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A structure-preserving relaxation Crank–Nicolson finite element method for the Schrödinger–Poisson equation

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In this paper, we propose a mass- and modified energy-conservative relaxation Crank–Nicolson finite element method for the Schrödinger–Poisson (SP) equation. Utilising only a single auxiliary variable, we simultaneously reformulate the distinct nonlinear terms present in both the Schrödinger equation and the Poisson equation into their equivalent expressions, constructing a system equivalent to the original SP equation. Our proposed scheme, derived from this equivalent system, is implemented linearly, avoiding the need for iterative techniques to solve the nonlinear equation. Additionally, it is executed sequentially, eliminating the need to solve a coupled large linear system. We in turn rigorously derive the optimal error estimates for the proposed scheme, demonstrating second-order accuracy in time and $(k+1)$th-order accuracy in space when employing polynomials of degree up to k. Numerical experiments validate the accuracy and effectiveness of our method and emphasise its conservation properties over long-time simulations.

Keywords: Schrödinger–Poisson equation; mass and modified energy conservation; relaxation Crank–Nicolson scheme; finite element method; optimal error estimates.

1. Introduction

Consider the Schrödinger–Poisson (SP) equation, also known as the Gross–Pitaevskii–Poisson equation (Shukla & Eliasson, 2006; Cai *et al.*, 2010; Cotner, 2016)

$$\mathbf{i}u_t = -\Delta u + \Phi u + V(x)u + |u|^2 u, \quad (x,t) \in \Omega \times (0,T], \tag{1.1a}$$

$$-\Delta \Phi = \mu(|u|^2 - c), \quad (x,t) \in \Omega \times [0,T], \tag{1.1b}$$

$$u(x,0) = u_0(x), \quad x \in \Omega. \tag{1.1c}$$

Here, the symbol $\mathbf{i} = \sqrt{-1}$ represents the imaginary unit, $\Omega \subset \mathbb{R}^2$ is a convex bounded domain, and $T > 0$ is the final time. The complex-valued function $u(x, t)$ represents the single-particle wave function, while the real-valued function $\Phi(x, t)$ denotes the Poisson potential. Both functions satisfy the homogeneous Dirichlet boundary condition. The nonlinear term $|u|^2 u$ in the Schrödinger equation is known as the self-repulsion, whereas the nonlinear term $|u|^2$ in the Poisson equation represents the charge density. The constant $\mu = \pm 1$ is a rescaled physical constant, reflecting the nature of the underlying forcing: repulsive for $\mu > 0$ and attractive for $\mu < 0$. The parameter c denotes a background charge of the particle independent of time t. $V(x)$ is a specified external potential, and $u_0(x)$ is the initial condition.

The SP equation was first introduced by (Ruffini & Bonazzola, 1969) to study self-gravitating boson stars. Later on, it was explored in various fields of application, including quantum mechanics (Cai *et al.*, 2010), semiconductors (Markowich *et al.*, 1990; Ringhofer & Soler, 2000), plasma physics (Bertrand & Van Tuan, 1980; Shukla & Eliasson, 2006, 2011; Sakaguchi & Malomed, 2020), optics (Paredes *et al.*, 2020). A significant body of literature is dedicated to the mathematical analysis and numerical approximation of the SP equation, including the well-posedness (Lange *et al.*, 1995; Castella, 1997; Arriola & Soler, 2001; Masaki, 2011).

In studies of Bose–Einstein condensates, boundary conditions for both u and Φ in (1.1) typically vanish at infinity and are often scaled to bounded domains as homogeneous Dirichlet boundary conditions (Cotner, 2016). For simplicity of presentation, we focus on the homogeneous Dirichlet boundary condition:

$$u(x,t) = 0 \quad \text{and} \quad \Phi(x,t) = 0, \quad (x,t) \in \partial\Omega \times [0,T]. \tag{1.2}$$

However, various types of boundary conditions can be imposed on the SP equation (1.1), including (homogeneous) Dirichlet boundary conditions (Arriola & Soler, 2001; Cotner, 2016), zero-flux (Neumann) boundary conditions (Sakaguchi & Malomed, 2020) and periodic boundary conditions (Lange *et al.*, 1995; Sakaguchi & Malomed, 2020; Verma *et al.*, 2021). More discussions about boundary conditions can be found in (Lange *et al.*, 1995; Lange & Zweifel, 1997) and the references therein. The method to be proposed later and its analysis are applicable to all these boundary conditions. Under the homogeneous Dirichlet boundary conditions (1.2), the solution of the SP equation (1.1) preserves the mass conservation

$$M(t) = \int_\Omega |u|^2 \, \mathrm{d}x = M(0),$$

and the energy conservation

$$E(t) = \int_\Omega \left(|\nabla u|^2 + \frac{1}{2\mu} |\nabla \Phi|^2 + V(x)|u|^2 + \frac{1}{2}|u|^4 \right) \mathrm{d}x = E(0), \tag{1.3}$$

which are important invariant properties that are also desired at the discrete level. In literature, a modified energy is often selected as an alternative structure to the original energy, particularly in numerical methods that involve reformulating the SP equation (1.1) into an equivalent enlarged system (Gong *et al.*, 2022; Yi & Liu, 2022).

