Time Integration 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). The approximation is defined by equations of motion resulting from the *Dirac-Frenkel variational principle*,

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

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

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

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

The *Pauli exclusion principle* implies antisymmetry in the coefficient tensor $a = (a_{j_1,\ldots,j_f})$ 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*

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

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 $\hat{T} := -\mathrm{i}(0,T)^T$, $\quad \hat{V} := -\mathrm{i}(\mathcal{A}_V,\mathcal{B}_V)$. 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, $u_j \mapsto u_{j+1} = \mathcal{S}_{\Delta t}u_j$, $j = 0,1,\ldots$. Then the convergence estimates*

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

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

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

[1]Supported by the Austrian Academy of Sciences, APART program.

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