this thesis, the time dependent wavepacket method is presented in comparison with other approaches, and the approximations used are discussed. Different applications, such as calculation of absorption spectra, Raman spectra, calculation of eigenstates and description of femtosecond experiments, are presented.

An exact calculation of absorption spectra of polyatomic molecules is a complicated task. To explain the phenomenon, time dependent and time independent methods for solving the Schrödinger equation are used. For some particular problems, for example, photodissociation, the time dependent methods are known to be very efficient. In the time dependent approach the absorption spectrum is found by propagating the initial state wavefunction on the excited state potential energy surface. The time dependent Schrödinger equation is solved using a grid representation of the wave function. The split operator method together with the fast Fourier transform is used in the present work in order to propagate a wavepacket. This approach also allows us to describe femtosecond experiments.

In the second part of the summary, the included articles describing calculations on photodissociation of the $CH_2I_2$, OClO, $O_3$ and $NO_2$ molecules using the split operator method in hyperspherical coordinates are presented. Connections between properties, such as absorption spectra, and photodissociation dynamics in these molecules are revealed.

The time dependent methods can be used to find eigenstates of the Schrödinger equation. Often an efficient way to do this is to use the filter diagonalization method. It allows one to use the time dependent methods efficiently for finding and characterizing bound and quasi-bound states. The filter diagonalization method is described in the summary and the convergence of the method is discussed.