

Analysis and Numerical Approximation of the Multi-Configuration Time-Dependent Hartree-Fock Equations

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We describe and analyze an approach to the approximate solution of the time-dependent Schrödinger equation for a gas of unbound Fermions interacting by Coulomb forces. Our method of choice to make the original, linear Schrödinger equation tractable for numerical computation, is the multiconfiguration time-dependent Hartree-Fock method, MCTDHF, which is closely related to the MCTDH method in quantum molecular dynamics, additionally accounting for the antisymmetry implied by the Pauli exclusion principle. The approximation is defined by partially uncoupled, nonlinear equations of motion resulting from the *Dirac-Frenkel variational principle*,

$$(1) \quad i \frac{da_J}{dt} = \mathcal{A}_V(\phi)a, \quad \forall J = (j_1, \dots, j_f),$$

$$(2) \quad i \frac{\partial \phi_j}{\partial t} = T\phi_j + \mathcal{B}_V(a, \phi), \quad j = 1, \dots, N,$$

where the orbitals ϕ_j depend on only one degree of freedom each, T is the kinetic energy operator and $\mathcal{A}_V(\phi)$, $\mathcal{B}_V(a, \phi)$ are nonlinear functions depending on the Coulomb potential V . The wave function is thus approximated by

$$u(x, t) = \sum_{(j_1, \dots, j_f)} a_{j_1, \dots, j_f}(t) \phi_{j_1}(x_1, t) \cdots \phi_{j_f}(x_f, t), \quad j_k = 1, \dots, N.$$

The *Pauli exclusion principle* implies antisymmetry in the coefficient tensor $a = (a_{j_1, \dots, j_f})$ under exchange of any two indices. We prove the following result:

Theorem 1. *Consider the system (1)–(2). If the initial data for ϕ_j is in the Sobolev space H^2 , then there exists a unique classical solution of the MCTDHF equations satisfying*

$$a_J \in C^2([0, t^*), \mathbb{C}), \quad \phi_j \in C^1([0, t^*), L^2) \cap C([0, t^*), H^2),$$

where either $t^* = \infty$ or the density matrix appearing in the definition of \mathcal{B}_V becomes singular for $t = t^*$.

Moreover, we analyze the convergence of a time integrator based on the symmetric (‘Strang’) splitting of the vector field into its component parts $\hat{T} := -i(0, T)^T$, $\hat{V} := -i(\mathcal{A}_V, \mathcal{B}_V)$. The convergence result can be stated as follows:

Theorem 2. *Consider the numerical approximation of (1)–(2) given by time semidiscretization based on splitting with step size Δt , $u_j \mapsto u_{j+1} = \mathcal{S}_{\Delta t} u_j$, $j = 0, 1, \dots$. Then the convergence estimates*

$$(3) \quad \|u_n - u(t_n)\|_{H^1} \leq \text{const.} \Delta t, \quad \text{for } t_n = n\Delta t,$$

$$(4) \quad \|u_n - u(t_n)\|_{L^2} \leq \text{const.} (\Delta t)^2,$$

hold if the exact solution satisfies $u \in H^2$ for (3) and $u \in H^3$ for (4).

Extension of the result of **Theorem 1** to atoms with a nuclear attractive potential is straightforward, the extension of the result of **Theorem 2** is currently investigated.

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