Variational Approximations in Quantum Dynamics and Multilinear Algebra

FR 08:00

*O. Koch** (Vienna Univ. of Technology),
and C. Lubich (Univ. Tübingen)

We describe and analyze an approach to the approximate solution of the time-dependent electronic Schrödinger equation. 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 nonlinear, solution-dependent manifold is defined by a variational principle and implies equations of motion which correspond to nonlinear, 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.

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

Finally we consider the approximation error of a related model reduction by variational approximation on a nonlinear manifold in a finite-dimensional, spatially discrete setting. The resulting approximation of time-dependent tensors and matrices as well as of tensor differential equations yields a quasi-optimal approximation whose error as compared to a pointwise best approximation grows only linearly even over 'long' time intervals.

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