If the self-repulsion term $|u|^2 u$ in (1.1a) vanishes, several numerical methods have been proposed to handle the nonlinearity caused by the charge density $|u|^2$ in the Poisson equation, including the Strang splitting types of methods (Lubich, 2008; Auzinger *et al.*, 2017). To preserve the invariant properties at the discrete level, Ringhofer *et al.* introduced a Crank–Nicolson scheme (Ringhofer & Soler, 2000) and employed the prediction-correction technique to handle the nonlinearity. An extension work of the Crank–Nicolson-type method was carried out by Ehrhardt *et al.* to develop an approximation for the spherically symmetric SP system (Ehrhardt & Zisowsky, 2006). A structure-preserving discontinuous Galerkin (DG) method proposed in (Yi & Liu, 2022) also treated the nonlinear term implicitly, but an iterative technique was employed to handle the nonlinear term. More recently, structure-preserving relaxation Crank–Nicolson types of methods were proposed for the nonlinear Schrödinger equation (Besse, 2004; Besse *et al.*, 2021) and the SP equation (Athanassoulis *et al.*, 2023). The relaxation methods introduce an intermediate function to handle the nonlinearity and find solutions of Schrödinger equation and Poisson equation at different time levels. Therefore, the corresponding schemes are linear.

For the nonlinear SP equation (1.1) that incorporates both the self-repulsion $|u|^2u$ and the charge density $|u|^2$, different techniques may be necessary to handle the two distinct nonlinear terms. In addition, it is challenging to handle the two nonlinear terms while simultaneously conserving the invariant properties (Wang *et al.*, 2018). A scalar auxiliary variable (SAV) Crank–Nicolson scheme was proposed in (Gong *et al.*, 2022) that preserves both mass and modified energy properties. It is interesting to note that the SAV approach is only applied to the nonlinear term $|u|^2u$ while treating the nonlinear term $|u|^2$ simply implicitly. Therefore, the method remains implicit and nonlinear, requiring iterative methods (IMs) for convergence. Another noteworthy DG method (Yi & Liu, 2022) applies the relaxation techniques described in (Besse, 2004) for the Schrödinger equation, but treats the nonlinear term $|u|^2$ in the Poisson equation implicitly. Therefore, iterative techniques are still needed to solve the coupled system formed by the Schrödinger equation and the Poisson equation.

It is natural to inquire whether it is possible to handle the nonlinear terms efficiently while conserving the invariant properties. Motivated by effectiveness and the ability of the structure-preserving relaxation-type of schemes to preserve the invariants for the Schrödinger equation and the general SP equation (Besse, 2004; Besse *et al.*, 2021; Athanassoulis *et al.*, 2023), we propose a linear and structure-preserving relaxation Crank–Nicolson finite element method (FEM) tailored for solving the nonlinear SP equation (1.1). More specifically, we introduce only one auxiliary variable to reformulate two different nonlinear terms in two equations simultaneously: the self-repulsion term $|u|^2u$ in the Schrödinger equation (1.1a), and the charge density $|u|^2$ in the Poisson equation (1.1b). This transforms the SP equation (1.1) into an equivalent system, facilitating its discretization into a linear fully discrete finite element scheme. This approach conserves both mass and modified energy, while also allowing for a linear implementation without the need for iterative techniques. To the best of our knowledge, the approach that introduces only one auxiliary variable to simultaneously reformulate different nonlinear terms in two distinct equations in a system, as described, has not been explored in the literature for the SP equation (1.1).

Error analysis of the numerical methods for the SP equations is crucial for assessing their stability and accuracy, but much attention has been given to optimal error analysis for the SP equations without the self-repulsion term. (Lubich, 2008) pioneered the error analysis of the Strang-type splitting method in the semi-discretization system. (Auzinger *et al.*, 2017) analyzed the convergence analysis for the fully discrete scheme for the SP equation by using the splitting FEM. Later on, (Zhang, 2013) studied the optimal error estimates of the finite difference method under proper regularity assumptions. The optimal L^2 error estimate of semi-discrete conservative DG scheme was also proved in (Yi & Liu, 2022). However, limited research on error analysis has been established for numerical methods incorporating the nonlinear self-repulsion term. (Gong *et al.*, 2022) established unconditional energy stability and performed convergence analysis for the SAV Crank–Nicolson spectral method.

In this work, we rigorously derive optimal a priori error estimates for the relaxation Crank–Nicolson FEM using the method of induction. Various tools have been introduced and developed to obtain the desired results, such as the uniform boundedness of the finite element approximations, and the dependence of the errors between different equations. Specially, the L^2 error of the solution in the Poisson equation is bounded by the L^2 error of auxiliary variable and an optimal spatial error bound. As a result, we obtain second order accuracy in time and $(k+1)$th order accuracy in space when employing polynomials of degrees no more than k. To the best of our knowledge, there are currently no rigorous convergence results in the literature for relaxation Crank–Nicolson types of methods for the SP equation. The analysis technique developed in this work can be extended to other similar numerical methods, offering a broader applicability. An extension of the error analysis for the structure-preserving relaxation Crank–Nicolson FEM to the SP equation, without the self-repulsion term $|u|^2u$ in (1.1a), was also provided.

The contributions, innovations and significance of this work include:

- Different from the existing methods that use various techniques to handle the two distinct nonlinear terms in the SP equation (1.1), we employ only one technique, namely the relaxation method, for both nonlinear terms. Consequently, the proposed method is easy to implement.
- Though we use only one technique to handle the two different nonlinear terms, we prove that the proposed method preserves both mass and modified energy.
- The proposed method is implemented linearly without resorting to any iterative techniques and sequentially without the need to solve a coupled system. Therefore, it is computationally efficient and cheap.
- We derived the optimal error estimates for the proposed method, obtaining second-order accuracy in time and $(k+1)$th order accuracy in space for the L^2 errors when applying polynomials with a maximal degree k.
- We conduct numerical examples to verify the performance of the proposed method, including accuracy tests, conservation verification and comparisons with existing results.

The organization of this paper is as follows. In Section 2, we present the relaxation Crank–Nicolson FEM for the SP equation, and we demonstrate the structure-preserving properties of both the continuous problem and the fully discrete scheme. In Section 3, we establish the optimal error estimates in L^2 norm for the solutions of a fully discrete system, comprising second-order accuracy in time and $(k+1)$th order accuracy in space. We further extend the convergence results to the relaxation Crank–Nicolson scheme (Athanassoulis *et al.*, 2023) in Section 4. In Section 5, some numerical experiments are carried out to validate the theoretical analysis and verify the performance of the proposed conservative method.

