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Title: Time-Dependent Simulations of Large-Scale Quantum Mechanical Processes

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Abstract: Time-Dependent Simulations of Large-Scale Quantum Mechanical Processes

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Time dependent linear and nonlinear equations govern the evolution of an extensive set of physical systems and processes, describing, to enumerate just a few, Bose-Einstein condensates; soliton propagation in optical and photonic band-gap fibers; quantum control of atomic and molecular collisions and reactions; highly-compressed liquids; and dense and ultra-cold plasmas. While the media vary substantially, the basic computational procedures have many common features. We focus on the nonlinear Schrodinger equation and discuss two powerful approaches to its propagation: the Arnoldi/Lanczos(AL)[1] and Real Space Product Formula(RSPF)[2]. Both provide efficient, systematic approximations to the short-time exponential propagator that moves the solution between time steps. We implement the former in a discrete variable representation (DVR)[3] both in spatial grid and finite element forms and the latter in a spatial mesh with a finite difference representation of the kinetic energy operator. Both approaches require O(N) operations to propagate the wavefunction between time steps and handle multidimensional systems. We shall also draw connections with Liouville formulations used in quantum molecular dynamics simulations of large collections of atoms and molecules. After briefly outlining these formulations, we shall discuss some of the varied applications.

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[1] B. I. Schneider,ITAMP Workshop: Computational Approaches to Time-Dependent Quantum Dynamics, ¡http://itamp.harvard.edu/quantum.html¿

[2] L. Collins, J. Kress, and R. Walker, Comp. Phys. Comm. **114**, 15 (1998)

[3] B. Schneider and D. Feder, Phys. Rev. A **59**,2232 (1999)