INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 16, Number 1, Pages 139–166

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.

Received by the editors March 5, 2018 and, in revised form, June 22, 2018.
2000 *Mathematics Subject Classification.* 65L20, 65M12, 65M60.

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

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

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

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

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:

$$
\Psi \longrightarrow \Psi' = e^{\mathrm{i}q\chi}\Psi, \quad \mathbf{A} \longrightarrow \mathbf{A}' = \mathbf{A} + \nabla\chi, \quad \phi \longrightarrow \phi' = \phi - \frac{\partial\chi}{\partial t}, \tag{7}
$$

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:

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

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

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

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

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

Remark 1.1 The boundary condition of the Schrödinger's equation, $\Psi(\mathbf{x}, t) = 0$ on $\partial\Omega$, implies that it is a closed quantum system and the electron is trapped within the domain. For the Maxwell's equations, we use the perfect conductive boundary condition (PEC), i.e. $\mathbf{A}(\mathbf{x}, t) \times \mathbf{n} = 0$ and $\phi(\mathbf{x}, t) = 0$ on $\partial\Omega$. We refer readers to [8] for the determination of the boundary conditions for the vector potential $\mathbf{A}$ and the scalar potential ϕ in different electromagnetic environment.

The existence and uniqueness of the solutions to the M-S system (5) in the whole space of $\mathbb{R}^2$ or $\mathbb{R}^3$ have been investigated in [13, 20, 21, 22]. However, these results don't hold for bounded domains because some important tools used in these work can't apply to bounded domains. For example, Strichartz estimates and many other tools from Fourier analysis. To the best of our knowledge, there seems no results on the wellposedness of the M-S system in a bounded domain.

Due to the development of nanophotonics in recent years, the Maxwell–Schrödinger coupled model is widely used to simulate light-matter interaction at the nanoscale, such as self-induced transparency in quantum dot systems [14], laser-molecule interaction [15], carrier dynamics in nanodevices [24] and molecular nanopolaritonics [17]. In the existing numerical methods, the Maxwell's equations of field type (3), instead of the potential type in (5), are usually coupled to the Schrödinger's equation through the dipole approximation or by extracting the vector potential $\mathbf{A}$ and the scalar potential ϕ from the electric field $\mathbf{E}$ and the magnetic field $\mathbf{H}$ [1, 23, 29, 32]. In part because there exists robust numerical algorithms for the Maxwell's equations (3), for example, the time domain finite difference (FDTD) method, the transmission line matrix (TLM) method, etc. In the context of the M-S system (5), the FDTD method [25] and a Hamiltonian approach together with the eigenmode expansion technique [6] have been proposed. In our recent work [18], an alternating Crank–Nicolson Galerkin finite element method together with the optimal error estimates are studied for the M-S system (5) in the Lorentz gauge. But so far, there are rather limited studies on the numerical algorithms of the M-S system (5) as well as their convergence analysis.

In this paper we present two equivalent fully discrete finite element methods for solving the problem (8)-(9) and show that they keep the total charge and the total energy of the discrete system conserved. A difficulty in solving the M-S-C system numerically lies in the mixed derivative term $\frac{\partial(\nabla\phi)}{\partial t}$ in the second equation of (8). The presence of this term would make the discrete system more involved and the analysis of the numerical schemes much more difficult. To overcome this difficulty, in the discrete system, we find the vector potential $\mathbf{A}$ and the associated test functions $\mathbf{v}$ in a finite element space $\mathbf{X}_h$ satisfying the discrete divergence-free condition, i.e.,

$$(\nabla \cdot \mathbf{v}_h,\, \varphi_h) = 0,\ \forall \mathbf{v}_h \in \mathbf{X}_h,\ \varphi_h \in X_h, \tag{11}$$

where X_h is a finite element subspace of $H_0^1(\Omega)$, and then approximate the scalar potential ϕ in X_h. Thanks to this technique, we make the mixed derivative term vanish in the discrete system (36). At first look, the M-S-C system (8)-(9) doesn't involve the divergence-free constraint on the vector potential $\mathbf{A}$, which makes the discrete divergence-free approximation of $\mathbf{A}$ a bit dubious. However, in section 2 we prove that the weak solution to the M-S-C system (8)-(9) implies that $\nabla\cdot\mathbf{A} = 0$ and thus the discrete divergence-free approximation of $\mathbf{A}$ is justified. More importantly, by approximating $\mathbf{A}$ and ϕ respectively in the finite element subspaces $\mathbf{X}_h$ and X_h satisfying (11), we can tackle the mixed derivative term and make the numerical computations and the theoretical analysis a lot easier.

The main result of this paper is the (almost) unconditionally error estimates of the numerical scheme in which we only require the time step τ sufficiently small. In comparison, in the error analysis of numerical algorithms for many nonlinear PDEs in $\mathbb{R}^2$ or $\mathbb{R}^3$, the CFL-type condition $\tau \leq C\,h^\alpha$ is often needed [19, 34, 35, 36]. In practice, many authors usually derive the L^∞ bounds of the numerical solutions first and then use them to establish the error bounds of the numerical methods. To get the L^∞ estimates of the numerical solutions, in $\mathbb{R}^2$ or $\mathbb{R}^3$, a traditional and widely used technique is to apply the inverse inequalities, which thus often leads to certain restriction like $\tau \leq C\,h^\alpha$ on the time step. In this paper, we avoid using the inverse inequalities to obtain the L^∞ boundedness of the numerical solutions by taking a deep analysis of the error equations and making some difficult nonlinear terms in the Schrödinger's equation and the Maxwell's equations respectively cancel out. Thanks to this technique, we remove the above restriction on the time step. It is worth mentioning that in [18], we proved the optimal error estimates of a fully discrete finite element method for the M-S system in the Lorentz gauge by the mathematical induction method. However, due to the different system nature, the method used in [18] can't be applied in this paper.

The rest of this paper is organized as follows. In section 2, we introduce some notation and give some useful lemmas. In section 3, we present two fully discrete finite element schemes for the M-S-C system and show that they are equivalent. In section 4, conservation and the stability are established for the method. In section 5, we prove the existence and uniqueness of solutions to the discrete system. The error estimates of the scheme are provided in section 6. We present some numerical experiments in section 7 to confirm our theoretical analysis.

2. Notation and preliminaries

In this section, we first introduce some notation and give the definition of weak solutions to the M-S-C system (8)-(9). Then we give several lemmas which are used in the following sections.

For any nonnegative integer s, we denote $W^{s,p}(\Omega)$ as the conventional Sobolev spaces of the real-valued functions defined in Ω and $W_0^{s,p}(\Omega)$ as the subspace of $W^{s,p}(\Omega)$ consisting of functions whose traces are zero on $\partial\Omega$. As usual, we denote $H^s(\Omega) = W^{s,2}(\Omega)$, $H_0^s(\Omega) = W_0^{s,2}(\Omega)$, and $L^p(\Omega) = W^{0,p}(\Omega)$, respectively. We use $\mathcal{H}^s(\Omega) = \{u + \mathrm{i}v \,|\, u, v \in H^s(\Omega)\}$ and $\mathcal{L}^p(\Omega) = \{u + \mathrm{i}v \,|\, u, v \in L^p(\Omega)\}$ with calligraphic letters for Sobolev spaces and Lebesgue spaces of the complex-valued functions, respectively. Furthermore, let $\mathbf{H}^s(\Omega) = [H^s(\Omega)]^d$ and $\mathbf{L}^p(\Omega) = [L^p(\Omega)]^d$ with bold faced letters be Sobolev spaces and Lebesgue spaces of the vector-valued functions with d components (d=2, 3). The dual spaces of $\mathcal{H}_0^s(\Omega)$, $H_0^s(\Omega)$, and $\mathbf{H}_0^s(\Omega)$ are denoted by $\mathcal{H}^{-s}(\Omega)$, $H^{-s}(\Omega)$, and $\mathbf{H}^{-s}(\Omega)$, respectively. L^2 inner-products in $H^s(\Omega)$, $\mathcal{H}^s(\Omega)$, and $\mathbf{H}^s(\Omega)$ are denoted by $(\cdot,\cdot)$ without ambiguity.

We consider the following subspaces of $\mathbf{H}^1(\Omega)$ and $\mathbf{L}^2(\Omega)$:

$$\begin{aligned}
&\mathbf{H}_t^1(\Omega) = \{\mathbf{v} \in \mathbf{H}^1(\Omega) \,|\, \mathbf{v} \times \mathbf{n} = 0 \ \text{ on } \partial\Omega\},\\
&\mathbf{H}_{t,0}^1(\Omega) = \{\mathbf{v} \in \mathbf{H}_t^1(\Omega) \,|\, \nabla \cdot \mathbf{v} = 0\},\\
&\mathbf{L}_0^2(\Omega) = \{\mathbf{v} \in \mathbf{L}^2(\Omega) \,|\, \nabla \cdot \mathbf{v} = 0 \text{ weakly }\}.
\end{aligned}$$

The semi-norms on $\mathbf{H}_t^1(\Omega)$ and $\mathbf{H}_{t,0}^1(\Omega)$ are defined by

$$|\mathbf{u}|_{\mathbf{H}_t^1} := \|\nabla \cdot \mathbf{u}\|_{L^2(\Omega)} + \|\nabla \times \mathbf{u}\|_{\mathbf{L}^2(\Omega)}, \quad |\mathbf{u}|_{\mathbf{H}_{t,0}^1} := \|\nabla \times \mathbf{u}\|_{\mathbf{L}^2(\Omega)},$$

both of which are equivalent to the standard $\mathbf{H}^1(\Omega)$-norm $\|\mathbf{u}\|_{\mathbf{H}^1(\Omega)}$ (see, e.g., [12]).

To take into account the time dependence, for any Banach space W and integer $s \geq 1$, we define function spaces $C\big([0,T],\ W\big)$, $C\big((0,T),\ W\big)$, and $C_0^s\big((0,T),\ W\big)$ consisting of W-valued functions in $C[0,T]$, $C(0,T)$, and $C_0^s(0,T)$, respectively.

We define the weak solution to the M-S-C system (8)-(9) as follows:

Definition 2.1 $(\Psi,\ \mathbf{A},\ \phi)$ is a weak solution to (8)-(9), if

$$\Psi \in C\big([0,T];\mathcal{L}^2(\Omega)\big) \cap L^\infty\big(0,T;\mathcal{H}_0^1(\Omega)\big),\ \frac{\partial \Psi}{\partial t} \in L^\infty\big(0,T;\mathcal{H}^{-1}(\Omega)\big), \tag{12a}$$

$$\phi \in C\big([0,T];L^2(\Omega)\big) \cap L^\infty\big(0,T;H_0^1(\Omega)\big),\ \frac{\partial \phi}{\partial t} \in L^\infty\big(0,T;L^2(\Omega)\big), \tag{12b}$$

$$\mathbf{A} \in C\big([0,T];\ \mathbf{L}^2(\Omega)\big) \cap L^\infty\big(0,T;\ \mathbf{H}_t^1(\Omega)\big), \tag{12c}$$

$$\frac{\partial \mathbf{A}}{\partial t} \in C\big([0,T];\ \big(\mathbf{H}_t^1(\Omega)\big)'\,\big) \cap L^\infty\big(0,T;\ \mathbf{L}^2(\Omega)\big), \tag{12d}$$

with the initial condition $\Psi(\cdot,0) \in \mathcal{H}_0^1(\Omega)$, $\mathbf{A}(\cdot,0) \in \mathbf{H}_{t,0}^1(\Omega)$, $\mathbf{A}_t(\cdot,0) \in \mathbf{L}_0^2(\Omega)$, and the variational equations

$$\int_0^T \Big[\mathrm{i}\big(\Psi,\ \frac{\partial \widetilde{\Psi}}{\partial t}\big) + \frac{1}{2}\big(\,(\mathrm{i}\nabla + \mathbf{A})\,\Psi,\ (\mathrm{i}\nabla + \mathbf{A})\,\widetilde{\Psi}\big) + \big(V\Psi, \widetilde{\Psi}\big) + \big(\phi\Psi, \widetilde{\Psi}\big)\Big]\mathrm{d}t = 0, \tag{13}$$

$$\begin{aligned} \int_0^T \Big[\big(\mathbf{A}, \frac{\partial^2 \widetilde{\mathbf{A}}}{\partial t^2}\big) + \big(\nabla \times \mathbf{A}, \nabla \times \widetilde{\mathbf{A}}\big) + \big(\frac{\mathrm{i}}{2}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*),\ \widetilde{\mathbf{A}}\big) \\ -\big(\frac{\partial \phi}{\partial t},\ \nabla \cdot \widetilde{\mathbf{A}}\big) + \big(|\Psi|^2\mathbf{A},\ \widetilde{\mathbf{A}}\big)\Big]\mathrm{d}t = 0, \end{aligned} \tag{14}$$

$$\int_0^T \Big[\big(\nabla\phi,\ \nabla\widetilde{\phi}\big) - \big(|\Psi|^2,\ \widetilde{\phi}\big)\Big]\,\mathrm{d}t = 0, \tag{15}$$

hold for all $\widetilde{\Psi} \in C_0^1\big((0,T);\ \mathcal{H}_0^1(\Omega)\big)$, $\widetilde{\mathbf{A}} \in C_0^2\big((0,T);\ \mathbf{H}_t^1(\Omega)\big)$ and $\widetilde{\phi} \in C\big((0,T);\ H_0^1(\Omega)\big)$.

We now give some useful lemmas.

Lemma 2.1 The weak solution to the M-S-C system defined in Definition 2.1 satisfies $\nabla \cdot \mathbf{A} = 0$.

Proof. For any $\eta(t) \in C_0^2(0,T)$, $\varphi \in H_0^1(\Omega) \cap H^2(\Omega)$, take $\widetilde{\mathbf{A}} = \eta\nabla\varphi$ in (14) and we have

$$\int_0^T (\nabla \cdot \mathbf{A},\ \varphi)\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2}\,\mathrm{d}t - \int_0^T \Big[\big(\frac{\partial \phi}{\partial t},\ \Delta\varphi\big) + \big(\mathbf{J},\ \nabla\varphi\big)\Big]\frac{\mathrm{d}\eta}{\mathrm{d}t}\,\mathrm{d}t = 0, \tag{16}$$

where

$$\mathbf{J} = -\frac{\mathrm{i}}{2}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - |\Psi|^2\mathbf{A}. \tag{17}$$

Next we will show that

$$\big(\frac{\partial \phi}{\partial t},\ \Delta\varphi\big) + \big(\mathbf{J},\ \nabla\varphi\big) = 0, \quad \forall \varphi \in H_0^1(\Omega) \cap H^2(\Omega). \tag{18}$$

To this end, we choose $\widetilde{\Psi} = \eta\Psi\varphi$ in (13), $\widetilde{\phi} = \frac{\mathrm{d}\eta}{\mathrm{d}t}\varphi$ in (15), and take the imaginary part of (13) to find

$$\begin{aligned} &\int_0^T \Big[-\big(\frac{\partial \rho}{\partial t},\ \varphi\big) + \big(\mathbf{J},\ \nabla\varphi\big)\Big]\eta(t)\mathrm{d}t = 0, \\ &\int_0^T \Big[\big(\frac{\partial \phi}{\partial t},\ \Delta\varphi\big) + \big(\frac{\partial \rho}{\partial t},\ \varphi\big)\Big]\eta(t)\mathrm{d}t = 0, \end{aligned} \tag{19}$$

where $\rho = |\Psi|^2$ and $\mathbf{J}$ is defined in (17). Since $\eta(t)$ is arbitrary, by adding up two equations in (19) we obtain (18).