We employ $W^{m,p}(\Omega,\mathbb{R})$ and $W^{m,p}(\Omega,\mathbb{C})$ to denote real-valued and complex-valued Sobolev spaces, respectively. For brevity, we use $H^m(\Omega)$ for $W^{m,2}(\Omega,\mathbb{R})$ and $\mathbf{H}^m(\Omega)$ for $W^{m,2}(\Omega,\mathbb{C})$, with norms denoted by $\|\cdot\|_m$ and semi-norms by $|\cdot|_m$. When $m=0$, $\|\cdot\|$ represents the L^2 norm of either $L^2(\Omega)$ or $\mathbf{L}^2(\Omega)$. Unless explicitly stated otherwise, the constants denoted by C, possibly accompanied by a suitable subscript, represent generic positive constants that are independent of τ, h, n and N, but may depend on final time T and the regularity of exact solutions u and Φ.

2. The relaxation Crank–Nicolson FEM

In the following presentation, the inner product and norm of the standard complex-valued Hilbert space $\mathbf{L}^2(\Omega)$ are expressed as $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$, respectively,

$$\langle u,v\rangle := \int_\Omega uv^*\,\mathrm{d}x \quad \text{and} \quad \|u\| = \sqrt{\langle u,u\rangle},$$

where v^* denotes the complex conjugate of v. Similarly, the inner product and norm of the real-valued Hilbert space $L^2(\Omega)$ are defined by

$$(u, v) := \int_\Omega uv \, \mathrm{d}x \quad \text{and} \quad \|u\| = \sqrt{(u, u)}.$$

Then the weak formulation of problem (1.1) reads as: find $u \in C^1([0, T], \mathbf{H}_0^1(\Omega))$ and $\Phi \in H_0^1(\Omega)$,

$$\mathbf{i}\left\langle u_t, \omega\right\rangle = A_0\left(u, \omega\right) + \langle \Phi u, \omega\rangle + \langle V(x)u, \omega\rangle + \left\langle |u|^2 u, \omega\right\rangle, \quad \forall \omega \in \mathbf{H}_0^1(\Omega), \tag{2.1}$$

$$A_1\left(\Phi, \chi\right) = \mu\left(|u|^2 - c, \chi\right), \quad \forall \chi \in H_0^1(\Omega), \tag{2.2}$$

where the bilinear forms $A_0(\cdot,\cdot)$ and $A_1(\cdot,\cdot)$ are defined as follows

$$A_0(\omega, v) = \langle \nabla\omega, \nabla v\rangle, \quad \forall \omega, v \in \mathbf{H}_0^1(\Omega), \tag{2.3}$$

$$A_1(\phi, \chi) = (\nabla\phi, \nabla\chi), \quad \forall \phi, \chi \in H_0^1(\Omega), \tag{2.4}$$

and they both satisfy the coercivity and continuity properties, namely, there exist constants $\gamma_1 > 0$ and $\gamma_2 > 0$ such that

$$A_j(v, v) \geq \gamma_1 \|v\|_1^2, \quad A_j(\omega, v) \leq \gamma_2 \|\omega\|_1 \|v\|_1, \quad j = 0, 1, \tag{2.5}$$

for any $\omega, v \in H_0^1(\Omega)$ or $\mathbf{H}_0^1(\Omega)$.

2.1 *Mass and conservation properties*

We begin with the review of the continuous mass and energy conservation for the SP equation (1.1). Then, we propose a FEM that conserves these properties.

The SP equation (1.1) is nonlinear, containing two nonlinear terms: the self-repulsion term $|u|^2 u$ in the Schrödinger equation (1.1a), and the charge density $|u|^2$ in the Poisson equation (1.1b). Observing that two nonlinearities share a common factor, we introduce a real auxiliary variable $\Psi = |u|^2$. The SP equation (1.1) can then be equivalently written as

$$\begin{cases} \Psi = |u|^2, \\ \mathbf{i}u_t = -\Delta u + \Phi u + V(x)u + \Psi u, \\ -\Delta\Phi = \mu(\Psi - c), \end{cases} \tag{2.6}$$

whose weak formulation is to find $u \in C^1([0, T], \mathbf{H}_0^1(\Omega))$ and $\Psi, \Phi \in H_0^1(\Omega)$ such that

$$(\Psi, v) = \left(|u|^2, v\right), \quad \forall v \in H_0^1(\Omega), \tag{2.7a}$$

$$\mathbf{i}\left\langle u_t, \omega\right\rangle = A_0\left(u, \omega\right) + \langle \Phi u, \omega\rangle + \langle V(x)u, \omega\rangle + \langle \Psi u, \omega\rangle, \quad \forall \omega \in \mathbf{H}_0^1(\Omega), \tag{2.7b}$$

$$A_1\left(\Phi, \chi\right) = \mu\left(\Psi - c, \chi\right), \quad \forall \chi \in H_0^1(\Omega). \tag{2.7c}$$

Similar to (1.1), the following invariants are preserved for the new SP system:

$$\text{mass conservation} \quad M(t) = \int_\Omega |u|^2 \,\mathrm{d}x = M(0), \tag{2.8}$$

$$\text{energy conservation} \quad E(t) = \int_\Omega \left(|\nabla u|^2 + \frac{1}{2\mu}|\nabla \Phi|^2 + V(x)|u|^2 + \frac{1}{2}\Psi^2 \right) \mathrm{d}x = E(0). \tag{2.9}$$

Indeed, by substituting $\omega = u$ in (2.7b), we obtain

$$\mathbf{i}\left\langle u_t, u \right\rangle = A_0(u,u) + \langle \Phi u, u\rangle + \langle V(x)u, u\rangle + \langle \Psi u, u\rangle. \tag{2.10}$$

Taking the imaginary part of (2.10) yields

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega |u|^2 \,\mathrm{d}x = 0, \tag{2.11}$$

which proves the mass conservation (2.8).

