Mathematical and Numerical Analysis of the MCTDH Equations in Quantum Dynamics

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Joint work with Christian Lubich

We describe and analyze an approach to the approximate solution of the time-dependent multi-particle Schrödinger equation. Our method of choice to make the original, linear Schrödinger equation tractable for numerical computation, is the multiconfiguration time-dependent Hartree method, MCTDH. The approximation is defined by partially uncoupled, nonlinear equations of motion resulting from the *Dirac-Frenkel variational principle*. We first discuss existence of a unique, regular solution of the equations of motion in the presence of bounded potentials which occur in quantum molecular dynamics. We prove existence of a solution in the Sobolev space H^m by employing commutator techniques. By different arguments, the result can also be extended to unbounded potentials in the multiconfiguration time-dependent Hartree-Fock method (MCTDHF) for systems of fermions, based on appropriate estimates of the singular 'Hartree terms'.

Moreover, we analyze the convergence of a time integrator for the MCTDHF equations based on the symmetric ('Strang') splitting of the vector field into its kinetic and potential parts. We prove first order convergence in H^1 and quadratic convergence in L^2 when the exact solution is in H^2 and H^3, respectively. This time integrator thus enables to treat separately the fast varying modes associated with the kinetic part of the Hamiltonian and the solution modes related to the computationally expensive meanfield integrals given by the Hartree terms.

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