Numerical Treatment of the Multi-Particle Time-Dependent Schrödinger Equation

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We study the solution of the time-dependent Schrödinger equation for an atom or molecule with f degrees of freedom in a time-dependent electric field (typically arising from ultrashort laser pulses),

$$\mathrm{i}\frac{\partial\psi(x_1,\dots,x_f,t)}{\partial t} = H(t)\psi(x_1,\dots,x_f,t).$$

In the Hamiltonian H, the kinetic part includes a time-dependent drift term to model the influence of the electric field, and the potential part is given by the classical Coulomb potential. To reduce the computational complexity, we approximate the wave function using the *multi-configuration time-dependent Hartree-Fock method (MCTDHF)*. In this approach, the problem is reduced to a set of partially uncoupled, nonlinear PDEs. These are solved numerically using the method of lines. We demonstrate the success of our solution approach by giving results computed for a one-dimensional model, where a screened Coulomb potential is used. Moreover, low rank approximations for the computationally demanding *meanfield terms* are discussed. In the case of smooth potential, it is also possible to prove the existence, uniqueness and regularity of the solution of the MCTDHF equations. Finally, it is demonstrated how MCTDHF for the time-dependent Schrödinger equation relates to low rank approximations of time-dependent finite matrices and tensors, and an outlook on current developments is given.