On the other hand, by taking $\omega = u_t$ in (2.7b), it holds

$$\mathbf{i}\left\langle u_t, u_t \right\rangle = A_0(u,u_t) + \left\langle \Phi u, u_t\right\rangle + \left\langle V(x)u, u_t\right\rangle + \left\langle \Psi u, u_t\right\rangle. \tag{2.12}$$

The real part of (2.12) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \int_\Omega \Phi \frac{\mathrm{d}}{\mathrm{d}t}|u|^2 \,\mathrm{d}x + \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega V(x)\,|u|^2 \,\mathrm{d}x + \int_\Omega \Psi \frac{\mathrm{d}}{\mathrm{d}t}|u|^2 \,\mathrm{d}x = 0. \tag{2.13}$$

By taking $v = \Phi$ in $(2.7a)_t$, which is a resulting equation from differentiation of (2.7a) in t, it follows

$$\int_\Omega \Phi \frac{\mathrm{d}}{\mathrm{d}t}|u|^2 \,\mathrm{d}x = \int_\Omega \Phi \frac{\mathrm{d}}{\mathrm{d}t}(\Psi - c)\,\mathrm{d}x. \tag{2.14}$$

Similarly, by taking $\chi = \Phi$ in $(2.7c)_t$, the second term in (2.13) can be rewritten as

$$\int_\Omega \Phi \frac{\mathrm{d}}{\mathrm{d}t}|u|^2 \,\mathrm{d}x = \frac{1}{\mu}\int_\Omega \nabla\Phi_t \cdot \nabla\Phi \,\mathrm{d}x. \tag{2.15}$$

Setting $v = \Psi$ in $(2.7a)_t$, the last term in (2.13) can be rewritten as

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Psi^2 \,\mathrm{d}x = \int_\Omega \Psi \frac{\mathrm{d}}{\mathrm{d}t}|u|^2 \,\mathrm{d}x. \tag{2.16}$$

Therefore, (2.13) reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \frac{1}{2\mu}\int_\Omega |\nabla\Phi|^2 \,\mathrm{d}x + \int_\Omega V(x)\,|u|^2 \,\mathrm{d}x + \frac{1}{2}\int_\Omega \Psi^2 \,\mathrm{d}x \right) = 0. \tag{2.17}$$

Hence, the energy conservation (2.9) holds.

2.2 *Fully discrete scheme*

To preserve the properties mentioned above at the discrete level, we investigate a relaxation Crank–Nicolson FEM in this subsection.

Let $\mathcal{T}_h$ be a shape-regular and quasi-uniform triangulation of $\Omega \subset \mathbb{R}^2$, $K \in \mathcal{T}_h$ be an element, and $h := \max_{K\in\mathcal{T}_h} h_K$ be the mesh size with h_K being the diameter of K. We denote the real-valued finite element space V_h by

$$V_h = \left\{ v \in C(\Omega) : v \in \mathbb{P}^k(K), \quad \forall K \in \mathcal{T}_h \right\}, \tag{2.18}$$

where $\mathbb{P}^k$ is the space of real-valued polynomials of degree up to the k ($k \geq 1$). Similarly, the complex-valued finite element space V_h^c, associated with the triangulation $\mathcal{T}_h$, is denoted by

$$V_h^c = \left\{ v \in C(\Omega) : v \in \mathbb{Q}^k(K), \quad \forall K \in \mathcal{T}_h \right\}, \tag{2.19}$$

where $\mathbb{Q}^k$ denotes the space of complex-valued polynomials of degree up to k ($k \geq 1$) in space.

Denote by $\{t_n \mid t_n = n\tau, 0 \leq n \leq N\}$ a uniform partition of time interval $[0, T]$ with time step size $\tau = T/N$, where N is a positive integer. We also introduce $t_{n-1/2} = (t_n + t_{n-1})/2 = (n - \frac{1}{2})\tau$. For any function $\varphi(x,t)$ and $n \geq 0$, we denote $\varphi_h^{n-\theta} \in V_h$ or V_h^c as an approximation of $\varphi(x, t_{n-\theta})$, where $\theta = 0, \frac{1}{2}$.

For a sequence of functions $\{\varphi^n\}_{n=0}^N$, we define the operators

$$D_\tau \varphi^{n+1} := \frac{\varphi^{n+1} - \varphi^n}{\tau}, \quad \overline{\varphi}^{n+1/2} := \frac{\varphi^{n+1} + \varphi^n}{2}. \tag{2.20}$$

The relaxation Crank–Nicolson method introduces an intermediate function, and solves the intermediate function and the solution of the Schrödinger equation at different time levels. Therefore, the corresponding scheme can be implemented linearly. For the linearity of the scheme when coupled with the Poisson equation, we further solve the Poisson equation in the same time level as the intermediate function. More specifically, for given $(\Psi_h^{n-1/2}, u_h^n, \Phi_h^{n-1/2}) \in V_h \times V_h^c \times V_h$, the relaxation Crank–Nicolson finite element scheme, derived from (2.6) or its weak formualation (2.7), is to find $(\Psi_h^{n+1/2}, u_h^{n+1}, \Phi_h^{n+1/2}) \in V_h \times V_h^c \times V_h$ such that

$$(\Psi_h^{n+1/2} + \Psi_h^{n-1/2}, v_h) = (2|u_h^n|^2, v_h), \quad \forall v_h \in V_h, \tag{2.21a}$$