Combining (16) and (18) we see that

$$\int_0^T (\nabla \cdot \mathbf{A},\, \varphi)\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2}\,\mathrm{d}t = 0, \tag{20}$$

which implies that

$$\nabla \cdot \mathbf{A} = 0. \tag{21}$$

Consequently we complete the proof of this lemma. □

Lemma 2.2 Let $2 < p < 6$. Suppose that $\Omega \subset \mathbb{R}^d$, $d \geq 2$ is a bounded Lipschitz domain. Then for each $\epsilon > 0$, there exists some constant C_ϵ depending on ϵ (and on Ω and p) such that

$$\|u\|_{\mathcal{L}^p} \leq \epsilon\|\nabla u\|_{\mathbf{L}^2} + C_\epsilon\|u\|_{\mathcal{L}^2}, \qquad \forall u \in \mathcal{H}_0^1(\Omega).$$

Lemma 2.2 can be proved by applying Sobolev's embedding theorems, Poincaré's inequality, and the following lemma in [30]:

lemma 2.3 Let W_0, W, and W_1 be three Banach spaces such that $W_0 \subset W \subset W_1$, the injection of W into W_1 being continuous, and the injection of W_0 into W is compact. Then for each $\epsilon > 0$, there exists some constant C_ϵ depending on ϵ (and on the spaces W_0, W, W_1) such that

$$\|u\|_W \leq \epsilon\|u\|_{W_0} + C_\epsilon\|u\|_{W_1}, \qquad \forall u \in W_0.$$

Lemma 2.4 Suppose that $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ is a bounded Lipschitz domain and $\psi \in \mathcal{H}_0^1(\Omega)$, $\mathbf{A} \in \mathbf{L}^6(\Omega)$. There exists a constant C dependent of $\mathbf{A}$ such that

$$\frac{9}{32}\|\nabla\psi\|_{\mathbf{L}^2}^2 \leq \|(\mathrm{i}\nabla + \mathbf{A})\psi\|_{\mathbf{L}^2}^2 + C\|\psi\|_{\mathcal{L}^2}^2.$$

Proof. By applying Lemma 2.2, we have

$$\begin{aligned}\|\nabla\psi\|_{\mathbf{L}^2} &\leq \|(\mathrm{i}\nabla + \mathbf{A})\psi\|_{\mathbf{L}^2} + \|\mathbf{A}\psi\|_{\mathbf{L}^2} \leq \|(\mathrm{i}\nabla + \mathbf{A})\psi\|_{\mathbf{L}^2} + \|\mathbf{A}\|_{\mathbf{L}^6}\|\psi\|_{\mathcal{L}^3}\\ &\leq \|(\mathrm{i}\nabla + \mathbf{A})\psi\|_{\mathbf{L}^2} + \frac{1}{4}\|\nabla\psi\|_{\mathbf{L}^2} + C\|\psi\|_{\mathcal{L}^2}.\end{aligned}$$

Consequently,

$$\frac{9}{32}\|\nabla\psi\|_{\mathbf{L}^2}^2 \leq \|(\mathrm{i}\nabla + \mathbf{A})\psi\|_{\mathbf{L}^2}^2 + C\|\psi\|_{\mathcal{L}^2}^2. \qquad \square$$

We finally give a lemma in [5] which will be used to prove the existence of solutions to the discrete system.

Lemma 2.5 Let $(H, \langle\cdot,\cdot\rangle)$ be a finite-dimensional inner product space, $\|\cdot\|_H$ be the associated norm, and $g : H \longrightarrow H$ be continuous. Assume that

$$\exists\, \alpha > 0, \quad \forall z \in H, \;\; \|z\|_H = \alpha, \;\; \mathrm{Re}\langle g(z), z\rangle > 0.$$

Then there exists a $z_0 \in H$ such that $g(z_0) = 0$ and $\|z_0\|_H \leq \alpha$.

3. Fully discrete finite element schemes

In this section, we present the fully discrete schemes for the M-S-C system (8)-(9) using the Galerkin finite element method in space together with the Crank-Nicolson scheme in time. In the following of the paper, we assume that Ω is a bounded Lipschitz polyhedron convex domain in $\mathbb{R}^3$.

Let $\mathcal{T}_h = \{K\}$ be a regular partition of Ω into tetrahedrons of maximal diameter h. Without loss of generality, we assume that $0 < h < 1$. We denote by $P_r(K)$ the space of polynomials of degree r defined on the element K. For a given partition $\mathcal{T}_h$, we define the classical Lagrange finite element space

$$Y_h^r = \{u_h \in C(\Omega) :\ u_h|_K \in P_r(K),\ \forall\, K \in \mathcal{T}_h\}. \tag{22}$$

We have the following finite element subspaces of $H_0^1(\Omega)$, $\mathcal{H}_0^1(\Omega)$, and $\mathbf{H}_{\rm t}^1(\Omega)$

$$X_h = Y_h^1 \cap H_0^1(\Omega), \quad \mathcal{X}_h = X_h \oplus {\rm i}X_h, \quad \mathbf{X}_h = \big(Y_h^2\big)^3 \cap \mathbf{H}_{\rm t}^1(\Omega). \tag{23}$$

Let $\mathcal{I}_h$, I_h, and $\mathbf{I}_h$ be the commonly used Lagrange interpolation on $\mathcal{X}_h$, X_h, and $\mathbf{X}_h$, respectively. We have the following interpolation error estimates [3]:

$$\|\psi - \mathcal{I}_h\psi\|_{\mathcal{L}^2} + h\|\psi - \mathcal{I}_h\psi\|_{\mathcal{H}^1} \le Ch^2\|\psi\|_{\mathcal{H}^2},\ \forall\psi \in \mathcal{H}_0^1(\Omega) \cap \mathcal{H}^2(\Omega), \tag{24a}$$

$$\|u - I_h u\|_{L^2} + h\|u - I_h u\|_{H^1} \le Ch^2\|u\|_{H^2},\ \forall u \in H_0^1(\Omega) \cap H^2(\Omega), \tag{24b}$$

and for $s = 1, 2$,

$$\|\mathbf{v} - \mathbf{I}_h\mathbf{v}\|_{\mathbf{L}^2} + h\|\mathbf{v} - \mathbf{I}_h\mathbf{v}\|_{\mathbf{H}^1} \le Ch^{s+1}\|\mathbf{v}\|_{\mathbf{H}^{s+1}},\ \forall \mathbf{v} \in \mathbf{H}_{\rm t}^1(\Omega) \cap \mathbf{H}^{s+1}(\Omega). \tag{25}$$

We approximate the scalar potential ϕ and the wave function Ψ in X_h and $\mathcal{X}_h$ respectively, and find the approximate solution of the vector potential $\mathbf{A}$ in a subspace of $\mathbf{X}_h$:

$$\mathbf{X}_{0h} = \{\mathbf{v}_h \in \mathbf{X}_h \mid (\nabla \cdot \mathbf{v}_h,\, q_h) = 0,\ \forall q_h \in X_h\}. \tag{26}$$

Note that $\mathbf{X}_{0h}$ is the second-order finite element subspace of $\mathbf{H}_{\rm t}^1(\Omega)$. Besides, $\mathbf{X}_{0h} \not\subseteq \mathbf{H}_{t,0}^1(\Omega)$ since for each $\mathbf{v}_h \in \mathbf{X}_{0h}$, we only have $\rho_h(\nabla \cdot \mathbf{v}_h) = 0$, where ρ_h is the orthogonal projection of $L^2(\Omega)$ onto X_h.

We now claim that there exists an interpolation operator $\boldsymbol{i}_h : \mathbf{H}_{t,0}^1(\Omega) \to \mathbf{X}_{0h}$, such that for every $\mathbf{v} \in \mathbf{H}_{t,0}^1(\Omega) \cap \mathbf{H}^{s+1}(\Omega)$, $s = 1, 2$,

$$\|\mathbf{v} - \boldsymbol{i}_h\mathbf{v}\|_{\mathbf{H}^1} \le Ch^s\|\mathbf{v}\|_{\mathbf{H}^{s+1}}. \tag{27}$$

By the mixed finite element theory [2, 4, 12], we can ensure (27) by applying (25) and the following discrete inf-sup condition: there exists a positive constant β, independent of h, such that

$$\sup_{\mathbf{v}_h \in \mathbf{X}_h} \frac{\big(\nabla \cdot \mathbf{v}_h,\, q_h\big)}{\|\mathbf{v}_h\|_{\mathbf{H}^1}} \ge \beta\, \|q_h\|_{L^2}, \quad \forall\, q_h \in X_h. \tag{28}$$

For $\widetilde{\mathbf{X}}_h = \big(Y_h^2\big)^3 \cap \mathbf{H}_0^1(\Omega)$, $\widetilde{X}_h = Y_h^1$, the following discrete inf-sup condition for Hood-Taylor element is proved in [4] by Verfürth's trick:

$$\sup_{\mathbf{v}_h \in \widetilde{\mathbf{X}}_h} \frac{\big(\nabla \cdot \mathbf{v}_h,\, q_h\big)}{\|\mathbf{v}_h\|_{\mathbf{H}^1}} \ge \beta\, \|q_h\|_{L^2/R}, \quad \forall\, q_h \in \widetilde{X}_h. \tag{29}$$

The technique used in the proof of (29) can be applied directly to prove (28) by virtue of the fact that $\widetilde{\mathbf{X}}_h \subset \mathbf{X}_h$, $X_h \subset \widetilde{X}_h$ and the following continuous inf-sup condition:

$$\sup_{\mathbf{v} \in \mathbf{H}_{\rm t}^1(\Omega)} \frac{\big(\nabla \cdot \mathbf{v},\, q\big)}{\|\mathbf{v}\|_{\mathbf{H}^1}} \ge \beta\, \|q\|_{L^2}, \quad \forall\, q \in L^2(\Omega). \tag{30}$$

For more details, see [2, 4]. Thus (27) is verified.

Let $\boldsymbol{\pi}_h : \mathbf{H}_{\rm t}^1(\Omega) \to \mathbf{X}_{0h}$ be a Ritz projection as follows: $\forall\, \mathbf{A} \in \mathbf{H}_{\rm t}^1(\Omega)$, find $\boldsymbol{\pi}_h\mathbf{A} \in \mathbf{X}_{0h}$ such that

$$\big(\nabla \cdot (\mathbf{A} - \boldsymbol{\pi}_h\mathbf{A}),\, \nabla \cdot \mathbf{v}\big) + \big(\nabla \times (\mathbf{A} - \boldsymbol{\pi}_h\mathbf{A}),\, \nabla \times \mathbf{v}\big) = 0, \quad \forall\, \mathbf{v} \in \mathbf{X}_{0h}. \tag{31}$$

Owing to (27), we have the following error estimate of $\boldsymbol{\pi}_h$. For $s = 1, 2$,

$$\|\mathbf{v} - \boldsymbol{\pi}_h\mathbf{v}\|_{\mathbf{H}^1} \le Ch^s\|\mathbf{v}\|_{\mathbf{H}^{s+1}}, \quad \forall \mathbf{v} \in \mathbf{H}_{t,0}^1(\Omega) \cap \mathbf{H}^{s+1}(\Omega). \tag{32}$$

To define the fully discrete schemes, we divide the time interval $(0,T)$ into M uniform subintervals using the nodal points

$$0 = t^0 < t^1 < \cdots < t^M = T,$$

with $t^k = k\tau$ and $\tau = T/M$. We denote $u^k = u(\cdot, t^k)$ for any given functions $u \in C\big((0,T); W\big)$ with a Banach space W. For a given sequence $\{u^k\}_{k=0}^M$, we introduce the following notation:

$$\begin{aligned} &\partial_\tau u^k = (u^k - u^{k-1})/\tau, \quad \partial_\tau^2 u^k = (\partial_\tau u^k - \partial_\tau u^{k-1})/\tau, \\ &\overline{u}^k = (u^k + u^{k-1})/2, \quad \widetilde{u}^k = (u^k + u^{k-2})/2, \end{aligned} \tag{33}$$

For convenience, Let us assume that $\mathbf{A}^{-1}$ is defined by

$$\mathbf{A}^{-1} = \mathbf{A}(\cdot, 0) - \tau \frac{\partial \mathbf{A}}{\partial t}(\cdot, 0) = \mathbf{A}_0 - \tau \mathbf{A}_1, \tag{34}$$

which is an approximation of $\mathbf{A}(\cdot, -\tau)$ with second order accuracy.

Using the above notation, we can formulate our first fully discrete finite element scheme for the M-S-C system as follows.

Scheme I. For $k = 0, 1, \cdots, M$, find $(\Psi_h^k, \mathbf{A}_h^k, \phi_h^k) \in \mathcal{X}_h \times \mathbf{X}_{0h} \times X_h$ such that

$$\Psi_h^0 = \mathcal{I}_h \Psi_0, \quad \mathbf{A}_h^0 = \boldsymbol{\pi}_h \mathbf{A}_0, \quad \mathbf{A}_h^{-1} = \mathbf{A}_h^0 - \tau\, \boldsymbol{\pi}_h \mathbf{A}_1, \tag{35}$$

and for any $\varphi \in \mathcal{X}_h$, $\mathbf{v} \in \mathbf{X}_{0h}$, $u \in X_h$, the following equations hold:

$$\begin{cases} -\mathrm{i}(\partial_\tau \Psi_h^k, \varphi) + \dfrac{1}{2}\Big((\mathrm{i}\nabla + \overline{\mathbf{A}}_h^k)\overline{\Psi}_h^k, (\mathrm{i}\nabla + \overline{\mathbf{A}}_h^k)\varphi\Big) + \Big((V + \overline{\phi}_h^k)\overline{\Psi}_h^k, \varphi\Big) = 0, \\ (\partial_\tau^2 \mathbf{A}_h^k, \mathbf{v}) + \big(\nabla \times \widetilde{\mathbf{A}}_h^k, \nabla \times \mathbf{v}\big) + \big(\nabla \cdot \widetilde{\mathbf{A}}_h^k, \nabla \cdot \mathbf{v}\big) + \Big(|\Psi_h^{k-1}|^2 \dfrac{\overline{\mathbf{A}}_h^k + \overline{\mathbf{A}}_h^{k-1}}{2}, \mathbf{v}\Big) \\ \quad + \Big(\dfrac{\mathrm{i}}{2}\big((\Psi_h^{k-1})^* \nabla \Psi_h^{k-1} - \Psi_h^{k-1} \nabla (\Psi_h^{k-1})^*\big), \mathbf{v}\Big) = 0, \\ (\nabla \phi_h^k, \nabla u) = (|\Psi_h^k|^2, u). \end{cases} \tag{36}$$

Remark 3.1 In section 2 we see that the vector potential $\mathbf{A}$ in Definition 2.1 is divergence-free, and thus in the discrete level we approximate $\mathbf{A}$ and the associated test functions in $\mathbf{X}_{0h}$ to ensure a discrete divergence-free constraint on $\mathbf{A}$ and to tackle the mixed derivative term $\frac{\partial(\nabla\phi)}{\partial t}$ in the discrete system. Moreover, for the purpose of theoretical analysis and practical computations, we add an extra term $\big(\nabla \cdot \widetilde{\mathbf{A}}_h^k, \nabla \cdot \mathbf{v}\big)$ to the discrete system (36). It turns out that this term is indispensable to the proof of the error estimates and the existence of solutions to the discrete system (36).

Apart from introducing the subspace $\mathbf{X}_{0h}$ of $\mathbf{X}_h$, we can also introduce a Lagrangian multiplier p_h^k to relax the divergence-free constraint of $\mathbf{A}_h^k$ at each time step. We now give another fully discrete scheme based on the mixed finite element method as follows.

