

Efficient High-Order Splitting Methods for Nonlinear Evolution Equations

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We discuss high-order split-step time integrators for the semi-discretization of nonlinear evolution equations defined by the right-hand side $H = A + B$ on a Banach space, where generally A and B are nonlinear, unbounded operators. Our particular focus is on the equations of motion associated with the multi-configuration time-dependent Hartree–Fock (MCTDHF) method used in numerical computations of 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 operators A , B remain bounded for the exact solution. This assumption is verified for the unbounded operators defining the MCTDHF equations if the exact solution is sufficiently regular.

For an efficient implementation of splitting methods, adaptive step-size control is of paramount importance. To this end, we construct pairs of related split-step formulae where several of the compositions coincide, yielding a computationally cheap estimate for the local truncation error.

Finally, we demonstrate that our approach enables reliable and efficient time integration of evolution equations by numerical examples. These comprise the cubic nonlinear Schrödinger equation with a focussing singularity in two space dimensions and a dissipative parabolic problem in 3D.