$$\mathbf{i}\langle D_\tau u_h^{n+1}, \omega_h\rangle = A_0(\overline{u}_h^{n+1/2}, \omega_h) + \langle(\Phi_h^{n+1/2} + V(x) + \Psi_h^{n+1/2})\overline{u}_h^{n+1/2}, \omega_h\rangle, \quad \forall \omega_h \in V_h^c, \tag{2.21b}$$

$$A_1(\Phi_h^{n+1/2}, \chi_h) = \mu(\Psi_h^{n+1/2} - c, \chi_h), \quad \forall \chi_h \in V_h, \tag{2.21c}$$

where the initial data $u_h^0 = \Pi_h u_0$ and $\Psi_h^{-1/2} = \Pi_h |u_h^0|^2$. Here, $\Pi_h : H^1(\Omega) \to V_h$ is the nodal interpolation operator. To compute the initial energy, we need $\Phi_h^{-1/2} \in V_h$, which is obtained by

$$A_1(\Phi_h^{-1/2}, \chi_h) = \mu(\Psi_h^{-1/2} - c, \chi_h), \quad \forall \chi_h \in V_h.$$

LEMMA 2.1. Given $(\Psi_h^{n-1/2}, u_h^n, \Phi_h^{n-1/2}) \in V_h \times V_h^c \times V_h$ and $\tau > 0$, the relaxation Crank–Nicolson finite element scheme (2.21) admits a unique solution $(\Psi_h^{n+1/2}, u_h^{n+1}, \Phi_h^{n+1/2}) \in V_h \times V_h^c \times V_h$.

Proof. The scheme (2.21) is a finite dimensional system, whose existence is equivalent to its uniqueness, thus we only need to show its uniqueness. Assume that (2.21) has two possible solutions and their difference is denoted by $(\delta\Psi_h^{n+1/2}, \delta u_h^{n+1}, \delta\Phi_h^{n+1/2})$, then it satisfies

$$(\delta\Psi_h^{n+1/2}, v_h) = 0, \quad \forall v_h \in V_h, \tag{2.22a}$$

$$\mathbf{i}\langle \delta u_h^{n+1}/\tau, \omega_h\rangle = \frac{1}{2}A_0(\delta u_h^{n+1}, \omega_h) + \frac{1}{2}\left\langle \left(\Phi_h^{n+1/2} + V(x) + \Psi_h^{n+1/2}\right)\delta u_h^{n+1}, \omega_h \right\rangle, \quad \forall \omega_h \in V_h^c, \tag{2.22b}$$

$$A_1(\delta\Phi_h^{n+1/2}, \chi_h) = \mu(\delta\Psi_h^{n+1/2}, \chi_h), \quad \forall \chi_h \in V_h. \tag{2.22c}$$

Taking $v_h = \delta\Psi_h^{n+1/2}$ in (2.22a) gives $\|\delta\Psi_h^{n+1/2}\| = 0$, namely $\delta\Psi_h^{n+1/2} = 0$. Then (2.22c) gives

$$A_1(\delta\Phi_h^{n+1/2}, \chi_h) = 0, \quad \forall \chi_h \in V_h. \tag{2.23}$$

By taking $\chi_h = \delta\Phi_h^{n+1/2}$ in (2.23) and applying (2.5), it follows

$$\|\delta\Phi_h^{n+1/2}\|_1 \le 0,$$

which implies $\delta\Phi_h^{n+1/2} = 0$. Finally, taking $\omega_h = \tau\delta u_h^{n+1}$ in (2.22b) yields

$$\mathbf{i}\|\delta u_h^{n+1}\|^2 = \frac{\tau}{2}A_0(\delta u_h^{n+1}, \delta u_h^{n+1}) + \frac{\tau}{2}\left\langle \left(\Phi_h^{n+1/2} + V(x) + \Psi_h^{n+1/2}\right)\delta u_h^{n+1}, \delta u_h^{n+1} \right\rangle,$$

and the imaginary part gives $\|\delta u_h^{n+1}\| = 0$, or equivalently, $\delta u_h^{n+1} = 0$. Thus, the conclusion holds. □

By solving the intermediate function, the Poisson equation, and the solutions of the Schrödinger equation at different time levels, namely the intermediate function and the Poisson solution at $t_{n+1/2}$, and the Schrödinger at t_{n+1}, the relaxation Crank–Nicolson FEM (2.21) can be implemented in the following algorithm.

Algorithm 2.1 The relaxation Crank–Nicolson FEM (2.21) is solved sequentially and linearly as follows.

- Solve $\Psi_h^{n+1/2} \in V_h$ from (2.21a).
- Solve $\Phi_h^{n+1/2} \in V_h$ from (2.21c).
- Solve $u_h^{n+1} \in V_h^c$ from (2.21b).

REMARK 2.1. The proposed relaxation Crank–Nicolson FEM (2.21) is linear without resorting to any interaction techniques, Algorithm 2.1 additionally implies that it does not require solving a couple system.

2.3 *Structure-preserving properties*

From the literature, to conserve the invariant properties is challenging to solve the SP equation (1.1). Next, we explore the conservation properties of the proposed relaxation Crank–Nicolson finite element scheme (2.21) and obtain the following statement.