Scheme II. Let $\Psi_h^0 = \mathcal{I}_h \Psi_0, \quad \mathbf{A}_h^0 = \boldsymbol{\pi}_h \mathbf{A}_0, \quad \mathbf{A}_h^{-1} = \mathbf{A}_h^0 - \tau\, \boldsymbol{\pi}_h \mathbf{A}_1,$

and for $k = 1, 2, \cdots, M$, find $(\Psi_h^k,\, \mathbf{A}_h^k,\, p_h^k,\, \phi_h^k) \in \mathcal{X}_h \times \mathbf{X}_h \times X_h \times X_h$ satisfying

(37)
$$\begin{cases} -\mathrm{i}(\partial_\tau \Psi_h^k, \varphi) + \dfrac{1}{2}\Big((\mathrm{i}\nabla + \overline{\mathbf{A}}_h^k)\overline{\Psi}_h^k, (\mathrm{i}\nabla + \overline{\mathbf{A}}_h^k)\varphi\Big) + \Big((V + \overline{\phi}_h^k)\overline{\Psi}_h^k, \varphi\Big) = 0, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall \varphi \in \mathcal{X}_h, \\ (\partial_\tau^2 \mathbf{A}_h^k, \mathbf{v}) + \big(\nabla \times \widetilde{\mathbf{A}}_h^k, \nabla \times \mathbf{v}\big) + \big(\nabla \cdot \widetilde{\mathbf{A}}_h^k, \nabla \cdot \mathbf{v}\big) + \big(|\Psi_h^{k-1}|^2 \dfrac{\overline{\mathbf{A}}_h^k + \overline{\mathbf{A}}_h^{k-1}}{2},\, \mathbf{v}\big) \\ \quad + \big(p_h^k,\, \nabla \cdot \mathbf{v}\big) + \Big(\dfrac{\mathrm{i}}{2}\big((\Psi_h^{k-1})^* \nabla \Psi_h^{k-1} - \Psi_h^{k-1} \nabla (\Psi_h^{k-1})^*\big),\, \mathbf{v}\Big) = 0, \quad \forall \mathbf{v} \in \mathbf{X}_h, \\ \big(\nabla \cdot \mathbf{A}_h^k,\, q\big) = 0, \quad \forall\, q \in X_h, \\ (\nabla \phi_h^k,\, \nabla u) = (|\Psi_h^k|^2,\, u), \quad \forall\, u \in X_h. \end{cases}$$

At each time step, the equation

$$\begin{aligned} &(\partial_\tau^2 \mathbf{A}_h^k, \mathbf{v}) + \big(\nabla \times \widetilde{\mathbf{A}}_h^k, \nabla \times \mathbf{v}\big) + \big(\nabla \cdot \widetilde{\mathbf{A}}_h^k, \nabla \cdot \mathbf{v}\big) + \big(|\Psi_h^{k-1}|^2 \frac{\overline{\mathbf{A}}_h^k + \overline{\mathbf{A}}_h^{k-1}}{2},\, \mathbf{v}\big) \\ &\quad + \Big(\frac{\mathrm{i}}{2}\big((\Psi_h^{k-1})^* \nabla \Psi_h^{k-1} - \Psi_h^{k-1} \nabla (\Psi_h^{k-1})^*\big), \mathbf{v}\Big) = 0, \quad \forall \mathbf{v} \in \mathbf{X}_{0h} \end{aligned} \tag{38}$$

in scheme I and

(39)
$$\begin{cases} (\partial_\tau^2 \mathbf{A}_h^k, \mathbf{v}) + \big(\nabla \times \widetilde{\mathbf{A}}_h^k, \nabla \times \mathbf{v}\big) + \big(\nabla \cdot \widetilde{\mathbf{A}}_h^k, \nabla \cdot \mathbf{v}\big) + \big(|\Psi_h^{k-1}|^2 \dfrac{\overline{\mathbf{A}}_h^k + \overline{\mathbf{A}}_h^{k-1}}{2},\, \mathbf{v}\big) \\ \quad + \big(p_h^k,\, \nabla \cdot \mathbf{v}\big) + \Big(\dfrac{\mathrm{i}}{2}\big((\Psi_h^{k-1})^* \nabla \Psi_h^{k-1} - \Psi_h^{k-1} \nabla (\Psi_h^{k-1})^*\big),\, \mathbf{v}\Big) = 0, \quad \forall \mathbf{v} \in \mathbf{X}_h, \\ \big(\nabla \cdot \mathbf{A}_h^k,\, q\big) = 0, \quad \forall\, q \in X_h \end{cases}$$

in scheme II are decoupled from the other two equations, respectively. Due to the discrete inf-sup condition (28) and the coerciveness of the bilinear functional $a_h^k(\cdot,\, \cdot)$ in $\mathbf{X}_h$, where

$$\begin{aligned} a_h^k(\mathbf{u},\, \mathbf{v}) &= \big(\nabla \times \mathbf{u}, \nabla \times \mathbf{v}\big) + \big(\nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v}\big) + \frac{2}{\tau^2}(\mathbf{u}, \mathbf{v}) \\ &\quad + \frac{1}{2}\big(|\Psi_h^{k-1}|^2 \mathbf{u},\, \mathbf{v}\big), \qquad \forall\, \mathbf{u}, \mathbf{v} \in \mathbf{X}_h, \end{aligned} \tag{40}$$

we know that there exists a unique solution to (38) and (39), respectively. It is easy to see that $\mathbf{A}_h^k$ in (39) satisfies (38) and thus the two above equations admit the same solution $\mathbf{A}_h^k$. Consequently, scheme I and scheme II are mathematically equivalent. However, it is easier to carry out numerical computations with scheme II and more convenient to perform theoretical analysis with scheme I.

At each time step, we first solve (38) or (39) and obtain $\mathbf{A}_h^k$. Then we substitute it into (37) and solve the nonlinear subsystem concerning Ψ_h^k and ϕ_h^k. The existence and uniqueness of solutions to this subsystem is proved in section 5. In practical computations, we can apply the Picard simple iterative method or the Newton iterative method to solve the nonlinear subsystem.

For convenience, we define the following bilinear forms:

$$\begin{aligned} B(\mathbf{A}; \Psi, \varphi) &= \left((\mathrm{i}\nabla + \mathbf{A})\Psi, (\mathrm{i}\nabla + \mathbf{A})\varphi\right), \\ D(\mathbf{u},\, \mathbf{v}) &= (\nabla \cdot \mathbf{u},\, \nabla \cdot \mathbf{v}) + (\nabla \times \mathbf{u},\, \nabla \times \mathbf{v}), \\ f(\Psi, \varphi) &= \frac{\mathrm{i}}{2}(\varphi^* \nabla \Psi - \Psi \nabla \varphi^*). \end{aligned} \tag{41}$$

Then (36) in scheme I can be rewritten as follows: for $k = 1, 2, \cdots, M$,

(42)
$$\begin{cases} -\mathrm{i}(\partial_\tau \Psi_h^k, \varphi) + \dfrac{1}{2} B(\overline{\mathbf{A}}_h^k;\, \overline{\Psi}_h^k,\, \varphi) + (V\overline{\Psi}_h^k, \varphi) + (\overline{\phi}_h^k \overline{\Psi}_h^k, \varphi) = 0, \quad \forall \varphi \in \mathcal{X}_h, \\ (\partial_\tau^2 \mathbf{A}_h^k, \mathbf{v}) + D(\widetilde{\mathbf{A}}_h^k, \mathbf{v}) + \big(f(\Psi_h^{k-1}, \Psi_h^{k-1}), \mathbf{v}\big) + \big(|\Psi_h^{k-1}|^2 \dfrac{\overline{\mathbf{A}}_h^k + \overline{\mathbf{A}}_h^{k-1}}{2}, \mathbf{v}\big) = 0, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall \mathbf{v} \in \mathbf{X}_{0h}, \\ (\nabla \phi_h^k,\, \nabla u) = (|\Psi_h^k|^2,\, u), \quad \forall u \in X_h. \end{cases}$$

In this paper we assume that the M-S-C system (8)-(9) has one and only one weak solution $(\Psi, \mathbf{A}, \phi)$ defined in Definition 2.1 and the following regularity conditions are satisfied:

$$\begin{aligned} &\Psi, \Psi_t \in L^\infty(0,T;\mathcal{H}^2(\Omega)), \quad \Psi_{tt}, \Psi_{ttt} \in L^\infty(0,T;\mathcal{H}^1(\Omega)), \\ &\qquad \Psi_{tttt} \in L^2(0,T;\mathcal{L}^2(\Omega)), \\ &\mathbf{A}, \mathbf{A}_t \in L^\infty(0,T;\mathbf{H}^2(\Omega)), \quad \mathbf{A}_{tt} \in L^\infty(0,T;\mathbf{H}^1(\Omega)) \\ &\mathbf{A}_{ttt} \in L^2(0,T;\mathbf{H}^1(\Omega)), \quad \mathbf{A}_{tttt} \in L^2(0,T;\mathbf{L}^2(\Omega)), \\ &\phi, \phi_t \in L^\infty(0,T;H^2(\Omega)), \quad \phi_{tt} \in L^\infty(0,T;H^1(\Omega)), \\ &\phi_{ttt} \in L^\infty(0,T;L^2(\Omega)), \quad \phi_{tttt} \in L^2(0,T;L^2(\Omega)). \end{aligned} \tag{43}$$

For the initial conditions $(\Psi_0, \mathbf{A}_0, \mathbf{A}_1)$, we assume that

$$\Psi_0 \in \mathcal{H}^2(\Omega) \cap \mathcal{H}_0^1(\Omega), \quad \mathbf{A}_0, \mathbf{A}_1 \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_{t,0}^1(\Omega). \tag{44}$$

We now give the main convergence result in this paper as follows:

Theorem 3.1 Let $(\Psi, \mathbf{A}, \phi)$ be the unique solution to the M-S-C system (8)-(9), and let $(\Psi_h^k, \mathbf{A}_h^k, \phi_h^k)$ be the numerical solution to the discrete system (35)-(36). In addition, let the time step τ sufficiently small. Under the assumptions (43) and (44), we have the following error estimates

(45)
$$\max_{1 \le k \le M} \Big[\|\Psi_h^k - \Psi^k\|_{\mathcal{H}^1(\Omega)}^2 + \|\mathbf{A}_h^k - \mathbf{A}^k\|_{\mathbf{H}^1(\Omega)}^2 + \|\phi_h^k - \phi^k\|_{H^1(\Omega)}^2 \Big] \le C(h^2 + \tau^4),$$

where $\Psi^k = \Psi(\cdot, t^k)$, $\mathbf{A}^k = \mathbf{A}(\cdot, t^k)$, $\phi^k = \phi(\cdot, t^k)$, and C is a constant independent of h and τ.

4. Stability estimates

In this section we first show that the discrete system (35)-(36) maintains the conservation of the total charge and the total energy. Then we deduce some stability estimates of the discrete solution, which will be used to derive the error estimates in section 6.

First we define the energy of the discrete system (35)-(36) as follows:

$$\begin{aligned} \mathcal{E}_h^k = &\frac{1}{2} B(\overline{\mathbf{A}}_h^k;\, \Psi_h^k,\, \Psi_h^k) + (V\Psi_h^k,\, \Psi_h^k) + \frac{1}{2}\|\nabla \phi_h^k\|_{\mathbf{L}^2}^2 + \frac{1}{2}\|\partial_\tau \mathbf{A}_h^k\|_{\mathbf{L}^2}^2 \\ &+ \frac{1}{4} D(\mathbf{A}_h^k,\, \mathbf{A}_h^k) + \frac{1}{4} D(\mathbf{A}_h^{k-1},\, \mathbf{A}_h^{k-1}). \end{aligned} \tag{46}$$

Lemma 4.1 For $k = 1, 2 \cdots, M$, the solution $(\Psi_h^k, \mathbf{A}_h^k, \phi_h^k)$ of the discrete system (35)-(36) satisfies

$$\|\Psi_h^k\|_{\mathcal{L}^2}^2 = \|\Psi_h^0\|_{\mathcal{L}^2}^2, \quad \mathcal{E}_h^k = \mathcal{E}_h^0. \tag{47}$$

Proof. For $(47)_1$ we can simply choose $\varphi = \overline{\Psi}_h^k$ in $(42)_1$ and take its imaginary part.

To prove $(47)_2$, we first notice that

$$\begin{aligned}\mathrm{Re}\left[B\left(\overline{\mathbf{A}}_h^k;\overline{\Psi}_h^k,\partial_\tau\Psi_h^k\right)\right] &= \frac{1}{2}\partial_\tau B(\overline{\mathbf{A}}_h^k;\Psi_h^k,\Psi_h^k)\\ &+\frac{1}{2\tau}\left[B(\overline{\mathbf{A}}_h^{k-1};\Psi_h^{k-1},\Psi_h^{k-1})-B(\overline{\mathbf{A}}_h^k;\Psi_h^{k-1},\Psi_h^{k-1})\right]\\ &+\frac{1}{2\tau}\mathrm{Re}\left[B(\overline{\mathbf{A}}_h^k;\Psi_h^{k-1},\Psi_h^k)-B(\overline{\mathbf{A}}_h^k;\Psi_h^k,\Psi_h^{k-1})\right].\end{aligned}\tag{48}$$

We also have the following identities by direct calculations

$$\begin{aligned}&B(\mathbf{A};\psi,\varphi)=(\nabla\psi,\nabla\varphi)+(\mathbf{A}\psi,\mathbf{A}\varphi)+2(f(\psi,\varphi),\mathbf{A}),\\ &B(\mathbf{A};\psi,\varphi)-B(\tilde{\mathbf{A}};\psi,\varphi)=\left((\mathbf{A}+\tilde{\mathbf{A}})\psi\varphi^*,\mathbf{A}-\tilde{\mathbf{A}}\right)+2(f(\psi,\varphi),\mathbf{A}-\tilde{\mathbf{A}}),\end{aligned}\tag{49}$$

from which we deduce

$$\mathrm{Re}\left[B(\overline{\mathbf{A}}_h^k;\Psi_h^{k-1},\Psi_h^k)-B(\overline{\mathbf{A}}_h^k;\Psi_h^k,\Psi_h^{k-1})\right]=0.\tag{50}$$

Thus we get

$$\begin{aligned}&\mathrm{Re}\left[B\left(\overline{\mathbf{A}}_h^k;\overline{\Psi}_h^k,\partial_\tau\Psi_h^k\right)\right]=\frac{1}{2}\partial_\tau B(\overline{\mathbf{A}}_h^k;\Psi_h^k,\Psi_h^k)\\ &-\left(|\Psi_h^{k-1}|^2\frac{\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1}}{2},\frac{\overline{\mathbf{A}}_h^k-\overline{\mathbf{A}}_h^{k-1}}{\tau}\right)-\left(f(\Psi_h^{k-1},\Psi_h^{k-1}),\frac{\overline{\mathbf{A}}_h^k-\overline{\mathbf{A}}_h^{k-1}}{\tau}\right).\end{aligned}\tag{51}$$

Also we have

$$\mathrm{Re}\left[\left(V\overline{\Psi}_h^k,\partial_\tau\Psi_h^k\right)\right]=\frac{1}{2}\partial_\tau\left(V\Psi_h^k,\Psi_h^k\right),\quad \mathrm{Re}\left[\left(\overline{\phi}_h^k\overline{\Psi}_h^k,\partial_\tau\Psi_h^k\right)\right]=\frac{1}{2}\left(\overline{\phi}_h^k,\,\partial_\tau|\Psi_h^k|^2\right).\tag{52}$$

By choosing $\varphi=\partial_\tau\Psi_h^k$ in $(42)_1$, taking the real part of the equation and combining with (51) and (52), we get

$$\begin{aligned}&\frac{1}{2}\partial_\tau\|\left(\mathrm{i}\nabla+\overline{\mathbf{A}}_h^k\right)\Psi_h^k\|_{\mathbf{L}^2}^2+\partial_\tau\left(V\Psi_h^k,\Psi_h^k\right)+\left(\overline{\phi}_h^k,\,\partial_\tau|\Psi_h^k|^2\right)\\ &-\left(|\Psi_h^{k-1}|^2\frac{\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1}}{2},\frac{\overline{\mathbf{A}}_h^k-\overline{\mathbf{A}}_h^{k-1}}{\tau}\right)-\left(f(\Psi_h^{k-1},\Psi_h^{k-1}),\frac{\overline{\mathbf{A}}_h^k-\overline{\mathbf{A}}_h^{k-1}}{\tau}\right)=0.\end{aligned}\tag{53}$$

Next by taking $\mathbf{v}=\frac{1}{2\tau}(\mathbf{A}_h^k-\mathbf{A}_h^{k-2})$ and adding it to (53), we obtain

$$\begin{aligned}&\partial_\tau\left(\frac{1}{2}B(\overline{\mathbf{A}}_h^k;\Psi_h^k,\Psi_h^k)+\left(V\Psi_h^k,\Psi_h^k\right)+\frac{1}{2}\|\partial_\tau\mathbf{A}_h^k\|_{\mathbf{L}^2}^2\right)\\ &+\partial_\tau\left(\frac{1}{4}\|\nabla\times\mathbf{A}_h^k\|_{\mathbf{L}^2}^2+\frac{1}{4}\|\nabla\times\mathbf{A}_h^{k-1}\|_{\mathbf{L}^2}^2\right)+\left(\overline{\phi}_h^k,\,\partial_\tau|\Psi_h^k|^2\right)=0.\end{aligned}\tag{54}$$

Finally it is easy to deduce the following equation from the last equation of (42):

$$(\nabla\,\partial_\tau\phi_h^k,\,\nabla u)=(\partial_\tau|\Psi_h^k|^2,\,u),\quad \forall u\in X_h.\tag{55}$$

Take $u=\overline{\phi}_h^k$ in (55), insert it into (54) and we complete the proof of $(47)_2$. □

Theorem 4.1 For $k=1,2,\cdots,M$, the solution of the discrete system (41) fulfills the following estimate

$$\|\Psi_h^k\|_{\mathcal{H}^1}+\|\partial_\tau\mathbf{A}_h^k\|_{\mathbf{L}^2}+\|\mathbf{A}_h^k\|_{\mathbf{H}^1}+\|\phi_h^k\|_{H^1}\le C,\tag{56}$$

where C is independent of h and τ.

