Efficient High-Order Splitting Methods for the MCTDHF Equations

Othmar Koch

joint with Ch. Lubich, Ch. Neuhauser, and M. Thalhammer

September 20, 2010

We discuss high-order split-step time integrators for the semi-discretization of the multi-configuration time-dependent Hartree–Fock (MCTDHF) equations in electron dynamics. This approximation on a nonlinear, solution-dependent manifold is defined by the Dirac–Frenkel variational principle and implies equations of motion which correspond to coupled nonlinear single-particle Schrödinger equations.

We prove that the split-step time integrators have the classical convergence order under the assumption that iterated commutators of the kinetic and potential operators remain bounded for the exact solution, which is guaranteed if the exact solution is regular enough.

On the basis of the convergence analysis, we demonstrate that pairs of embedded split-step methods yield an estimate of the local error which can be used successfully in an adaptive time-stepping procedure.

The computationally most demanding part in an MCTDHF implementation is the evaluation of the nonlocal integral operators given by the "meanfield terms". By means of splitting methods, this part can be treated separately with respect to the choice of the step-size, with according increase in efficiency.

Finally, we prove that hierarchical matrices yield an approximation of the meanfield terms with reliable control of the approximation error and demonstrate the increase in efficiency as compared to global low rank approximation.