LEMMA 2.2. For any $\tau > 0$, the relaxation Crank–Nicolson FEM (2.21) satisfies the discrete conservation for both mass and modified energy with $0 \le n \le N-1$, respectively

$$M_h^{n+1} = M_h^0, \tag{2.24}$$

$$E_h^{n+1} = E_h^0, \tag{2.25}$$

where the mass $M_h^{n+1} := \int_\Omega |u_h^{n+1}|^2 \,\mathrm{d}x$, and the modified energy

$$E_h^{n+1} := A_0(u_h^{n+1}, u_h^{n+1}) + \frac{1}{2\mu} A_1(\Phi_h^{n+3/2}, \Phi_h^{n+1/2}) + \int_\Omega V(x)|u_h^{n+1}|^2 \,\mathrm{d}x + \frac{1}{2}\int_\Omega \Psi_h^{n+3/2}\Psi_h^{n+1/2} \,\mathrm{d}x.$$

Proof. Taking $\omega_h = \overline{u}_h^{n+1/2}$ in (2.21b) yields

$$\mathbf{i}\langle D_\tau u_h^{n+1}, \overline{u}_h^{n+1/2}\rangle = A_0(\overline{u}_h^{n+1/2}, \overline{u}_h^{n+1/2}) + \langle(\Phi_h^{n+1/2} + V(x) + \Psi_h^{n+1/2})\overline{u}_h^{n+1/2}, \overline{u}_h^{n+1/2}\rangle. \tag{2.26}$$

Then the imaginary part of (2.26) gives

$$\|u_h^{n+1}\|^2 - \|u_h^n\|^2 = 0, \tag{2.27}$$

which implies the conservation of the mass (2.24).

Next, taking $\omega_h = D_\tau u_h^{n+1}$ in (2.21b) gives

$$\mathbf{i}\langle D_\tau u_h^{n+1}, D_\tau u_h^{n+1}\rangle = A_0(\overline{u}_h^{n+1/2}, D_\tau u_h^{n+1}) + \langle(\Phi_h^{n+1/2} + V(x) + \Psi_h^{n+1/2})\overline{u}_h^{n+1/2}, D_\tau u_h^{n+1}\rangle. \tag{2.28}$$

The real part of (2.28) implies

$$\left[A_0(u_h^{n+1}, u_h^{n+1}) - A_0(u_h^n, u_h^n)\right] + \int_\Omega (\Phi_h^{n+1/2} + V(x) + \Psi_h^{n+1/2})(|u_h^{n+1}|^2 - |u_h^n|^2) \,\mathrm{d}x = 0. \tag{2.29}$$

Then we proceed to estimate the terms in (2.29). Upon calculation,

$$\begin{aligned}
&\int_\Omega \Phi_h^{n+1/2}\left(|u_h^{n+1}|^2-|u_h^n|^2\right)\,\mathrm{d}x\\
&=\int_\Omega \Phi_h^{n+1/2}\left(\frac{\Psi_h^{n+3/2}+\Psi_h^{n+1/2}}{2}-\frac{\Psi_h^{n+1/2}+\Psi_h^{n-1/2}}{2}\right)\mathrm{d}x \qquad \text{by (2.21a)}\\
&=\frac{1}{2}\int_\Omega \Phi_h^{n+1/2}(\Psi_h^{n+3/2}-c)-\Phi_h^{n+1/2}(\Psi_h^{n-1/2}-c)\,\mathrm{d}x\\
&=\frac{1}{2\mu}A_1\left(\Phi_h^{n+3/2},\Phi_h^{n+1/2}\right)-\frac{1}{2\mu}A_1\left(\Phi_h^{n+1/2},\Phi_h^{n-1/2}\right) \qquad \text{by (2.21c)}.
\end{aligned} \tag{2.30}$$

Similarly, by (2.21a), it holds

$$\int_\Omega \Psi_h^{n+1/2}\left(|u_h^{n+1}|^2-|u_h^n|^2\right)\mathrm{d}x=\frac{1}{2}\int_\Omega\left(\Psi_h^{n+3/2}\Psi_h^{n+1/2}-\Psi_h^{n+1/2}\Psi_h^{n-1/2}\right)\mathrm{d}x. \tag{2.31}$$

Plugging (2.30) and (2.31) into (2.29) and regrouping give the discrete energy conservation (2.25). □

REMARK 2.2. Handling the two nonlinear terms in the SP equation (1.1) while conserving the original energy at the discrete level remains a challenging task. The discrete energy has only been numerically verified for the splitting Chebyshev collocation method proposed in (Wang *et al.*, 2018), whereas the IMs in (Gong *et al.*, 2022; Yi & Liu, 2022) conserve modified rather than original energies. Although our proposed method also conserves a modified energy, it achieves this with much higher efficiency.

3. Error estimates for the fully discrete system

The main objective of this section is to establish the optimal error estimates of the relaxation Crank–Nicolson FEM (2.21) for the SP equation (1.1). To begin with, we review some useful results.

Recall that $\Pi_h : H^1(\Omega) \to V_h$ be the nodal interpolation operator. By the classical finite element approximation theory (Brenner & Scott, 2008), it follows

$$\|v-\Pi_h v\|+h\left\|\nabla\left(v-\Pi_h v\right)\right\|+h\|v-\Pi_h v\|_\infty \le Ch^{k+1}\|v\|_{k+1}, \quad \forall v\in H^{k+1}(\Omega). \tag{3.1}$$

We also define the Ritz projection operator $\mathrm{R}_h : H_0^1(\Omega)\to V_h$, which satisfies

$$\left(\nabla(v-\mathrm{R}_h v),\nabla\omega\right)=0, \quad \forall \omega\in V_h, \tag{3.2}$$

and holds the projection error estimate

$$\|v-\mathrm{R}_h v\|+h\left\|\nabla\left(v-\mathrm{R}_h v\right)\right\| \le Ch^{k+1}\|v\|_{k+1}, \quad \forall v\in H_0^1(\Omega)\cap H^{k+1}(\Omega). \tag{3.3}$$

The following inverse inequality (Ciarlet & Oden, 1978) will be widely used in the analysis,

$$\|v\|_\infty \le Ch^{-1}\|v\|, \quad \forall v\in V_h. \tag{3.4}$$

In addition, we also need the following result.

LEMMA 3.1. For the Ritz projection defined in (3.2), it holds for any $k \geq 1$,

$$\|\mathrm{R}_h v\|_\infty \leq C, \quad \forall v \in H_0^1(\Omega) \cap H^{k+1}(\Omega), \tag{3.5}$$

where C depends on $\|v\|_{k+1}$ and $\|v\|_\infty$, independent of h.