Proof. In view of Lemma 4.1 and the boundedness of $\mathcal{E}_h^0$, we have

$$B(\overline{\mathbf{A}}_h^k;\, \Psi_h^k,\, \Psi_h^k) + \|\partial_\tau \mathbf{A}_h^k\|_{\mathbf{L}^2} + D(\mathbf{A}_h^k,\, \mathbf{A}_h^k) + \|\nabla\phi_h^k\|_{\mathbf{L}^2} \le C. \tag{57}$$

Since the semi-norm in $\mathbf{H}_t^1(\Omega)$ is equivalent to $\mathbf{H}^1$-norm, we get

$$\|\mathbf{A}_h^k\|_{\mathbf{H}^1} \le C. \tag{58}$$

Then it follows from the Sobolev's embedding theorem that

$$\|\mathbf{A}_h^k\|_{\mathbf{L}^6} \le C. \tag{59}$$

Using Lemma 2.4, (57) and (59), we further prove

$$\|\Psi_h^k\|_{\mathcal{H}^1} \le C\big(B(\overline{\mathbf{A}}_h^k;\, \Psi_h^k,\, \Psi_h^k) + \|\Psi_h^k\|_{\mathcal{L}^2}\big) \le C. \tag{60}$$

By applying Poincaré's inequality and (57), we see that

$$\|\phi_h^k\|_{H^1} \le C. \tag{61}$$

Therefore, (56) is obtained by combining (58), (60), and (61). □

5. Solvability of the discrete system

In this section we prove the existence and uniqueness of the solutions to the discrete system (35)-(36).

Theorem 5.1 For any $\big(\Psi_h^{k-1}, \mathbf{A}_h^{k-2}, \mathbf{A}_h^{k-1}, \phi_h^{k-1}\big)$ satisfies (56), there exists a solution $\big(\Psi_h^k, \mathbf{A}_h^k, \phi_h^k\big)$ to the discrete system (36). Furthermore, if the time step τ is sufficiently small, the solution is unique.

Proof. As noted in section 3, to solve the discrete system (35)-(36), we need to solve (38) and the following subsystem alternately.

$$\begin{cases} -\mathrm{i}(\partial_\tau\Psi_h^k, \varphi) + \dfrac{1}{2}\Big((\mathrm{i}\nabla + \overline{\mathbf{A}}_h^k)\overline{\Psi}_h^k, (\mathrm{i}\nabla + \overline{\mathbf{A}}_h^k)\varphi\Big) + \Big((V + \overline{\phi}_h^k)\overline{\Psi}_h^k, \varphi\Big) = 0, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall\varphi \in \mathcal{X}_h, \\ (\nabla\phi_h^k,\, \nabla u) = (|\Psi_h^k|^2,\, u), \quad \forall u \in X_h, \end{cases} \tag{62}$$

Since we have proved the solvability of (38) in section 3, we only need to consider the solvability of (62), which can be rewritten as follows:

$$\begin{cases} (\overline{\Psi}_h^k,\, \varphi) = (\Psi_h^{k-1}, \varphi) - \mathrm{i}\dfrac{\tau}{4}B(\overline{\mathbf{A}}_h^k;\, \overline{\Psi}_h^k,\, \varphi) - \mathrm{i}\dfrac{\tau}{2}\Big((V + \overline{\phi}_h^k)\overline{\Psi}_h^k,\, \varphi\Big), \forall\varphi \in \mathcal{X}_h \\ (\nabla\overline{\phi}_h^k,\, \nabla u) = \big(\dfrac{1}{2}(|\Psi_h^{k-1}|^2 + |2\overline{\Psi}_h^k - \Psi_h^{k-1}|^2),\, u\big), \quad \forall u \in X_h. \end{cases} \tag{63}$$

For a given h, assume that $\{u_1, u_2, \cdots, u_N\}$ is a basis of X_h. Note that $\mathcal{X}_h = X_h \oplus \mathrm{i}X_h$. Then $\overline{\phi}_h^k$, $\overline{\Psi}_h^k$, and Ψ_h^{k-1} can be written as follows

$$\overline{\phi}_h^k = \sum_{j=1}^N a_j u_j, \quad \overline{\Psi}_h^k = \sum_{j=1}^N b_j u_j, \quad \Psi_h^{k-1} = \sum_{j=1}^N c_j u_j, \tag{64}$$

where

$$\vec{a} = (a_1, \cdots, a_N)^T \in \mathbb{R}^N,\ \vec{b} = (b_1, \cdots, b_N)^T \in \mathbb{C}^N,\ \vec{c} = (c_1, \cdots, c_N)^T \in \mathbb{C}^N. \tag{65}$$

Denote by

$$\begin{aligned} &W = \big(w_{ij}\big) \in \mathbb{R}^{N\times N}, \quad \vec{r} = (r_1, \cdots, r_N)^T \in \mathbb{R}^N, \\ &S = \big(s_{ij}\big) \in \mathbb{C}^{N\times N}, \quad Q = \big(q_{ij}\big) \in \mathbb{R}^{N\times N}, \end{aligned} \tag{66}$$

where

$$w_{ij} = (u_i, u_j),\ r_i = \frac{1}{2}\big(|\Psi_h^{k-1}|^2 + |2\overline{\Psi}_h^k - \Psi_h^{k-1}|^2,\, u_i\big), \tag{67}$$
$$s_{ij} = B(\overline{\mathbf{A}}_h^k;\, u_i,\, u_j), \quad q_{ij} = \big((V + \overline{\phi}_h^k)u_i,\, u_j\big) \quad i,j = 1,\cdots,N.$$

Using the above notation, we can write (63) in the form of matrix:

$$W\vec{b} = W\vec{c} - \mathrm{i}\frac{\tau}{4}S\vec{b} - \mathrm{i}\frac{\tau}{2}Q\vec{b}, \quad W\vec{a} = \vec{r}, \quad Q = Q(\vec{a}), \quad \vec{r} = \vec{r}(\vec{b}), \tag{68}$$

or a more compact form

$$\vec{b} = \vec{c} - \mathrm{i}\frac{\tau}{4}W^{-1}S\vec{b} - \mathrm{i}\frac{\tau}{2}W^{-1}Q(\vec{b})\vec{b}. \tag{69}$$

Now we define a finite dimensional space $\big(H, \langle\cdot,\cdot\rangle\big)$ and a mapping $g : H \longrightarrow H$ as following:

$$H = \mathbb{C}^N, \quad \langle\vec{e}_1, \vec{e}_2\rangle = (\vec{e}_2)^* W\vec{e}_1, \quad \forall\vec{e}_1,\ \vec{e}_2 \in H, \tag{70}$$
$$g(\vec{e}) = \vec{e} - \vec{c} + \mathrm{i}\frac{\tau}{4}W^{-1}S\vec{e} + \mathrm{i}\frac{\tau}{2}W^{-1}Q(\vec{e})\vec{e}, \quad \forall\vec{e} \in H,$$

where $(\vec{e}_2)^*$ denotes the conjugate transpose of $\vec{e}_2$ and W, S and Q are defined in (66)-(67). It is obvious that g is continuous. Moreover,

$$\mathrm{Re}\langle g(\vec{e}),\, \vec{e}\rangle = \|\vec{e}\|_H^2 - \mathrm{Re}\langle\vec{c},\, \vec{e}\rangle \geq \|\vec{e}\|_H\big(\|\vec{e}\|_H - \|\vec{c}\|_H\big), \quad \forall\,\vec{e} \in H, \tag{71}$$

which implies that

$$\mathrm{Re}\langle g(\vec{e}),\, \vec{e}\rangle > 0, \quad \text{if } \|\vec{e}\|_H = \|\vec{c}\|_H + 1. \tag{72}$$

Thus the existence of $\vec{b}$ and $\vec{a} = W^{-1}\vec{r}(\vec{b})$ for (69) follows from Lemma 2.5. Combining with the existence of $\mathbf{A}_h^k$, we obtain the existence of $\big(\Psi_h^k, \mathbf{A}_h^k, \phi_h^k\big)$ to the discrete system (36).

Now we study the uniqueness of the solutions to (62). Let (Ψ_h^k, ϕ_h^k) and $(\hat{\Psi}_h^k, \hat{\phi}_h^k)$ be two solutions of (62). Set $\eta = \Psi_h^k - \hat{\Psi}_h^k,\ \psi = \phi_h^k - \hat{\phi}_h^k$. They satisfy

$$\begin{cases} -\mathrm{i}(\eta,\varphi) + \dfrac{\tau}{4}B(\overline{\mathbf{A}}_h^k;\, \eta,\, \varphi) + \dfrac{\tau}{2}\big((V + \overline{\phi}_h^k)\eta,\, \varphi\big) + \dfrac{\tau}{4}\big((\hat{\Psi}_h^k + \Psi_h^{k-1})\psi,\, \varphi\big) = 0, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall\varphi \in \mathcal{X}_h, \\ (\nabla\psi,\, \nabla u) = ((\Psi_h^k)^*\eta + \eta^*\hat{\Psi}_h^k,\, u), \quad \forall u \in X_h, \end{cases} \tag{73}$$

By choosing $\varphi = \eta$ in the first equation of (73) and taking its imaginary part, we obtain

$$\|\eta\|_{\mathcal{L}^2} \leq C\tau\|\psi\|_{L^6}. \tag{74}$$

Take $u = \psi$ in the second equation of (73) and we get

$$\|\psi\|_{L^6} \leq C\|\nabla\psi\|_{\mathbf{L}^2} \leq C\|\eta\|_{\mathcal{L}^2}. \tag{75}$$

By substituting (75) into (74) and taking τ sufficiently small, we find $\eta = 0$ and consequently obtain the uniqueness of the solutions. □

6. The error estimates

We now turn to the proof of Theorem 3.1. Set $e_\Psi = \mathcal{I}_h\Psi - \Psi$, $e_{\mathbf{A}} = \boldsymbol{\pi}_h\mathbf{A} - \mathbf{A}$ and $e_\phi = I_h\phi - \phi$, where $\mathcal{I}_h$, $\boldsymbol{\pi}_h$ and I_h are defined in section 3. From the regularity assumption and the interpolation error estimates (24a), (24b) and (32), we deduce

$$\|e_\Psi\|_{\mathcal{H}^1} + \|e_{\mathbf{A}}\|_{\mathbf{H}^1} + \|e_\phi\|_{H^1} \le Ch. \tag{76}$$

By using standard finite element theory [3] and the regularity assumption (43), we also have

$$\|\mathcal{I}_h\Psi\|_{\mathcal{L}^\infty} + \|\nabla\mathcal{I}_h\Psi\|_{\mathbf{L}^3} + \|\boldsymbol{\pi}_h\mathbf{A}\|_{\mathbf{H}^1} \le C. \tag{77}$$

In the rest of this paper, we need the following discrete integration by parts formulas.

$$\begin{aligned} &\sum_{k=1}^{M}(a_k - a_{k-1})b_k = a_M b_M - a_0 b_1 - \sum_{k=1}^{M-1} a_k(b_{k+1} - b_k).\\ &\sum_{k=1}^{M}(a_k - a_{k-1})b_k = a_M b_M - a_0 b_0 - \sum_{k=1}^{M} a_{k-1}(b_k - b_{k-1}). \end{aligned} \tag{78}$$

To simplify the notation , we denote by $\theta_\Psi^k = \Psi_h^k - \mathcal{I}_h\Psi^k$, $\theta_{\mathbf{A}}^k = \mathbf{A}_h^k - \boldsymbol{\pi}_h\mathbf{A}^k$ and $\theta_\phi^k = \phi_h^k - I_h\phi^k$. In view of the interpolation error estimates (76), we only need to prove that for $k = 1, 2, \cdots, M$, there holds

$$\|\theta_\Psi^k\|_{\mathcal{H}^1} + \|\theta_{\mathbf{A}}^k\|_{\mathbf{H}^1} + \|\theta_\phi^k\|_{H^1} \le C(h + \tau^2). \tag{79}$$

By assuming that

$$\frac{\partial\Psi}{\partial t} \in L^2(0,T;\mathcal{L}^2(\Omega)), \quad \frac{\partial^2\mathbf{A}}{\partial t^2} \in L^2(0,T;\mathbf{L}^2(\Omega)), \tag{80}$$

the weak solution $(\Psi, \mathbf{A}, \phi)$ in Definition 2.1 satisfies

(81)

$$\begin{cases} -\mathrm{i}\big(\dfrac{\partial\Psi}{\partial t}, \varphi\big) + \dfrac{1}{2}B\big(\mathbf{A}; \Psi, \varphi\big) + \big(V\Psi, \varphi\big) + \big(\phi\Psi, \varphi\big) = 0, \quad \forall\varphi \in \mathcal{H}_0^1(\Omega),\\ \big(\dfrac{\partial^2\mathbf{A}}{\partial t^2}, \mathbf{v}\big) + \big(\nabla\times\mathbf{A}, \nabla\times\mathbf{v}\big) - \big(\dfrac{\partial\phi}{\partial t}, \nabla\cdot\mathbf{v}\big) + \big(f(\Psi,\Psi), \mathbf{v}\big) + \big(|\Psi|^2\mathbf{A}, \mathbf{v}\big) = 0,\\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall\mathbf{v} \in \mathbf{H}_{\mathrm{t}}^1(\Omega),\\ \big(\nabla\phi, \nabla u\big) = \big(|\Psi|^2, u\big), \quad \forall u \in H_0^1(\Omega). \end{cases}$$

Subtracting the discrete system (42) from (81) and noting that $\nabla\cdot\mathbf{A}^{k-1} = 0$, we have

$$\begin{aligned} &-2\mathrm{i}\big(\partial_\tau\theta_\Psi^k, \varphi\big) + B\big(\overline{\mathbf{A}}_h^k; \overline{\theta}_\Psi^k, \varphi\big) = 2\mathrm{i}\Big(\partial_\tau\mathcal{I}_h\Psi^k - (\Psi_t)^{k-\frac{1}{2}}, \varphi\Big)\\ &\quad +2\big(V(\Psi^{k-\frac{1}{2}} - \overline{\Psi}_h^k), \varphi\big) + B\big(\mathbf{A}^{k-\frac{1}{2}}; (\Psi^{k-\frac{1}{2}} - \mathcal{I}_h\overline{\Psi}^k), \varphi\big)\\ &\quad +2\big(\phi^{k-\frac{1}{2}}\Psi^{k-\frac{1}{2}} - \overline{\phi}_h^k\overline{\Psi}_h^k, \varphi\big) + \Big(B\big(\mathbf{A}^{k-\frac{1}{2}}; \mathcal{I}_h\overline{\Psi}^k, \varphi\big) - B\big(\overline{\mathbf{A}}_h^k; \mathcal{I}_h\overline{\Psi}^k, \varphi\big)\Big)\\ &:= \sum_{i=1}^{5} V_i^k(\varphi), \quad \forall\varphi \in \mathcal{X}_h, \end{aligned} \tag{82}$$

$$
\begin{aligned}
&\big(\partial_\tau^2\theta_{\mathbf{A}}^k,\,\mathbf{v}\big)+D\big(\widetilde{\theta}_{\mathbf{A}}^k,\,\mathbf{v}\big)=\Big((\mathbf{A}_{tt})^{k-1}-\partial_\tau^2\boldsymbol{\pi}_h\mathbf{A}^k,\,\mathbf{v}\Big)+D\big(\mathbf{A}^{k-1}-\widetilde{\boldsymbol{\pi}_h\mathbf{A}}^k,\,\mathbf{v}\big)\\
&\qquad-\Big((\phi_t)^{k-1},\,\nabla\cdot\mathbf{v}\Big)+\Big(|\Psi^{k-1}|^2\mathbf{A}^{k-1}-|\Psi_h^{k-1}|^2\frac{\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1}}{2},\,\mathbf{v}\Big)\\
&\qquad+\big(f(\Psi^{k-1},\Psi^{k-1})-f(\Psi_h^{k-1},\Psi_h^{k-1}),\,\mathbf{v}\big)\\
&\quad:=\sum_{i=1}^{5}U_i^k(\mathbf{v}),\quad\forall\mathbf{v}\in\mathbf{X}_{0h},
\end{aligned}\tag{83}
$$

$$
\big(\nabla\theta_\phi^k,\,\nabla u\big)=\big(\nabla(\phi^k-I_h\phi^k),\nabla u\big)+\big(|\Psi_h^k|^2-|\Psi^k|^2,\,u\big),\quad\forall u\in X_h.\tag{84}
$$

In the following of the section, we analyze the above three error equations term by term, respectively.

