

SPLITTING METHODS FOR THE MULTI-CONFIGURATION
TIME-DEPENDENT HARTREE-FOCK EQUATIONS

Othmar Koch¹

Joint with Christian Lubich²

We describe and analyze an approach to the approximate solution of the time-dependent Schrödinger equation for a gas of unbound Fermions interacting by Coulomb forces. To make the high-dimensional, linear Schrödinger 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 non-linear, single-particle Schrödinger 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 H^1 and of second order in L^2 if the exact solution is in H^2 and H^3 , respectively.

As a prerequisite, we prove that for initial data in the Sobolev space H^2 , there exists a unique classical solution of the MCTDHF equations in H^2 for all times where the density matrix appearing in the definition of the equations stays invertible.

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²Mathematisches Institut, Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen