The Variational Splitting Method for the Multi-Configuration Time-Dependent Hartree-Fock Equations

Othmar Koch[1] and Christian Lubich

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. Our method of choice to make the original, linear Schrödinger equation tractable for numerical computation, is the multiconfiguration time-dependent Hartree–Fock method, MCTDHF, which is closely related to the MCTDH method in quantum molecular dynamics, additionally accounting for the antisymmetry implied by the Pauli exclusion principle. The approximation is defined by 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 ('Strang') splitting of the vector field into its kinetic and potential parts. This was introduced as *variational splitting* by C. Lubich for MCTDH in quantum molecular dynamics. The convergence result in the presence of the unbounded Coulomb potential can be stated as follows:

Consider the numerical approximation of the MCTDHF equations given by time semidiscretization based on variational splitting with step size Δt, $u_j \mapsto u_{j+1} = \mathcal{S}_{\Delta t} u_j$, $j = 0, 1, \ldots$. Then the convergence estimates

$$(1) \qquad \|u_n - u(t_n)\|_{H^1} \quad \leq \quad \mathrm{const.}\, \Delta t, \qquad \text{for } t_n = n\Delta t,$$

$$(2) \qquad \|u_n - u(t_n)\|_{L^2} \quad \leq \quad \mathrm{const.}\, (\Delta t)^2,$$

hold if the exact solution satisfies $u \in H^2$ for (1) and $u \in H^3$ for (2).

As a prerequisite for the convergence proof, existence of a unique, regular solution to the MCTDHF equations is proven.