6.1. Estimates for (82). First, by taking $\varphi=\overline{\theta}_\Psi^k$ in (82), the imaginary part of the equation implies

$$
\frac{1}{\tau}\big(\|\theta_\Psi^k\|_{\mathcal{L}^2}^2-\|\theta_\Psi^{k-1}\|_{\mathcal{L}^2}^2\big)=-\mathrm{Im}\sum_{i=1}^{5}V_i^k(\overline{\theta}_\Psi^k)\le\sum_{i=1}^{5}|V_i^k(\overline{\theta}_\Psi^k)|.\tag{85}
$$

Now we are going to estimate the terms $V_i^k(\overline{\theta}_\Psi^k)$, $i=1,\cdots,5$ one by one. By the error estimates for the interpolation operator $\mathcal{I}_h$ and the regularity of Ψ in (43), we see that

$$
|V_1^k(\overline{\theta}_\Psi^k)|+|V_2^k(\overline{\theta}_\Psi^k)|\le C\big(\tau^4+h^2\big)+C\|\overline{\theta}_\Psi^k\|_{\mathcal{L}^2}^2.\tag{86}
$$

Thanks to

$$
\begin{aligned}
B(\mathbf{A};\psi,\varphi)&=(\nabla\psi,\nabla\varphi)+\big(|\mathbf{A}|^2\psi,\varphi\big)+\mathrm{i}\,(\varphi^*\nabla\psi-\psi\nabla\varphi^*,\mathbf{A})\\
&\le C\|\nabla\psi\|_{\mathbf{L}^2}\|\nabla\varphi\|_{\mathbf{L}^2},\quad\forall\mathbf{A}\in\mathbf{L}^6(\Omega),\ \ \psi,\varphi\in\mathcal{H}_0^1(\Omega),
\end{aligned}\tag{87}
$$

and

$$
V_3^k(\overline{\theta}_\Psi^k)=B(\mathbf{A}^{k-\frac12};(\overline{\Psi}^k-\mathcal{I}_h\overline{\Psi}^k),\overline{\theta}_\Psi^k)+B(\mathbf{A}^{k-\frac12};(\Psi^{k-\frac12}-\overline{\Psi}^k),\overline{\theta}_\Psi^k),\tag{88}
$$

we get

$$
|V_3^k(\overline{\theta}_\Psi^k)|\le C\big(h^2+\tau^4\big)+C\|\nabla\overline{\theta}_\Psi^k\|_{\mathbf{L}^2}^2.\tag{89}
$$

In order to estimate $V_4^k(\overline{\theta}_\Psi^k)$, we first decompose it as follows.

$$
\begin{aligned}
V_4^k(\overline{\theta}_\Psi^k)&=\Big((\Psi^{k-\frac12}-\mathcal{I}_h\Psi^{k-\frac12})\phi^{k-\frac12},\,\overline{\theta}_\Psi^k\Big)+\Big(\mathcal{I}_h(\Psi^{k-\frac12}-\overline{\Psi}^k)\phi^{k-\frac12},\,\overline{\theta}_\Psi^k\Big)\\
&\quad+\Big((\mathcal{I}_h\overline{\Psi}^k-\overline{\Psi}_h^k)\phi^{k-\frac12},\,\overline{\theta}_\Psi^k\Big)+\Big(\overline{\Psi}_h^k(\phi^{k-\frac12}-I_h\phi^{k-\frac12}),\,\overline{\theta}_\Psi^k\Big)\\
&\quad+\Big(\overline{\Psi}_h^kI_h(\phi^{k-\frac12}-\overline{\phi}^k),\,\overline{\theta}_\Psi^k\Big)+\Big(\overline{\Psi}_h^k(I_h\overline{\phi}^k-\overline{\phi}_h^k),\,\overline{\theta}_\Psi^k\Big)
\end{aligned}\tag{90}
$$

By using Theorem 4.1, the regularity assumption, and the properties of the interpolation operators, we obtain from (90) that

$$
|V_4^k(\overline{\theta}_\Psi^k)|\le C\big(h^2+\tau^4\big)+C\left(\|\nabla\overline{\theta}_\Psi^k\|_{\mathbf{L}^2}^2+\|\nabla\overline{\theta}_\phi^k\|_{\mathbf{L}^2}^2\right).\tag{91}
$$

Notice that

$$
\begin{aligned}
V_5^k(\overline{\theta}_\Psi^k)&=\Big[B(\overline{\mathbf{A}}_h^k;\mathcal{I}_h\overline{\Psi}^k,\overline{\theta}_\Psi^k)-B(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\overline{\theta}_\Psi^k)\Big]+\Big[B(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\overline{\theta}_\Psi^k)\\
&\quad-B(\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\overline{\theta}_\Psi^k)\Big]+\Big[B(\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\overline{\theta}_\Psi^k)-B(\mathbf{A}^{k-\frac12};\mathcal{I}_h\overline{\Psi}^k,\overline{\theta}_\Psi^k)\Big].
\end{aligned}\tag{92}
$$

By applying (49) and Theorem 4.1, it is easy to see that

$$|V_5^k(\overline{\theta}_{\Psi}^k)| \leq C\big(h^2+\tau^4\big) + C\left(D(\overline{\theta}_{\mathbf{A}}^k,\overline{\theta}_{\mathbf{A}}^k) + \|\nabla\overline{\theta}_{\Psi}^k\|_{\mathbf{L}^2}^2\right). \tag{93}$$

Now multiplying (85) by τ, summing over $k=1,2,\cdots,m$, and applying the above estimates , we have

$$\begin{aligned}\|\theta_{\Psi}^m\|_{\mathcal{L}^2}^2 &\leq C\big(h^2+\tau^4\big) + C\tau\sum_{k=1}^m\left(D(\overline{\theta}_{\mathbf{A}}^k,\overline{\theta}_{\mathbf{A}}^k) + \|\nabla\overline{\theta}_{\Psi}^k\|_{\mathbf{L}^2}^2 + \|\nabla\overline{\theta}_{\phi}^k\|_{\mathbf{L}^2}^2\right)\\ &\leq C\big(h^2+\tau^4\big) + C\tau\sum_{k=0}^m\left(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k) + \|\nabla\theta_{\Psi}^k\|_{\mathbf{L}^2}^2 + \|\nabla\theta_{\phi}^k\|_{\mathbf{L}^2}^2\right).\end{aligned} \tag{94}$$

Next, we take $\varphi = \partial_\tau\theta_{\Psi}^k$ in (82), which gives

$$-2\mathrm{i}(\partial_\tau\theta_{\Psi}^k,\partial_\tau\theta_{\Psi}^k) + B\Big(\overline{\mathbf{A}}_h^k;\,\overline{\theta}_{\Psi}^k,\partial_\tau\theta_{\Psi}^k\Big) = \sum_{j=1}^5 V_j^k(\partial_\tau\theta_{\Psi}^k). \tag{95}$$

From the real part of (95) and (49), we obtain

$$\begin{aligned}\frac{1}{2\tau}\left(B(\overline{\mathbf{A}}_h^k;\theta_{\Psi}^k,\theta_{\Psi}^k) - B(\overline{\mathbf{A}}_h^{k-1};\theta_{\Psi}^{k-1},\theta_{\Psi}^{k-1})\right) &= \sum_{j=1}^5 \mathrm{Re}\big[V_j^k(\partial_\tau\theta_{\Psi}^k)\big]\\ &+\Big(\frac{1}{2}(\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1})|\theta_{\Psi}^{k-1}|^2,\,\frac{1}{2}(\partial_\tau\mathbf{A}_h^k+\partial_\tau\mathbf{A}_h^{k-1})\Big)\\ &+\Big(f(\theta_{\Psi}^{k-1},\theta_{\Psi}^{k-1}),\,\frac{1}{2}(\partial_\tau\mathbf{A}_h^k+\partial_\tau\mathbf{A}_h^{k-1})\Big),\end{aligned} \tag{96}$$

which yields

$$\begin{aligned}\frac{1}{2}B(\overline{\mathbf{A}}_h^m;\theta_{\Psi}^m,\theta_{\Psi}^m) &= \frac{1}{2}B(\overline{\mathbf{A}}_h^0;\theta_{\Psi}^0,\theta_{\Psi}^0) + \tau\sum_{j=1}^5\sum_{k=1}^m \mathrm{Re}\big[V_j^k(\partial_\tau\theta_{\Psi}^k)\big]\\ &+\tau\sum_{k=1}^m\Big(\frac{1}{2}(\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1})|\theta_{\Psi}^{k-1}|^2,\,\partial_\tau\overline{\mathbf{A}}_h^k\Big) + \tau\sum_{k=1}^m\Big(f(\theta_{\Psi}^{k-1},\theta_{\Psi}^{k-1}),\,\partial_\tau\overline{\mathbf{A}}_h^k\Big).\end{aligned} \tag{97}$$

From Theorem 4.1, we deduce

$$\begin{aligned}\sum_{k=1}^m\Big(\frac{1}{2}(\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1})|\theta_{\Psi}^{k-1}|^2,\,\partial_\tau\overline{\mathbf{A}}_h^k\Big) &\leq \sum_{k=1}^m\|\overline{\mathbf{A}}_h^k+\overline{\mathbf{A}}_h^{k-1}\|_{\mathbf{L}^6}\|\theta_{\Psi}^{k-1}\|_{\mathcal{L}^6}^2\|\partial_\tau\overline{\mathbf{A}}_h^k\|_{\mathbf{L}^2}\\ &\leq C\sum_{k=1}^m\|\theta_{\Psi}^{k-1}\|_{\mathcal{L}^6}^2 \leq C\sum_{k=0}^m\|\nabla\theta_{\Psi}^k\|_{\mathbf{L}^2}^2,\\ \sum_{k=1}^m\Big(f(\theta_{\Psi}^{k-1},\theta_{\Psi}^{k-1}),\,\partial_\tau\overline{\boldsymbol{\pi}_h\mathbf{A}}^k\Big) &\leq \sum_{k=1}^m\|\nabla\theta_{\Psi}^{k-1}\|_{\mathbf{L}^2}\|\theta_{\Psi}^{k-1}\|_{\mathcal{L}^6}\|\partial_\tau\overline{\boldsymbol{\pi}_h\mathbf{A}}^k\|_{\mathbf{L}^3}\\ &\leq C\sum_{k=0}^m\|\nabla\theta_{\Psi}^k\|_{\mathbf{L}^2}^2.\end{aligned} \tag{98}$$

Denoting by

$$J_1^k = \Big(f(\theta_{\Psi}^{k-1},\theta_{\Psi}^{k-1}),\,\overline{\partial_\tau\theta_{\mathbf{A}}}^k\Big), \tag{99}$$

we have

$$\frac{1}{2}B(\overline{\mathbf{A}}_h^m;\theta_\Psi^m,\theta_\Psi^m)\le Ch^2+C\tau\sum_{k=0}^m\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}+\tau\sum_{k=1}^m J_1^k+\tau\sum_{j=1}^5\sum_{k=1}^m\mathrm{Re}\big[V_j^k(\partial_\tau\theta_\Psi^k)\big].\tag{100}$$

Now let us estimate $\sum_{k=1}^m\mathrm{Re}\big[V_j^k(\partial_\tau\theta_\Psi^k)\big]$, $j=1,\cdots,5$ term by term. In light of (78), we get

$$\begin{aligned}\tau\sum_{k=1}^m V_1^k(\partial_\tau\theta_\Psi^k)&=2\mathrm{i}\sum_{k=1}^m\Big(\partial_\tau\mathcal{I}_h\Psi^k-(\Psi_t)^{k-\frac{1}{2}},\ \theta_\Psi^k-\theta_\Psi^{k-1}\Big)\\&=2\mathrm{i}\Big(\partial_\tau\mathcal{I}_h\Psi^m-(\Psi_t)^{m-\frac{1}{2}},\ \theta_\Psi^m\Big)-2\mathrm{i}\Big(\partial_\tau\mathcal{I}_h\Psi^1-(\Psi_t)^{\frac{1}{2}},\ \theta_\Psi^0\Big)\\&\quad-2\mathrm{i}\sum_{k=1}^{m-1}\Big(\partial_\tau\mathcal{I}_h\Psi^{k+1}-\partial_\tau\mathcal{I}_h\Psi^k-(\Psi_t)^{k+\frac{1}{2}}+(\Psi_t)^{k-\frac{1}{2}},\ \theta_\Psi^k\Big).\end{aligned}\tag{101}$$

By employing the regularity assumption and the error estimates of interpolation operators, we see that

$$|\tau\sum_{k=1}^m V_1^k(\partial_\tau\theta_\Psi^k)|\le C\big(h^2+\tau^4\big)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+C\tau\sum_{k=1}^{m-1}\|\theta_\Psi^k\|_{\mathcal{L}^2}^2.\tag{102}$$

The second term can be rewritten as

$$\begin{aligned}\tau V_2^k(\partial_\tau\theta_\Psi^k)&=2\Big(V(\Psi^{k-\frac{1}{2}}-\overline{\Psi}_h^k),\ \theta_\Psi^k-\theta_\Psi^{k-1}\Big)\\&=2\Big(V(\Psi^{k-\frac{1}{2}}-\mathcal{I}_h\overline{\Psi}^k),\ \theta_\Psi^k-\theta_\Psi^{k-1}\Big)-2\Big(V(\frac{1}{2}(\theta_\Psi^k+\theta_\Psi^{k-1}),\ \theta_\Psi^k-\theta_\Psi^{k-1}\Big).\end{aligned}$$

Arguing as before, we obtain

$$\Big|\tau\sum_{k=1}^m\mathrm{Re}\big[V_2^k(\partial_\tau\theta_\Psi^k)\big]\Big|\le C\big(h^2+\tau^4\big)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+C\tau\sum_{k=1}^{m-1}\|\theta_\Psi^k\|_{\mathcal{L}^2}^2.\tag{103}$$

By the definition of the bilinear functional $B(\mathbf{A};\psi,\varphi)$ in (41), we can rewrite $\tau V_3^k(\partial_\tau\theta_\Psi^k)$ as follows:

$$\begin{aligned}\tau V_3^k(\partial_\tau\theta_\Psi^k)&=\Big(\nabla(\Psi^{k-\frac{1}{2}}-\mathcal{I}_h\overline{\Psi}^k),\ \nabla(\theta_\Psi^k-\theta_\Psi^{k-1})\Big)\\&\quad+\Big(|\mathbf{A}^{k-\frac{1}{2}}|^2(\Psi^{k-\frac{1}{2}}-\mathcal{I}_h\overline{\Psi}^k),\ \theta_\Psi^k-\theta_\Psi^{k-1}\Big)\\&\quad+\mathrm{i}\Big(\nabla(\Psi^{k-\frac{1}{2}}-\mathcal{I}_h\overline{\Psi}^k)\mathbf{A}^{k-\frac{1}{2}},\ \theta_\Psi^k-\theta_\Psi^{k-1}\Big)\\&\quad-\mathrm{i}\Big((\Psi^{k-\frac{1}{2}}-\mathcal{I}_h\overline{\Psi}^k)\mathbf{A}^{k-\frac{1}{2}},\ \nabla\theta_\Psi^k-\nabla\theta_\Psi^{k-1}\Big).\end{aligned}\tag{104}$$

By employing (78), (24a), the regularity assumption (43), and the Young's inequality, we can prove the following estimate

$$|\tau\sum_{k=1}^m V_3^k(\partial_\tau\theta_\Psi^k)|\le C\big(h^2+\tau^4\big)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+\frac{1}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2+C\tau\sum_{k=0}^m\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\tag{105}$$

by some standard but tedious arguments which are analogous to the estimate of $\sum_{k=1}^m V_1^k(\partial_\tau\theta_\Psi^k)$. Due to space limitations, we omit the proof here.

