Split-Step Time Propagation of the Multi-Configuration Time-Dependent Hartree-Fock Equations for Atoms

Othmar Koch[1] and Christian Lubich

We describe and analyze an approach to the approximate solution of the time-dependent Schroedinger equation governing electron dynamics in an atom. Our method of choice to make the original, linear Schroedinger equation tractable for numerical computation, is the multiconfiguration time-dependent Hartree-Fock method, MCTDHF. This variational approximation implies partially uncoupled, nonlinear equations of motion resulting from the Dirac-Frenkel variational principle.

For the MCTDHF equations, we analyze the convergence of a time integrator based on the symmetric splitting of the vector field into its kinetic and potential parts.

We establish the classical second-order convergence of this method assuming regularity of the exact solution in the Sobolev space with two bounded derivatives for systems of unbound fermions, and the same holds for electrons in an atom under additional regularity assumptions.

As a prerequisite we also discuss existence and regularity of the exact solution to the MCTDHF equations.

[1]Supported by the Austrian Academy of Sciences, APART program.