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,

\begin{align}
  i \frac{d a_J}{dt} &= \mathcal{A}_V(\phi) a, \quad \forall J = (j_1, \ldots, j_f), \\
  i \frac{\partial \phi_j}{\partial t} &= T\phi_j + \mathcal{B}_V(a, \phi), \quad j = 1, \ldots, N,
\end{align}

where the orbitals \( \phi_j \) 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 \( \phi_j \) 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 \( \Delta t \), \( u_j \mapsto u_{j+1} = S_{\Delta t} u_j, \quad j = 0, 1, \ldots \). Then the convergence estimates

\begin{align}
  \|u_n - u(t_n)\|_{H^1} &\leq \text{const.} \Delta t, \quad \text{for } t_n = n \Delta t, \\
  \|u_n - u(t_n)\|_{L^2} &\leq \text{const.} (\Delta t)^2,
\end{align}

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