To estimate the term $\tau V_4^k(\partial_\tau \theta_\Psi^k)$, we rewrite it by

$$\begin{aligned}\tau V_4^k(\partial_\tau \theta_\Psi^k) &= 2\left(\phi^{k-\frac{1}{2}}\Psi^{k-\frac{1}{2}} - I_h\overline{\phi}^k \mathcal{I}_h \overline{\Psi}^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\right) - 2\left(I_h\overline{\phi}^k \overline{\theta}_\Psi^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\right)\\ &\quad -2\left(\mathcal{I}_h\overline{\Psi}^k\overline{\theta}_\phi^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\right) - 2\left(\overline{\theta}_\phi^k\overline{\theta}_\Psi^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\right).\end{aligned} \tag{106}$$

Arguing as before, we can obtain

$$\begin{aligned}&\Big|\sum_{k=1}^m \big(\phi^{k-\frac{1}{2}}\Psi^{k-\frac{1}{2}} - I_h\overline{\phi}^k\mathcal{I}_h\overline{\Psi}^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\big)\Big| \le C(h^2+\tau^4)\\ &\qquad + C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 + C\tau\sum_{k=0}^m \|\theta_\Psi^k\|_{\mathcal{L}^2}^2,\\ &\Big|\mathrm{Re}\sum_{k=1}^m \big(I_h\overline{\phi}^k\overline{\theta}_\Psi^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\big)\Big| \le C(h^2+\tau^4) + C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 + \frac{1}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2\\ &\qquad + C\tau\sum_{k=0}^m \|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2.\end{aligned} \tag{107}$$

The real part of the last two terms on the right hand side of (106) can be decomposed as follows:

$$\begin{aligned}&\mathrm{Re}\big[\big(\mathcal{I}_h\overline{\Psi}^k\overline{\theta}_\phi^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\big) + \big(\overline{\theta}_\phi^k\overline{\theta}_\Psi^k,\ \theta_\Psi^k - \theta_\Psi^{k-1}\big)\big]\\ &= \mathrm{Re}\big[\big(\mathcal{I}_h\overline{\Psi}^k(\theta_\Psi^k - \theta_\Psi^{k-1})^*,\ \overline{\theta}_\phi^k\big)\big] + \frac{1}{2}\big(|\theta_\Psi^k|^2 - |\theta_\Psi^{k-1}|^2,\ \overline{\theta}_\phi^k\big)\\ &= \mathrm{Re}\big[\big(\mathcal{I}_h\Psi^k(\theta_\Psi^k)^* - \mathcal{I}_h\Psi^{k-1}(\theta_\Psi^{k-1})^*,\ \overline{\theta}_\phi^k\big)\big] + \frac{1}{2}\big(|\theta_\Psi^k|^2 - |\theta_\Psi^{k-1}|^2,\ \overline{\theta}_\phi^k\big)\\ &\quad -\mathrm{Re}\big[\big(\overline{\theta}_\phi^k(\mathcal{I}_h\Psi^k - \mathcal{I}_h\Psi^{k-1}),\ \overline{\theta}_\Psi^k\big)\big]\\ &= \frac{1}{2}\big(|\Psi_h^k|^2 - |\mathcal{I}_h\Psi^k|^2,\ \overline{\theta}_\phi^k\big) - \frac{1}{2}\big(|\Psi_h^{k-1}|^2 - |\mathcal{I}_h\Psi^{k-1}|^2,\ \overline{\theta}_\phi^k\big)\\ &\quad -\mathrm{Re}\big[\big(\overline{\theta}_\phi^k(\mathcal{I}_h\Psi^k - \mathcal{I}_h\Psi^{k-1}),\ \overline{\theta}_\Psi^k\big)\big].\end{aligned} \tag{108}$$

Combining (106)-(108) and setting

$$J_2^k = \big(|\Psi_h^k|^2 - |\mathcal{I}_h\Psi^k|^2,\ \overline{\theta}_\phi^k\big) - \big(|\Psi_h^{k-1}|^2 - |\mathcal{I}_h\Psi^{k-1}|^2,\ \overline{\theta}_\phi^k\big), \tag{109}$$

we obtain

$$\begin{aligned}\tau\sum_{k=1}^m \mathrm{Re}\big[V_4^k(\partial_\tau\theta_\Psi^k)\big] &\le C\big(h^2+\tau^4\big) + C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 + \frac{1}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2\\ &\quad + C\tau\sum_{k=0}^m\big(\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2 + \|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2\big) - \sum_{k=1}^m J_2^k.\end{aligned} \tag{110}$$

We now focus on the analysis of $\tau V_5^k(\partial_\tau\theta_\Psi^k)$, which can be rewritten as

$$\begin{aligned}\tau V_5^k(\partial_\tau\theta_\Psi^k) &= \Big[B(\mathbf{A}^{k-\frac{1}{2}};\mathcal{I}_h\overline{\Psi}^k,\theta_\Psi^k - \theta_\Psi^{k-1}) - B(\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\theta_\Psi^k - \theta_\Psi^{k-1})\Big]\\ &\quad + \Big[B(\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\theta_\Psi^k - \theta_\Psi^{k-1}) - B(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\theta_\Psi^k - \theta_\Psi^{k-1})\Big]\\ &\quad + \Big[B(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k;\mathcal{I}_h\overline{\Psi}^k,\theta_\Psi^k - \theta_\Psi^{k-1}) - B(\overline{\mathbf{A}}_h^k;\mathcal{I}_h\overline{\Psi}^k,\theta_\Psi^k - \theta_\Psi^{k-1})\Big]\\ &:= V_5^{k,1} + V_5^{k,2} + V_5^{k,3}.\end{aligned} \tag{111}$$

By applying (49) and (78) and arguing as before, we deduce

$$
\begin{aligned}
&|\sum_{k=1}^{m} V_5^{k,1}| + |\sum_{k=1}^{m} V_5^{k,2}| \leq C\big(h^2+\tau^4\big) + C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 \\
&\quad + \frac{1}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2 + C\tau\sum_{k=1}^{m}\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2.
\end{aligned}
\tag{112}
$$

In order to estimate $|\sum\limits_{k=1}^{m} V_5^{k,3}|$, we rewrite it as follows.

$$
\begin{aligned}
\sum_{k=1}^{m} V_5^{k,3} &= \sum_{k=1}^{m}\Big(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k + \overline{\mathbf{A}}_h^k)(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k - \overline{\mathbf{A}}_h^k),\ \theta_\Psi^k - \theta_\Psi^{k-1}\Big) \\
&\quad - \sum_{k=1}^{m}\mathrm{i}\Big(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k - \overline{\mathbf{A}}_h^k),\ \nabla\theta_\Psi^k - \nabla\theta_\Psi^{k-1}\Big) \\
&\quad + \sum_{k=1}^{m}\mathrm{i}\Big(\nabla\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k - \overline{\mathbf{A}}_h^k),\ \theta_\Psi^k - \theta_\Psi^{k-1}\Big) \\
&:= T_1 + T_2 + T_3.
\end{aligned}
\tag{113}
$$

We decompose the term T_1 as follows.

$$
\begin{aligned}
T_1 &= \sum_{k=1}^{m}\Big(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k + \overline{\mathbf{A}}_h^k)(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k - \overline{\mathbf{A}}_h^k),\ \theta_\Psi^k - \theta_\Psi^{k-1}\Big) \\
&= -\Big(\mathcal{I}_h\overline{\Psi}^m(\boldsymbol{\pi}_h\overline{\mathbf{A}}^m + \overline{\mathbf{A}}_h^m)\overline{\theta}_{\mathbf{A}}^m,\ \theta_\Psi^m\Big) + \Big(\mathcal{I}_h\overline{\Psi}^0(\boldsymbol{\pi}_h\overline{\mathbf{A}}^0 + \overline{\mathbf{A}}_h^0)\overline{\theta}_{\mathbf{A}}^0,\ \theta_\Psi^0\Big) \\
&\quad + \sum_{k=1}^{m}\Big(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k + \overline{\mathbf{A}}_h^k)\overline{\theta}_{\mathbf{A}}^k - \mathcal{I}_h\overline{\Psi}^{k-1}(\boldsymbol{\pi}_h\overline{\mathbf{A}}^{k-1} + \overline{\mathbf{A}}_h^{k-1})\overline{\theta}_{\mathbf{A}}^{k-1},\ \theta_\Psi^{k-1}\Big).
\end{aligned}
\tag{114}
$$

By applying the Young's inequality and Theorem 4.1, we can estimate the first two terms on the right side of (114) by

$$
\begin{aligned}
&|\Big(\mathcal{I}_h\overline{\Psi}^m(\boldsymbol{\pi}_h\overline{\mathbf{A}}^m + \overline{\mathbf{A}}_h^m)\overline{\theta}_{\mathbf{A}}^m,\ \theta_\Psi^m\Big)| + |\Big(\mathcal{I}_h\overline{\Psi}^0(\boldsymbol{\pi}_h\overline{\mathbf{A}}^0 + \overline{\mathbf{A}}_h^0)\overline{\theta}_{\mathbf{A}}^0,\ \theta_\Psi^0\Big)| \\
&\leq \frac{1}{16}D(\overline{\theta}_{\mathbf{A}}^m, \overline{\theta}_{\mathbf{A}}^m) + C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 + Ch^2.
\end{aligned}
\tag{115}
$$

Since

$$
\begin{aligned}
&\Big(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k + \overline{\mathbf{A}}_h^k)\overline{\theta}_{\mathbf{A}}^k - \mathcal{I}_h\overline{\Psi}^{k-1}(\boldsymbol{\pi}_h\overline{\mathbf{A}}^{k-1} + \overline{\mathbf{A}}_h^{k-1})\overline{\theta}_{\mathbf{A}}^{k-1},\ \theta_\Psi^{k-1}\Big) \\
&= \tau\left(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k + \overline{\mathbf{A}}_h^k)\frac{\overline{\theta}_{\mathbf{A}}^k - \overline{\theta}_{\mathbf{A}}^{k-1}}{\tau},\ \theta_\Psi^{k-1}\right) \\
&\quad + \tau\left(\frac{\mathcal{I}_h\overline{\Psi}^k - \mathcal{I}_h\overline{\Psi}^{k-1}}{\tau}(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k + \overline{\mathbf{A}}_h^k)\overline{\theta}_{\mathbf{A}}^{k-1},\ \theta_\Psi^{k-1}\right) \\
&\quad + \tau\left(\mathcal{I}_h\overline{\Psi}^{k-1}\overline{\theta}_{\mathbf{A}}^{k-1}\Big(\frac{\boldsymbol{\pi}_h\overline{\mathbf{A}}^k - \boldsymbol{\pi}_h\overline{\mathbf{A}}^{k-1}}{\tau} + \frac{\overline{\mathbf{A}}_h^k - \overline{\mathbf{A}}_h^{k-1}}{\tau}\Big),\ \theta_\Psi^{k-1}\right),
\end{aligned}
\tag{116}
$$

we deduce

$$
\begin{aligned}
&|\left(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k+\overline{\mathbf{A}}_h^k)\overline{\theta}_{\mathbf{A}}^k-\mathcal{I}_h\overline{\Psi}^{k-1}(\boldsymbol{\pi}_h\overline{\mathbf{A}}^{k-1}+\overline{\mathbf{A}}_h^{k-1})\overline{\theta}_{\mathbf{A}}^{k-1},\ \theta_\Psi^{k-1}\right)|\\
&\le\tau\|\mathcal{I}_h\overline{\Psi}^k\|_{\mathcal{L}^6}\|\boldsymbol{\pi}_h\overline{\mathbf{A}}^k+\overline{\mathbf{A}}_h^k\|_{\mathbf{L}^6}\|\partial_\tau\overline{\theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}\|\theta_\Psi^{k-1}\|_{\mathcal{L}^6}\\
&\quad+\tau\|\partial_\tau\mathcal{I}_h\overline{\Psi}^k\|_{\mathcal{L}^2}\|\boldsymbol{\pi}_h\overline{\mathbf{A}}^k+\overline{\mathbf{A}}_h^k\|_{\mathbf{L}^6}\|\overline{\theta}_{\mathbf{A}}^{k-1}\|_{\mathbf{L}^6}\|\theta_\Psi^{k-1}\|_{\mathcal{L}^6}\\
&\quad+\tau\|\mathcal{I}_h\overline{\Psi}^{k-1}\|_{\mathcal{L}^6}\|\overline{\theta}_{\mathbf{A}}^{k-1}\|_{\mathbf{L}^6}\|\partial_\tau\boldsymbol{\pi}_h\overline{\mathbf{A}}^k+\partial_\tau\overline{\mathbf{A}}_h^k\|_{\mathbf{L}^2}\|\theta_\Psi^{k-1}\|_{\mathcal{L}^6}\\
&\le C\tau\left(\|\partial_\tau\overline{\theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}+\|\overline{\theta}_{\mathbf{A}}^{k-1}\|_{\mathbf{H}^1}\right)\|\theta_\Psi^{k-1}\|_{\mathcal{H}^1}\\
&\le C\tau\left(\|\partial_\tau\overline{\theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+D(\overline{\theta}_{\mathbf{A}}^{k-1},\overline{\theta}_{\mathbf{A}}^{k-1})+\|\nabla\theta_\Psi^{k-1}\|_{\mathbf{L}^2}^2\right)
\end{aligned}
\tag{117}
$$

by applying Theorem 4.1.

Hence we get the estimate of T_1 as follows.

$$
\begin{aligned}
|T_1|\le&\frac{1}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+Ch^2\\
&+C\tau\sum_{k=0}^m\left(\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\right).
\end{aligned}
\tag{118}
$$

By virtue of (78) and integrating by parts, we discover

$$
\begin{aligned}
\mathrm{i}T_2=&\sum_{k=1}^m\left(\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k-\overline{\mathbf{A}}_h^k),\ \nabla\theta_\Psi^k-\nabla\theta_\Psi^{k-1}\right)\\
=&\left(\nabla\mathcal{I}_h\overline{\Psi}^m\overline{\theta}_{\mathbf{A}}^m,\ \theta_\Psi^m\right)+\left(\mathcal{I}_h\overline{\Psi}^m\nabla\cdot\overline{\theta}_{\mathbf{A}}^m,\ \theta_\Psi^m\right)+\left(\mathcal{I}_h\overline{\Psi}^0\overline{\theta}_{\mathbf{A}}^0,\ \nabla\theta_\Psi^0\right)\\
&+\sum_{k=1}^m\left(\mathcal{I}_h\overline{\Psi}^k\overline{\theta}_{\mathbf{A}}^k-\mathcal{I}_h\overline{\Psi}^{k-1}\overline{\theta}_{\mathbf{A}}^{k-1},\ \nabla\theta_\Psi^{k-1}\right),
\end{aligned}
\tag{119}
$$

By using Young's inequality and (77), we can estimate the first three terms on the right side of (119) as follows:

$$
\begin{aligned}
&|\left(\nabla\mathcal{I}_h\overline{\Psi}^m\overline{\theta}_{\mathbf{A}}^m,\ \theta_\Psi^m\right)|+|\left(\mathcal{I}_h\overline{\Psi}^m\nabla\cdot\overline{\theta}_{\mathbf{A}}^m,\ \theta_\Psi^m\right)|+|\left(\mathcal{I}_h\overline{\Psi}^0\overline{\theta}_{\mathbf{A}}^0,\ \nabla\theta_\Psi^0\right)|\\
&\le\|\nabla\mathcal{I}_h\overline{\Psi}^m\|_{\mathbf{L}^3}\|\overline{\theta}_{\mathbf{A}}^m\|_{\mathbf{L}^6}\|\theta_\Psi^m\|_{\mathcal{L}^2}+\|\mathcal{I}_h\overline{\Psi}^m\|_{\mathcal{L}^\infty}\|\nabla\cdot\overline{\theta}_{\mathbf{A}}^m\|_{L^2}\|\theta_\Psi^m\|_{\mathcal{L}^2}+Ch^2\\
&\le C\|\overline{\theta}_{\mathbf{A}}^m\|_{\mathbf{H}^1}\|\theta_\Psi^m\|_{\mathcal{L}^2}+Ch^2\le\frac{1}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+Ch^2.
\end{aligned}
\tag{120}
$$

The last term at the right side of (119) satisfies the following estimate.

$$
\begin{aligned}
&|\sum_{k=1}^m\left(\mathcal{I}_h\overline{\Psi}^k\overline{\theta}_{\mathbf{A}}^k-\mathcal{I}_h\overline{\Psi}^{k-1}\overline{\theta}_{\mathbf{A}}^{k-1},\ \nabla\theta_\Psi^{k-1}\right)|\\
&\le\tau\sum_{k=1}^m\left(\|\partial_\tau\mathcal{I}_h\overline{\Psi}^k\|_{\mathcal{L}^3}\|\overline{\theta}_{\mathbf{A}}^k\|_{\mathbf{L}^6}\|\nabla\theta_\Psi^{k-1}\|_{\mathbf{L}^2}+\|\mathcal{I}_h\overline{\Psi}^{k-1}\|_{\mathcal{L}^\infty}\|\partial_\tau\overline{\theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}\|\nabla\theta_\Psi^{k-1}\|_{\mathbf{L}^2}\right)\\
&\le C\tau\sum_{k=0}^m\left(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\right).
\end{aligned}
\tag{121}
$$

