Title: A new method for the solution of the Schrödinger equation

Author: Jakub Kocák

Department: Department of Physical and Macromolecular Chemistry

Supervisor: doc. RNDr. Filip Uhlík, Ph.D.

Abstract: In this thesis we study method for the solution of time-independent Schrödinger equation for ground state. The wave function, interpreted as probability density, is represented by samples. In each iteration we applied approximant of imaginary time propagator. Acting of the operator is implemented by Monte Carlo simulation. Part of the thesis is dedicated to methods of energy calculation from samples of wave function: method based on estimation of value of wave function, method of convolution with heat kernel, method of averaged energy weighed by wave function and exponential decay method. The method for the solution was used to find ground state and energy for 6-dimensional harmonic oscillator, anharmonic 3-dimensional octic oscillator and hydrogen atom.

Keywords: imaginary time propagation, Monte Carlo method, variational principle, ground state