

Analysis of the Multi-Configuration Time-Dependent Hartree-Fock Equations for Coulomb systems

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The multiconfiguration methods are a natural generalization of Hartree and Hartree-Fock methods for the approximation of the time-dependent Schrödinger for many electron systems in molecular quantum dynamics. They consist in approximating the N -particle Schrödinger wavefunction by a (time-dependent) linear combination of (time-dependent) Slater determinants. Electrons and (fixed) nuclei interact through the Coulomb potential. The equations of motion express as a system of ordinary differential equations for the expansion coefficients coupled to nonlinear Schrödinger-type equations for mono-electronic wavefunctions (orbitals).

In this talk, we discuss and establish existence and uniqueness of maximal solutions to the Cauchy problem in the energy space H^1 for the orbitals. Higher regularity spaces and well-posedness in L^2 is discussed as well. The solutions cease to exist at finite time if the density matrix becomes singular. We provide with a sufficient condition for existence of global solution. This is the first result in this direction.

This is a joint work with Claude Bardos, Norbert Mauser and Saber Trabelsi.