Hence we get

$$
\begin{aligned}
|T_2|\le&\frac{1}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+Ch^2\\
&+C\tau\sum_{k=0}^m\left(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\right).
\end{aligned}
\tag{122}
$$

Reasoning as before, we can estimate T_3 as follows.

$$
\begin{aligned}
|T_3| &= \big|\mathrm{i}\sum_{k=1}^{m}\big(\nabla\mathcal{I}_h\overline{\Psi}^k(\boldsymbol{\pi}_h\overline{\mathbf{A}}^k-\overline{\mathbf{A}}_h^k),\ \theta_\Psi^k-\theta_\Psi^{k-1}\big)\big| \\
&\le \frac{1}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+Ch^2 \\
&\quad +C\tau\sum_{k=0}^{m}\big(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\big)\,.
\end{aligned}\tag{123}
$$

Combining (118), (122), and (123) implies

$$
\begin{aligned}
|\sum_{k=1}^{m}V_5^{k,3}| &\le \frac{3}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+Ch^2 \\
&\quad +C\tau\sum_{k=0}^{m}\big(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\big)\,,
\end{aligned}\tag{124}
$$

and thus

$$
\begin{aligned}
|\tau\sum_{k=1}^{m}V_5^k(\partial_\tau\theta_\Psi^k)| &\le |\sum_{k=1}^{m}V_5^{k,1}|+|\sum_{k=1}^{m}V_5^{k,2}|+|\sum_{k=1}^{m}V_5^{k,3}| \\
&\le C\big(h^2+\tau^4\big)+\frac{3}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+\frac{1}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 \\
&\quad +C\tau\sum_{k=0}^{m}\big(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\big)\,.
\end{aligned}\tag{125}
$$

Now substituting (102), (103), (105), (110), and (125) into (100), we have

$$
\begin{aligned}
&\frac{1}{2}B(\overline{\mathbf{A}}_h^m;\theta_\Psi^m,\theta_\Psi^m)+\sum_{k=1}^{m}J_2^k\ \le C\big(h^2+\tau^4\big)+\frac{3}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2+\frac{3}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m) \\
&+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2+\tau\sum_{k=1}^{m}J_1^k+C\tau\sum_{k=0}^{m}\big(\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2+D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\big)\,.
\end{aligned}\tag{126}
$$

Applying Lemma 2.4, we have

$$
\frac{9}{32}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2\le B(\overline{\mathbf{A}}_h^m;\theta_\Psi^m,\theta_\Psi^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2.\tag{127}
$$

Consequently, by inserting (127) into (126), we find

$$
\begin{aligned}
&\frac{3}{64}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2+\sum_{k=1}^{m}J_2^k\ \le C\big(h^2+\tau^4\big)+\frac{3}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+C\|\theta_\Psi^m\|_{\mathcal{L}^2}^2 \\
&+\tau\sum_{k=1}^{m}J_1^k+C\tau\sum_{k=0}^{m}\big(\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2+D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\big)\,.
\end{aligned}\tag{128}
$$

By substituting (94) into (128), we end up with

$$
\begin{aligned}
&\frac{3}{64}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2+\sum_{k=1}^{m}J_2^k\ \le C\big(h^2+\tau^4\big)+\frac{3}{16}D(\overline{\theta}_{\mathbf{A}}^m,\overline{\theta}_{\mathbf{A}}^m)+\tau\sum_{k=1}^{m}J_1^k \\
&\quad +C\tau\sum_{k=0}^{m}\big(\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2+D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\big)\,.
\end{aligned}\tag{129}
$$

6.2. Estimates for (83). Taking $\mathbf{v} = \frac{1}{2\tau}(\theta_{\mathbf{A}}^k - \theta_{\mathbf{A}}^{k-2})$ in (83), we see that

$$\begin{aligned}&\Big(\partial_\tau^2\theta_{\mathbf{A}}^k,\ \frac{1}{2}(\partial_\tau\theta_{\mathbf{A}}^k + \partial_\tau\theta_{\mathbf{A}}^{k-1})\Big) + D\big(\widetilde{\theta_{\mathbf{A}}^k},\ \frac{1}{2}(\partial_\tau\theta_{\mathbf{A}}^k + \partial_\tau\theta_{\mathbf{A}}^{k-1})\big)\\ &\quad= \frac{1}{2\tau}\left(\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2 - \|\partial_\tau\theta_{\mathbf{A}}^{k-1}\|_{\mathbf{L}^2}^2\right) + \frac{1}{4\tau}\left(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k) - (D(\theta_{\mathbf{A}}^{k-2},\theta_{\mathbf{A}}^{k-2})\right)\\ &\quad= \sum_{i=1}^{5} U_i^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k),\end{aligned} \tag{130}$$

which leads to

$$\begin{aligned}&\frac{1}{2}\|\partial_\tau\theta_{\mathbf{A}}^m\|_{\mathbf{L}^2}^2 + \frac{1}{4}D(\theta_{\mathbf{A}}^m,\theta_{\mathbf{A}}^m) + \frac{1}{4}D(\theta_{\mathbf{A}}^{m-1},\theta_{\mathbf{A}}^{m-1})\\ &\quad= \frac{1}{2}\|\partial_\tau\theta_{\mathbf{A}}^0\|_{\mathbf{L}^2}^2 + \frac{1}{4}D(\theta_{\mathbf{A}}^0,\theta_{\mathbf{A}}^0) + \frac{1}{4}D(\theta_{\mathbf{A}}^{-1},\theta_{\mathbf{A}}^{-1}) + \tau\sum_{k=1}^{m}\sum_{i=1}^{5} U_i^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k)\\ &\quad\le Ch^2 + \tau\sum_{k=1}^{m}\sum_{i=1}^{5} U_i^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k).\end{aligned} \tag{131}$$

Now we estimate $\sum_{k=1}^{m} U_i^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k)$, $i = 1,2,3,4,5$. Under the regularity assumption of $\mathbf{A}$ in (43), we have

$$\tau\sum_{k=1}^{m}|U_1^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k)| \le C\left(h^2+\tau^4\right) + C\tau\sum_{k=1}^{m}\|\overline{\partial_\tau\theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2. \tag{132}$$

Applying (78), the regularity assumption, and the Young's inequality, we can bound $\tau\sum_{k=1}^{m} U_2^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k)$ as follows.

$$\begin{aligned}\tau\sum_{k=1}^{m} U_2^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k) &\le C\big(h^2+\tau^4\big) + C\tau\sum_{k=0}^{m} D\left(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k\right)\\ &\quad+\frac{1}{32}D\left(\theta_{\mathbf{A}}^m,\theta_{\mathbf{A}}^m\right) + \frac{1}{32}D\left(\theta_{\mathbf{A}}^{m-1},\theta_{\mathbf{A}}^{m-1}\right).\end{aligned} \tag{133}$$

Since $\overline{\partial_\tau\theta}_{\mathbf{A}}^k \in \mathbf{X}_{0h}$, we have

$$\Big(\frac{1}{2\tau}(I_h\phi^k - I_h\phi^{k-2}),\ \nabla\cdot\overline{\partial_\tau\theta}_{\mathbf{A}}^k\Big) = 0, \tag{134}$$

from which we deduce

$$\begin{aligned}U_3^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k) &= -\Big((\phi_t)^{k-1},\ \nabla\cdot\overline{\partial_\tau\theta}_{\mathbf{A}}^k\Big) = -\Big((\phi_t)^{k-1} - \frac{1}{2\tau}(\phi^k-\phi^{k-2}),\ \nabla\cdot\overline{\partial_\tau\theta}_{\mathbf{A}}^k\Big)\\ &\quad-\Big(\frac{1}{2\tau}(\phi^k-\phi^{k-2}) - \frac{1}{2\tau}(I_h\phi^k - I_h\phi^{k-2}),\ \nabla\cdot\overline{\partial_\tau\theta}_{\mathbf{A}}^k\Big).\end{aligned} \tag{135}$$

By applying (78) and reasoning as before, we have

$$\begin{aligned}\tau\sum_{k=1}^{m} U_3^k(\overline{\partial_\tau\theta}_{\mathbf{A}}^k) &\le C\big(h^2+\tau^4\big) + C\tau\sum_{k=0}^{m} D\left(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k\right)\\ &\quad+\frac{1}{32}D\left(\theta_{\mathbf{A}}^m,\theta_{\mathbf{A}}^m\right) + \frac{1}{32}D\left(\theta_{\mathbf{A}}^{m-1},\theta_{\mathbf{A}}^{m-1}\right).\end{aligned} \tag{136}$$

By applying Theorem 4.1 and the regularity assumption, the terms $\tau \sum_{k=1}^m U_4^k(\overline{\partial_\tau \theta}_{\mathbf{A}}^k)$ can be estimated by a standard argument.

$$\tau \sum_{k=1}^m U_4^k(\overline{\partial_\tau \theta}_{\mathbf{A}}^k) \leq C\big(h^2+\tau^4\big) + C\tau \sum_{k=0}^m \big(\|\nabla \theta_\Psi^k\|_{\mathbf{L}^2}^2 + \|\partial_\tau \theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\big). \tag{137}$$

To estimate $\sum\limits_{k=1}^m U_5^k(\overline{\partial_\tau \theta}_{\mathbf{A}}^k)$, we first rewrite $U_5^k(\overline{\partial_\tau \theta}_{\mathbf{A}}^k)$ as follows.

$$\begin{aligned} U_5^k(\overline{\partial_\tau \theta}_{\mathbf{A}}^k) &= \Big(f(\Psi^{k-1},\Psi^{k-1}) - f(\mathcal{I}_h\Psi^{k-1},\mathcal{I}_h\Psi^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\Big) \\ &\quad + \Big(f(\mathcal{I}_h\Psi^{k-1},\mathcal{I}_h\Psi^{k-1}) - f(\Psi_h^{k-1},\Psi_h^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\Big) \\ &\quad := U_5^{k,1}(\overline{\partial_\tau \theta}_{\mathbf{A}}^k) + U_5^{k,2}(\overline{\partial_\tau \theta}_{\mathbf{A}}^k). \end{aligned} \tag{138}$$

A simple calculation shows that

$$\begin{aligned} & f(\psi,\psi) - f(\varphi,\varphi) = \frac{\mathrm{i}}{2}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{\mathrm{i}}{2}(\varphi^*\nabla\varphi - \varphi\nabla\varphi^*) \\ & = -\frac{\mathrm{i}}{2}\left(\varphi^*\nabla(\varphi-\psi) - \varphi\nabla(\varphi-\psi)^*\right) + \frac{\mathrm{i}}{2}\left((\varphi-\psi)\nabla\psi^* - (\varphi-\psi)^*\nabla\psi\right), \end{aligned} \tag{139}$$

and consequently, we have

$$\begin{aligned} U_5^{k,1}(\overline{\partial_\tau \theta}_{\mathbf{A}}^k) &= \Big(f(\Psi^{k-1},\Psi^{k-1}) - f(\mathcal{I}_h\Psi^{k-1},\mathcal{I}_h\Psi^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\Big) \\ &\leq C\left(h^2 + \|\overline{\partial_\tau \theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\right) \end{aligned} \tag{140}$$

by applying (76) and (77).

Similarly, by employing (77), we deduce

$$\begin{aligned} U_5^{k,2}(\overline{\partial_\tau \theta}_{\mathbf{A}}^k) &= \Big(f(\mathcal{I}_h\Psi^{k-1},\mathcal{I}_h\Psi^{k-1}) - f(\Psi_h^{k-1},\Psi_h^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\Big) \\ &= -\frac{\mathrm{i}}{2}\left((\theta_\Psi^{k-1})^*\nabla\theta_\Psi^{k-1} - \theta_\Psi^{k-1}\nabla(\theta_\Psi^{k-1})^*,\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\right) \\ &\quad -\frac{\mathrm{i}}{2}\left((\mathcal{I}_h\Psi^{k-1})^*\nabla\theta_\Psi^{k-1} - \mathcal{I}_h\Psi^{k-1}\nabla(\theta_\Psi^{k-1})^*,\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\right) \\ &\quad +\frac{\mathrm{i}}{2}\left(\theta_\Psi^{k-1}\nabla(\mathcal{I}_h\Psi^{k-1})^* - (\theta_\Psi^{k-1})^*\nabla\mathcal{I}_h\Psi^{k-1},\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\right) \\ &\leq -\left(f(\theta_\Psi^{k-1},\theta_\Psi^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\right) + C\|\mathcal{I}_h\Psi^{k-1}\|_{\mathcal{L}^\infty}\|\nabla\theta_\Psi^{k-1}\|_{\mathbf{L}^2}\|\overline{\partial_\tau \theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2} \\ &\quad + C\|\nabla\mathcal{I}_h\Psi^{k-1}\|_{\mathbf{L}^3}\|\theta_\Psi^{k-1}\|_{\mathcal{L}^6}\|\overline{\partial_\tau \theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2} \\ &\leq -\left(f(\theta_\Psi^{k-1},\theta_\Psi^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\right) + C\left(\|\nabla\theta_\Psi^{k-1}\|_{\mathbf{L}^2}^2 + \|\overline{\partial_\tau \theta}_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\right). \end{aligned} \tag{141}$$

Therefore, we have

$$\begin{aligned} \tau\sum_{k=1}^m U_5^k(\overline{\partial_\tau \theta}_{\mathbf{A}}^k) &\leq Ch^2 - \tau\sum_{k=1}^m \left(f(\theta_\Psi^{k-1},\theta_\Psi^{k-1}),\ \overline{\partial_\tau \theta}_{\mathbf{A}}^k\right) \\ &\quad + C\tau\sum_{k=0}^m \left(\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2 + \|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\right). \end{aligned} \tag{142}$$

Substituting (132), (133), (136), (137), and (142) into (131) and recalling the definition of J_1^k in (99), we obtain

$$\begin{aligned}&\frac{1}{2}\|\partial_\tau\theta_{\mathbf{A}}^m\|_{\mathbf{L}^2}^2+\frac{3}{16}D(\theta_{\mathbf{A}}^m,\theta_{\mathbf{A}}^m)+\frac{3}{16}D(\theta_{\mathbf{A}}^{m-1},\theta_{\mathbf{A}}^{m-1})\\&\le C\big(h^2+\tau^4\big)+C\tau\sum_{k=0}^m\big(D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2\big)-\tau\sum_{k=1}^m J_1^k.\end{aligned}\tag{143}$$

6.3. Estimates for (84). We can deduce the estimate of $\nabla\theta_\phi^k$ by a standard argument.

$$\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2\le Ch^2+C\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2,\quad k=0,1,\cdots,m.\tag{144}$$

From (84) we know that

$$\big(\partial_\tau\nabla\theta_\phi^k,\,\nabla u\big)=\big(\partial_\tau\nabla e_\phi^k,\,\nabla u\big)+\frac{1}{\tau}\big(|\Psi_h^k|^2-|\Psi^k|^2-|\Psi_h^{k-1}|^2+|\Psi^{k-1}|^2,\,u\big),\ \forall u\in X_h.\tag{145}$$

By taking $u=\overline{\theta}_\phi^k$ in (145) and recalling the definition of J_2^k in (109), we find

$$\begin{aligned}\frac{1}{2\tau}\big(\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2-\|\nabla\theta_\phi^{k-1}\|_{\mathbf{L}^2}^2\big)&=\big(\partial_\tau\nabla e_\phi^k,\,\nabla\overline{\theta}_\phi^k\big)+\frac{1}{\tau}J_2^k\\&+\frac{1}{\tau}\big(|\mathcal{I}_h\Psi^k|^2-|\Psi^k|^2-|\mathcal{I}_h\Psi^{k-1}|^2+|\Psi^{k-1}|^2,\,\overline{\theta}_\phi^k\big),\end{aligned}\tag{146}$$

which implies that

$$\begin{aligned}\frac{1}{2}\|\nabla\theta_\phi^m\|_{\mathbf{L}^2}^2&=\frac{1}{2}\|\nabla\theta_\phi^0\|_{\mathbf{L}^2}^2+\tau\sum_{k=1}^m\big(\partial_\tau\nabla e_\phi^k,\,\nabla\overline{\theta}_\phi^k\big)+\sum_{k=1}^m J_2^k\\&+\sum_{k=1}^m\big(|\mathcal{I}_h\Psi^k|^2-|\Psi^k|^2-|\mathcal{I}_h\Psi^{k-1}|^2+|\Psi^{k-1}|^2,\,\overline{\theta}_\phi^k\big).\end{aligned}\tag{147}$$

