Presentation

Numerical Computation of the Multi-Particle Time-Dependent Schrödinger Equation

Abstract

We describe and analyze an approach to the approximate solution of the time-dependent Schroedinger equation for electrons. To make the high-dimensional, linear Schroedinger equation tractable for numerical computation, we use the multiconfiguration time-dependent Hartree-Fock method (MCTDHF). This approximation on a manifold is defined by a variational principle and implies equations of motion which correspond to nonlinear, single-particle Schroedinger equations.

For the numerical integration of the MCTDHF equations we analyze the convergence of time semidiscretization based on symmetric additive (`Strang') splitting of the vector field. It is proven that the convergence is of first order in the Sobolev space H^1 and of second order in L^2 if the exact solution is in H^2 for unbound fermions and in H^3 for an atom, respectively.

As a prerequisite, we prove that for initial data in the Sobolev space H2, there exists a unique classical solution of the MCTDHF equations in H2 for all times where the density matrix appearing in the definition of the equations stays invertible.

Finally, we demonstrate how analogous model reduction techniques based on a variational principle can be used successfully in the spatially discrete setting, i.e. for the low-rank approximation of time-dependent tensors and matrices.