Proof. By the embedding theorem, it follows $H^2(\Omega) \subset L^\infty(\Omega)$. Then $v \in H^{k+1}(\Omega)$ implies $v \in L^\infty(\Omega)$. Let $\Pi_h v$ be the nodal interpolation of v. By (3.1), (3.3), and the triangle inequality,

$$\begin{aligned}\|v - \mathrm{R}_h v\|_\infty \leq& \|v - \Pi_h v\|_\infty + \|\Pi_h v - \mathrm{R}_h v\|_\infty \leq \|v - \Pi_h v\|_\infty + Ch^{-1}\|\Pi_h v - \mathrm{R}_h v\| \\ \leq& \|v - \Pi_h v\|_\infty + Ch^{-1}\left(\|v - \Pi_h v\| + \|v - \mathrm{R}_h v\|\right) \leq Ch^k \|v\|_{k+1}.\end{aligned}$$

Therefore, applying the triangle inequality gives

$$\|\mathrm{R}_h v\|_\infty \leq \|v - \mathrm{R}_h v\|_\infty + \|v\|_\infty \leq C.$$

□

REMARK 3.1. Specially, the result in Lemma 3.1 holds for any $v \in H_0^1(\Omega) \cap H^{s+1}(\Omega)$ with $s > 0$. The projection errors (3.1), (3.3), (3.4), and the bound (3.5) also hold for functions in complex-valued Sobolev space and the corresponding projections in complex-valued finite element space V_h^c.

LEMMA 3.2 (Discrete Gronwall's inequality (Heywood & Rannacher, 1990)). Let τ, B and a_k, b_k, c_k, γ_k, for $k \geq 0$, be non-negative numbers satisfying

$$a_n + \tau \sum_{k=0}^{n} b_k \leq \tau \sum_{k=0}^{n} \gamma_k a_k + \tau \sum_{k=0}^{n} c_k + B, \quad \text{for} \quad n \geq 0. \tag{3.6}$$

Suppose that $\tau\gamma_k < 1$, for all k and $\sigma_k = (1 - \tau\gamma_k)^{-1}$. Then

$$a_n + \tau \sum_{k=0}^{n} b_k \leq \exp\left(\tau \sum_{k=0}^{n} \sigma_k \gamma_k\right)\left(\tau \sum_{k=0}^{n} c_k + B\right). \tag{3.7}$$

LEMMA 3.3. (Zouraris, 2023) Let $v^a, v^b, z^a, z^b \in \mathbb{C}$ and $\mathrm{S}\left(v^a, v^b, z^a, z^b\right) := |v^a|^2 - |v^b|^2 - |z^a|^2 + |z^b|^2$. Then,

$$\left\|\mathrm{S}\left(v^a, v^b, z^a, z^b\right)\right\| \leq 2\left\|z^a - z^b\right\|_\infty \left\|v^b - z^b\right\| + \mathrm{H}\left(v^a, v^b, z^a, z^b\right)\left\|v^a - v^b - z^a + z^b\right\|, \tag{3.8}$$

where $\mathrm{H}\left(v^a, v^b, z^a, z^b\right) := \|v^a\|_\infty + \left\|v^b\right\|_\infty + \left\|z^a - z^b\right\|_\infty$.

For the finite element approximation related to the Poisson problem, the following estimate holds.

LEMMA 3.4. Given $f \in L^2(\Omega)$. If $a \in H_0^1(\Omega)$ satisfies

$$A_1(a, \chi_h) = (f, \chi_h), \quad \forall \chi_h \in V_h. \tag{3.9}$$

Then there exists a constant $C > 0$ such that

$$\|a\| \le C\left(\|f\| + h \min_{a_h \in V_h} \|a_h - a\|_1\right). \tag{3.10}$$

Proof. Let $a_h \in V_h$ be an approximation of a. Then (3.9) can be reformulated as

$$A_1(a_h, \chi_h) = A_1(a_h - a, \chi_h) + (f, \chi_h). \tag{3.11}$$

Taking $\chi_h = a_h$ in (3.11) and applying (2.5) give

$$\|a_h\|_1^2 \le \frac{\gamma_2}{\gamma_1}\|a_h - a\|_1\|a_h\|_1 + \frac{1}{\gamma_1}\|f\|\|a_h\|. \tag{3.12}$$

Note that $\|a_h\| \le C\|a_h\|_1$. We obtain

$$\|a_h\|_1 \le C\left(\|a_h - a\|_1 + \|f\|\right). \tag{3.13}$$

By using the triangle inequality $\|a\|_1 - \|a - a_h\|_1 \le \|a_h\|_1$, (3.13) yields

$$\|a\|_1 \le C\left(\min_{a_h \in V_h} \|a_h - a\|_1 + \|f\|\right). \tag{3.14}$$

On the other hand, we introduce a function ψ solving the elliptic problem

$$-\Delta\psi = a \quad \text{in } \Omega, \qquad \psi = 0 \quad \text{on } \partial\Omega, \tag{3.15}$$

which holds the regularity estimate $\psi \in H^2(\Omega)$ and

$$\|\psi\|_2 \le \|a\|. \tag{3.16}$$

From (3.15), it follows

$$\|a\|^2 = \int_\Omega a \cdot (-\Delta\psi)\,\mathrm{d}x = \int_\Omega (\nabla a \cdot \nabla\psi)\,\mathrm{d}x = A_1(a, \psi). \tag{3.17}$$