Employing the error estimates of interpolation operators and the regularity assumption, we obtain

$$\begin{aligned}&\tau\sum_{k=1}^m\big(\partial_\tau\nabla e_\phi^k,\,\nabla\overline{\theta}_\phi^k\big)\le Ch^2+C\tau\sum_{k=0}^m\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2,\\&\sum_{k=1}^m\big(|\mathcal{I}_h\Psi^k|^2-|\Psi^k|^2-|\mathcal{I}_h\Psi^{k-1}|^2+|\Psi^{k-1}|^2,\,\overline{\theta}_\phi^k\big)\le Ch^2+C\tau\sum_{k=0}^m\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2.\end{aligned}\tag{148}$$

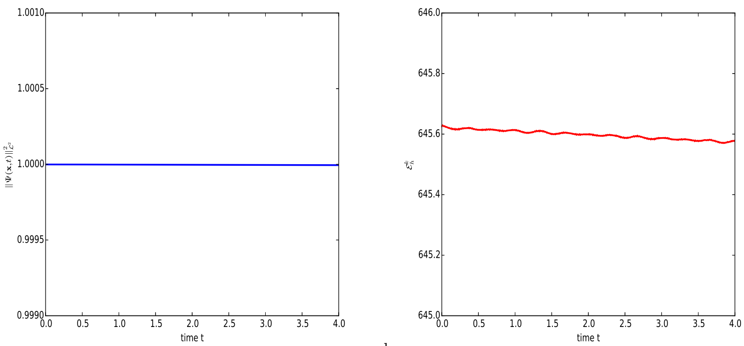
It follows that

$$\frac{1}{2}\|\nabla\theta_\phi^m\|_{\mathbf{L}^2}^2\le Ch^2+C\tau\sum_{k=0}^m\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2+\sum_{k=1}^m J_2^k.\tag{149}$$

By combining (129), (143), and (149), we finally obtain

$$\begin{aligned}&\frac{3}{64}\|\nabla\theta_\Psi^m\|_{\mathbf{L}^2}^2+\frac{1}{2}\|\nabla\theta_\phi^m\|_{\mathbf{L}^2}^2+\frac{1}{2}\|\partial_\tau\theta_{\mathbf{A}}^m\|_{\mathbf{L}^2}^2+\frac{3}{32}D(\theta_{\mathbf{A}}^m,\theta_{\mathbf{A}}^m)+\frac{3}{32}D(\theta_{\mathbf{A}}^{m-1},\theta_{\mathbf{A}}^{m-1})\\&\le C\big(h^2+\tau^4\big)+C\tau\sum_{k=0}^m\big(\|\nabla\theta_\Psi^k\|_{\mathbf{L}^2}^2+\|\nabla\theta_\phi^k\|_{\mathbf{L}^2}^2+D(\theta_{\mathbf{A}}^k,\theta_{\mathbf{A}}^k)+\|\partial_\tau\theta_{\mathbf{A}}^k\|_{\mathbf{L}^2}^2\big),\end{aligned}\tag{150}$$

which yields the desired estimate (79) by assuming the time step τ sufficiently small and then using the discrete Gronwall's inequality.



a b

FIGURE 1. Example 7.1: (a) The evolution of the total charge $\|\Psi_h^k\|_{\mathcal{L}^2}^2$; (b) The evolution of the total energy $\mathcal{E}_h^k$ of the discrete system.

7. Numerical Experiments

In this section, we present two numerical examples to confirm our theoretical analysis.

Example 7.1 To verify the conservation of the total charge and the total energy of our scheme, we consider the M-S-C system (8)-(9) with the initial conditions:

$$\begin{aligned}
&\Psi(\mathbf{x},0) = 2\sin(\pi x_1)\sin(\pi x_2)\sin(\pi x_3) + 2\sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3),\\
&\mathbf{A}(\mathbf{x},0) = \mathbf{A}_0(\mathbf{x}) = \big(5\sin(2\pi x_3)(1-\cos(2\pi x_1))\sin(\pi x_2), \;\; 0,\\
&\qquad\qquad 5\sin(2\pi x_1)(1-\cos(2\pi x_3))\sin(\pi x_2)\big),\\
&\mathbf{A}_t(\mathbf{x},0) = \mathbf{A}_1(\mathbf{x}) = 0.
\end{aligned}$$

In this example we take $\Omega = (0,1)^3$, $V(\mathbf{x}) = 5.0$, $T = 4.0$, $\tau = 0.01$, $h = 0.02$, and solve the M-S-C system by the proposed scheme (37).

The numerical results of this example are displayed in Fig. 1, which clearly show that our algorithm almost exactly keeps the conservation of the total charge and the total energy of the discrete system.

Example 7.2 We consider the following system:

$$\begin{cases}
-\mathrm{i}\dfrac{\partial \Psi}{\partial t} + \dfrac{1}{2}\left(\mathrm{i}\nabla + \mathbf{A}\right)^2\Psi + V\Psi + \phi\Psi = g(\mathbf{x},t), \;\; (\mathbf{x},t) \in \Omega\times(0,T),\\
\dfrac{\partial^2 \mathbf{A}}{\partial t^2} + \nabla\times(\nabla\times\mathbf{A}) + \dfrac{\partial(\nabla\phi)}{\partial t} + \dfrac{\mathrm{i}}{2}\big(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\big)\\
\qquad\qquad +|\Psi|^2\mathbf{A} = \mathbf{f}(\mathbf{x},t), \qquad (\mathbf{x},t)\in\Omega\times(0,T),\\
\nabla\cdot\mathbf{A} = 0, \quad -\Delta\phi - |\Psi|^2 = h(\mathbf{x},t), \;\; (\mathbf{x},t)\in\Omega\times(0,T)\\
\Psi(\mathbf{x},t) = 0, \quad \mathbf{A}(\mathbf{x},t)\times\mathbf{n} = 0, \quad \phi(\mathbf{x},t) = 0, \;\; (\mathbf{x},t)\in\partial\Omega\times(0,T).
\end{cases} \tag{151}$$

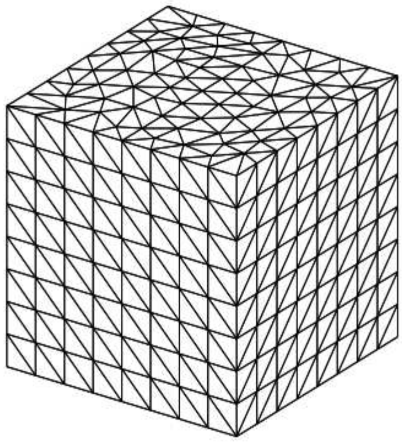


FIGURE 2. The mesh with $N = 8$.

with the exact solution $(\Psi, \mathbf{A}, \phi)$

$$\Psi(\mathbf{x}, t) = 5.0e^{\mathrm{i}\pi t}\sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3),$$

$$\mathbf{A}(\mathbf{x}, t) = \sin(\pi t)\Big(\cos(\pi x_1)\sin(\pi x_2)\sin(\pi x_3),\ \sin(\pi x_1)\cos(\pi x_2)\sin(\pi x_3),$$
$$-2\sin(\pi x_1)\sin(\pi x_2)\cos(\pi x_3)\Big) + \cos(\pi t)\Big(\sin(2\pi x_3)(1-\cos(2\pi x_1))\sin(\pi x_2),$$
$$0,\ \sin(2\pi x_1)(1-\cos(2\pi x_3))\sin(\pi x_2)\Big),$$

$$\phi(\mathbf{x}, t) = 4\sin(\pi t)x_1x_2x_3(1-x_1)(1-x_2)(1-x_3)$$
$$+\ cos(\pi t)\sin(\pi x_1)\sin(\pi x_2)\sin(\pi x_3).$$

where $V(\mathbf{x}) = \frac{1}{2}(x_1^2 + x_2^2 + x_3^2)$ and the right-hand side functions $g(\mathbf{x}, t)$, $\mathbf{f}(\mathbf{x}, t)$ and $h(\mathbf{x}, t)$ are determined by the exact solution.

In this example, we set $\Omega = (0, 1)^3$, $T = 2$, and take a uniform tetrahedral partition of the domain with $N + 1$ nodes in each direction and $6N^3$ elements in total. The schematic diagram of the mesh with $N = 8$ is shown in Fig. 2. The system (151) is solved by the proposed scheme (37). To test the convergence order of our method, we take $\tau = h^{\frac{1}{2}}$ for the scheme. The numerical results at the final time $T = 2.0$ are presented in Tables 1. We can see that our method has better convergence order than the theoretical analysis, which is partially because we use a quadratic element approximation of the vector potential $\mathbf{A}$.

TABLE 1. H^1 error of the scheme with $h = \frac{1}{N}$ and $\tau = h^{\frac{1}{2}}$.

	$\|\Psi_h^M - \Psi(\cdot, 2)\|_{\mathcal{H}^1}$	$\|\mathbf{A}_h^M - \mathbf{A}(\cdot, 2)\|_{\mathbf{H}^1}$	$\|\phi_h^M - \phi(\cdot, 2)\|_{H^1}$
N=25	3.3481e-01	2.8513e-01	4.0193e-02
N=50	1.5649e-01	1.1960e-01	1.6210e-02
N=100	6.9587e-02	4.5826e-02	7.0549e-03
order	1.13	1.33	1.25

Acknowledgements

This work is supported by National Natural Science Foundation of China (grant 11571353, 91330202), and Project supported by the Funds for Creative Research Group of China (grant 11321061)

References

[1] I. Ahmed and E. Li, Simulation of plasmonics nanodevices with coupled Maxwell and Schrödinger equations using the FDTD method, Advanced Electromagnetics (2012), 1: 76–83.
[2] D. Boffi, F. Brezzi and M. Fortin, Mixed Finite Elements and Applications, Springer, Berlin, 2013.
[3] S. Brenner and L. Scott, The Mathematical Theory of Finite Element Methods, Springer, New York, 2002.
[4] F. Brezzi and M. Fortin, Mixed and Hybrid Finite Element Methods, Springer, New York, 1991.
[5] F. E. Browder, Existence and uniqueness theorems for solutions of nonlinear boundary value problems, Proc. Sympos. Appl. Math (1965), 17: 24–49.
[6] Y.P. Chen, et al, A unified Hamiltonian solution to Maxwell–Schrödinger equations for modelling electromagnetic field-particle interaction, Computer Physics Communications (2017), 215: 63–70.
[7] Z. Chen and K.H. Hoffmann, Numerical studies of a non-stationary Ginzburg-Landau model for superconductivity, Adv. Math. Sci. Appl. (1995), 5: 363–389.
[8] W. C. Chew, Vector Potential Electromagnetics with Generalized Gauge for Inhomogeneous Media: Formulation, Progress In Electromagnetics Research (2014), 149: 69–84.
[9] Q. Du, M. Gunzburger and J. Peterson, Analysis and approxiamtion of the GL model of superconductivity, SIAM Rev (1992), 34: 54–81.
[10] L.C. Evans, Partial Differential Equations, American Mathematical Society, 1998.
[11] H.D. Gao, B.Y. Li and W.W. Sun, Optimal error estimates of linearized Crank-Nicolson Galerkin FEMs for the time-dependent Ginzburg-Landau equations in superconductivity, SIAM J. Numer. Anal. (2014), 52: 1183–1202.
[12] V. Girault, P.A. Raviart, Finite Element Methods for Navier-Stokes Equations, Springer-Verlag, Berlin, 1986.
[13] Y. Guo, K. Nakamitsu and W. Strauss, Global finite-energy solutions of the Maxwell-Schrödinger system, Commun. Math. Phys. (1995), 170: 181–196.
[14] O. Karni, et al, Rabi oscillations and self-induced transparency in InAs/InP quantum dot semiconductor optical amplifier operating at room temperature, Optics Express (2013), 21: 26786–26796.
[15] E. Lorin, S. Chelkowski and A.D. Bandrauk, A numerical Maxwell-Schrödinger model for intense laser-matter interaction and propagation, Comput. Phys. Comm. (2007), 177: 908–932.
[16] E. Lorin and A.D. Bandrauk, Efficient and accurate numerical modeling of a micro-macro nonlinear optics model for intense and short laser pulses, J. Comput. Sci. (2012), 3: 159–168.
[17] K. Lopata and D. Neuhauser, Multiscale Maxwell–Schrödinger modeling: A split field finite-difference time-domain approach to molecular nanopolaritonics, J. Chem. Phys (2009), 130: 104707–.
[18] C.P. Ma, L.Q. Cao and Y.P. Lin, Error estimates of the Crank–Nicolson Galerkin method for the time-dependent Maxwell–Schrödinger equations under the Lorentz gauge, IMA Journal of Numerical Analysis, drx060.
[19] M. Mu and Y.Q. Huang, An alternating Crank-Nicolson method for decoupling the Ginzburg–Landau equations, SIAM J. Numer. Anal. (1998), 35: 1740–1761.
[20] K. Nakamitsu and M. Tsutsumi, The Cauchy problem for the coupled Maxwell-Schródinger equations, J. Math. Phys. (1986), 27: 211–216.
[21] M. Nakamura and T. Wada, Local well-posedness for the Maxwell-Schrödinger equation, Mathematische Annalen (2005), 332: 565–604.
[22] M. Nakamura and T. Wada, Global existence and uniqueness of solutions to the Maxwell-Schrödinger equations, Commun. Math. Phys. (2007), 276: 315–339.
[23] S. Ohnuki et al., Coupled analysis of Maxwell-schrödinger equations by using the length gauge: harmonic model of a nanoplate subjected to a 2D electromagnetic field, Intern. J. of Numer. Model.: Electronic Networks, Devices and Fields (2013), 26: 533–544.

[24] L. Pierantoni, D. Mencarelli and T. Rozzi, A new 3-D transmission line matrix scheme for the combined Schrödinger-Maxwell problem in the electronic/electromagnetic characterization of nanodevices, IEEE Transactions on Microwave Theory and Techniques (2008), 56: 654–662.

[25] C.J. Ryu, A.Y. Liu and W.E.I Sha, Finite-Difference Time-Domain Simulation of the Maxwell–Schrödinger System, IEEE Journal on Multiscale and Multiphysics Computational Techniques (2016), 1: 40–47.

[26] S.A. Sato and K. Yabana, Maxwell+ TDDFT multi-scale simulation for laser-matter interactions, Adv. Simul. Sci. Engng. (2014), 1: 98–110.

[27] A. Shimomura, Modified wave operator for Maxwell-Schrödinger equations in three space dimensions, Ann. Henri Poincaré (2003), 4: 661–683.

[28] J. Simon, Compact sets in the space $L^p(0,T;B)$., Ann. Mat. Pura. Appl.(1987), 146: 65–96.

[29] W. Sui, J. Yang, X. H. Yun and C. Wang, Including quantum effects in electromagnetic system for FDTD solution to Maxwell-Schrödinger equations, Microwave Symposium, IEEE/MTT-S International (2007), 1979–1982.

[30] R. Temma, Navier–Stokes Equations: Theory and Numerical Analysis, North Holland, Amsterdam-New York-Oxford, 1977.

[31] Y. Tsutsumi, Global existence and asymptotic behavior of solutions for the Maxwell-Schrödinger equations in three space dimensions, Commun. Math. Phys. (1993), 151: 543–576.

[32] P. Turati and Y. Hao, A FDTD solution to the Maxwell-Schrödinger coupled model at the microwave range, Electromagnetics in Advanced Applications (ICEAA), 2012 International Conference on IEEE (2012), 363–366.

[33] T. Wada, Smoothing effects for Schrödinger equations with electro-magnetic potentials and applications to the Maxwell-Schrödinger equations, J. Functional Analysis (2012), 263: 1–24.

[34] T.C. Wang and X.F. Zhao, Optimal l^∞ error estimates of finite difference methods for the coupled Gross–Pitaevskii equations in high dimensions, Sci China Math (2014), 57: 2189–2214.

[35] C. Yang, A linearized Crank–Nicolson–Galerkin FEM for the time-dependent Ginzburg–Landau equations under the temporal gauge, Numerical Methods for Partial Differential Equations (2014), 30: 1740–1761.

[36] H. Yang and F.Y. Li, Error Estimates of Runge-Kutta Discontinuous Galerkin Methods for the Vlasov-Maxwell System, ESAIM: Mathematical Modelling and Numerical Analysis (2015), 49: 69–99.

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