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ANALYSIS OF A FULLY DISCRETE FINITE ELEMENT METHOD FOR THE MAXWELL–SCHRÖDINGER SYSTEM IN THE COULOMB GAUGE

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Abstract. In this paper, we consider the initial-boundary value problem for the time-dependent Maxwell–Schrödinger system in the Coulomb gauge. We propose a fully discrete finite element scheme for the system and prove the conservation of energy and the stability estimates of the scheme. By approximating the vector potential $\mathbf{A}$ and the scalar potential ϕ respectively in two finite element spaces satisfying certain orthogonality relation, we tackle the mixed derivative term in the discrete system and make the numerical computations and the theoretical analysis more easier. The existence and uniqueness of solutions to the discrete system are also investigated. The (almost) unconditionally error estimates are derived for the numerical scheme without certain restriction like $\tau \leq Ch^{\alpha}$ on the time step τ by using a new technique. Finally, numerical experiments are carried out to support our theoretical analysis.

Key words. Maxwell–Schrödinger, finite element method, energy conserving, error estimates.

1. Introduction

In this paper, we consider one of the fundamental equations of nonrelativistic quantum mechanics, the Maxwell–Schrödinger (M-S) system, which describes the time-evolution of an electron within its self-consistent generated and external electromagnetic fields. In this system, the Schrödinger's equation can be written as follows:

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \left\{\frac{1}{2m}\left[\mathrm{i}\hbar\nabla + q\mathbf{A}\right]^2 + q\phi + V\right\}\Psi \quad \text{in } \Omega_T, \tag{1}$$

where $\Omega_T = \Omega \times (0,T)$, Ψ, m, and q are respectively the wave function, the mass, and the charge of the electron. V is the time-independent potential energy and is assumed to be bounded in this paper. The vector potential $\mathbf{A}$ and the scalar potential ϕ are obtained by solving the following equations:

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \qquad \mathbf{B} = \nabla\times\mathbf{A}, \tag{2}$$

where the electric fields $\mathbf{E}$ and the magnetic fields $\mathbf{B}$ satisfy the Maxwell's equations:

$$\begin{aligned} &\nabla\times\mathbf{E} + \frac{\partial\mathbf{B}}{\partial t} = 0, \qquad \nabla\cdot\mathbf{B} = 0,\\ &\frac{1}{\mu}\nabla\times\mathbf{B} - \epsilon\frac{\partial\mathbf{E}}{\partial t} = \mathbf{J}, \quad \nabla\cdot(\epsilon\mathbf{E}) = \rho. \end{aligned} \tag{3}$$

Here ϵ and μ denote the electric permittivity and the magnetic permeability of the material, respectively. The charge density ρ and the current density $\mathbf{J}$ are defined as follows:

$$\rho = q|\Psi|^2, \qquad \mathbf{J} = -\frac{\mathrm{i}q\hbar}{2m}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) - \frac{|q|^2}{m}|\Psi|^2\mathbf{A}. \tag{4}$$

Here Ψ^* denotes the conjugate of Ψ.

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Substituting (2) into (3) and combining (1) and (4), we obtain the following M-S system

$$(5)\quad \begin{cases} i\hbar\dfrac{\partial\Psi}{\partial t} = \left\{\dfrac{1}{2m}\left[i\hbar\nabla + q\mathbf{A}\right]^2 + q\phi + V\right\}\Psi \quad \text{in } \Omega_T, \\ -\dfrac{\partial}{\partial t}\nabla\cdot\big(\epsilon\mathbf{A}\big) - \nabla\cdot\big(\epsilon\nabla\phi\big) = q|\Psi|^2 \quad \text{in } \Omega_T, \\ \epsilon\dfrac{\partial^2\mathbf{A}}{\partial t^2} + \nabla\times\big(\mu^{-1}\nabla\times\mathbf{A}\big) + \epsilon\dfrac{\partial(\nabla\phi)}{\partial t} = \mathbf{J} \quad \text{in } \Omega_T, \\ \mathbf{J} = -\dfrac{iq\hbar}{2m}\big(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\big) - \dfrac{|q|^2}{m}|\Psi|^2\mathbf{A} \quad \text{in } \Omega_T, \\ \Psi, \phi, \mathbf{A} \text{ subject to the appropriate initial and boundary conditions.} \end{cases}$$

We assume that $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ is a bounded Lipschitz domain. The total energy of the system, at time t, is defined as follows

$$(6)\quad \begin{aligned} \mathcal{E}(t) = \int_\Omega \Big(\frac{1}{2}\big|\left(i\nabla + q\mathbf{A}\right)\Psi(t,\mathbf{x})\big|^2 + V|\Psi(t,\mathbf{x})|^2 \\ + \frac{\epsilon}{2}|\mathbf{E}(t,\mathbf{x})|^2 + \frac{1}{2\mu}|\mathbf{B}(t,\mathbf{x})|^2\Big)\mathrm{d}\mathbf{x}. \end{aligned}$$

For a smooth solution $(\Psi, \mathbf{A}, \phi)$ satisfying certain appropriate boundary conditions, the energy is a conserved quantity.

It is well known that the solutions of the above M-S system are not uniquely determined. In fact, the M-S system is invariant under the gauge transformation:

$$(7)\quad \Psi \longrightarrow \Psi' = e^{iq\chi}\Psi, \quad \mathbf{A} \longrightarrow \mathbf{A}' = \mathbf{A} + \nabla\chi, \quad \phi \longrightarrow \phi' = \phi - \frac{\partial\chi}{\partial t},$$

for any sufficiently smooth function $\chi : \Omega\times(0,T) \to \mathbb{R}$. That is, if $(\Psi, \mathbf{A}, \phi)$ satisfies the M-S system, then so does $(\Psi', \mathbf{A}', \phi')$.

In view of the gauge freedom, to obtain mathematically well-posed equations, we can impose some extra constraint, commonly known as gauge choice, on the solutions of the M-S system. In this paper, we study the M-S system in the Coulomb gauge, i.e. $\nabla\cdot\mathbf{A} = 0$.

In this paper, we employ the atomic units, i.e. $\hbar = m = q = 1$. For simplicity, we assume that $\epsilon = \mu = 1$. The M-S system in the Coulomb gauge (M-S-C) can be reformulated as follow:

$$(8)\quad \begin{cases} -i\dfrac{\partial\Psi}{\partial t} + \dfrac{1}{2}\left(i\nabla + \mathbf{A}\right)^2\Psi + V\Psi + \phi\Psi = 0 \quad \text{in } \Omega_T, \\ \dfrac{\partial^2\mathbf{A}}{\partial t^2} + \nabla\times(\nabla\times\mathbf{A}) + \dfrac{\partial(\nabla\phi)}{\partial t} + \dfrac{i}{2}\big(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\big) \\ \qquad + |\Psi|^2\mathbf{A} = 0 \quad \text{in } \Omega_T, \\ -\Delta\phi = |\Psi|^2 \quad \text{in } \Omega_T. \end{cases}$$

In this paper, the M-S-C system (8) is considered in conjunction with the following initial boundary conditions:

$$(9)\quad \begin{cases} \Psi(\mathbf{x},t) = 0, \quad \mathbf{A}(\mathbf{x},t)\times\mathbf{n} = 0, \quad \phi(\mathbf{x},t) = 0 \quad \text{on } \partial\Omega\times(0,T), \\ \Psi(\mathbf{x},0) = \Psi_0(\mathbf{x}), \quad \mathbf{A}(\mathbf{x},0) = \mathbf{A}_0(\mathbf{x}), \quad \mathbf{A}_t(\mathbf{x},0) = \mathbf{A}_1(\mathbf{x}) \quad \text{in } \Omega, \end{cases}$$

with $\nabla\cdot\mathbf{A}_0 = \nabla\cdot\mathbf{A}_1 = 0$.

For the M-S-C system, the energy $\mathcal{E}(t)$ takes the following form

$$(10)\quad \mathcal{E}(t) = \int_\Omega \left(\frac{1}{2}\big|\left[i\nabla + q\mathbf{A}\right]\Psi\big|^2 + V|\Psi|^2 + \frac{1}{2}\Big|\frac{\partial\mathbf{A}}{\partial t}\Big|^2 + \frac{1}{2}|\nabla\times\mathbf{A}|^2 + \frac{1}{2}|\nabla\phi|^2\right)\mathrm{d}\mathbf{x}.$$