Let $\psi_I \in V_h$ be a piecewise linear interpolant of ψ. Then

$$
\begin{aligned}
\|a\|^2 &= A_1(a,\psi) = A_1(a,\psi_I) + A_1(a,\psi-\psi_I)\\
&= (f,\psi_I) + A_1(a,\psi-\psi_I)\\
&\le \|f\|(\|\psi\| + \|\psi-\psi_I\|) + \gamma_2\|a\|_1\|\psi-\psi_I\|_1\\
&\le \|f\|(\|\psi\| + Ch^2\|\psi\|_2) + Ch\|a\|_1\|\psi\|_2\\
&\le C(\|f\| + h\|a\|_1)\|a\|,
\end{aligned}
\tag{3.18}
$$

where we have used the regularity (3.16) and the projection errors

$$
\|\psi-\psi_I\| \le Ch^2\|\psi\|_2, \quad \|(\psi-\psi_I)\|_1 \le Ch\|\psi\|_2.
$$

(3.18) together with (3.14) yields the estimate (3.10). □

We define the discrete Laplacian operator $\Delta_h : \mathbf{H}_0^1(\Omega) \to V_h^c$ as

$$
\langle -\Delta_h v, \chi_h\rangle = \langle \nabla v, \nabla \chi_h\rangle, \quad \forall \chi_h \in V_h^c. \tag{3.19}
$$

We also introduce linear operators $\mathbf{S}_h, \mathbf{T}_h : V_h^c \to V_h^c$,

$$
\left\langle \mathbf{S}_h v_h, \omega_h\right\rangle = \left\langle \left(\mathbf{I}_h - \mathbf{i}\frac{\tau}{2}\Delta_h\right) v_h, \omega_h\right\rangle, \quad \forall \omega_h \in V_h^c, \tag{3.20}
$$

$$
\left\langle \mathbf{T}_h v_h, \omega_h\right\rangle = \left\langle \left(\mathbf{I}_h + \mathbf{i}\frac{\tau}{2}\Delta_h\right) v_h, \omega_h\right\rangle, \quad \forall \omega_h \in V_h^c, \tag{3.21}
$$

where $\mathbf{I}_h$ is an identity operator on V_h^c. Denoting by $\mathbf{O}_h = \mathbf{S}_h, \mathbf{T}_h$ and setting $\omega_h = v_h$ in (3.20) and (3.21) give

$$
\mathrm{Re}(\mathbf{O}_h v_h, v_h) = \|v_h\|^2, \quad \forall v_h \in V_h^c, \tag{3.22}
$$

which implies $\ker(\mathbf{O}_h) = \{0\}$. Therefore, the operators $\mathbf{S}_h$ and $\mathbf{T}_h$ are invertible.

Similar to (Zouraris, 2023, Lemma 2.4), the following statement holds.

LEMMA 3.5. The operators $\mathbf{S}_h$ defined in (3.20) and $\mathbf{T}_h$ in (3.21) are invertible and fulfil

$$
\|\mathbf{S}_h^{-1}(v_h)\| \le \|v_h\|, \quad \forall v_h \in V_h^c, \tag{3.23}
$$

$$
\|\mathbf{B}_h(v_h)\| \le \|v_h\|, \quad \forall v_h \in V_h^c, \tag{3.24}
$$

where the linear operator $\mathbf{B}_h : V_h^c \to V_h^c$ is given by

$$
\mathbf{B}_h := \mathbf{S}_h^{-1}\mathbf{T}_h. \tag{3.25}
$$

LEMMA 3.6. Let $\mathbf{I}_h$, $\mathbf{S}_h$ and $\mathbf{B}_h$ be the operators in (3.20), (3.21) and (3.25), and let $\{y^n\}_{n=1}^N$ be a sequence in V_h^c satisfying:

$$y^{n+1} = (\mathbf{B}_h - \mathbf{I}_h)y^n + \mathbf{B}_h y^{n-1} + \mathbf{S}_h^{-1}\Gamma^{n+1}, \tag{3.26}$$

where $\{\Gamma^{n+1}\}_{n=1}^N$ are given functions in V_h^c. Then, for $n \geq 2$ it follows

$$\|y^{n+1}\| + \|y^n\| \leq 2\left\|\mathbf{S}_h(y^2)\right\| + 2\left\|\mathbf{S}_h(y^1)\right\| + 2\sum_{l=2}^{n}\|\Gamma^{l+1}\|. \tag{3.27}$$

Proof. The proof is summarised from Part 9 in the proof of Theorem 3.1 in (Zouraris, 2023), we present it here for completeness. If $n = 1$ in (3.27), the estimate is obvious by using Lemma 3.5 and $y^i = \mathbf{S}_h^{-1}\mathbf{S}_h y^i$ for $i = 1, 2$. Next, we will focus on $n \geq 2$. Note that (3.26) can be written in a vector form

$$\begin{bmatrix} y^{n+1} \\ y^n \end{bmatrix} = M \begin{bmatrix} y^n \\ y^{n-1} \end{bmatrix} + \begin{bmatrix} F^{n+1} \\ 0 \end{bmatrix}, \tag{3.28}$$

where

$$M = \begin{bmatrix} \mathbf{B}_h - I_h & \mathbf{B}_h \\ \mathbf{I}_h & 0 \end{bmatrix} \quad \text{and} \quad F^{n+1} := \mathbf{S}_h^{-1}\Gamma^{n+1}. \tag{3.29}$$

A simple induction argument yields

$$\begin{bmatrix} y^{n+1} \\ y^n \end{bmatrix} = M^{n-1}\begin{bmatrix} y^2 \\ y^1 \end{bmatrix} + \sum_{l=2}^{n} M^{n-l}\begin{bmatrix} F^{l+1} \\ 0 \end{bmatrix}, \tag{3.30}$$

where

$$M^\kappa = \frac{1}{2}\begin{bmatrix} ((-1)^\kappa \mathbf{I}_h + \mathbf{B}_h^{\kappa+1})\mathbf{S}_h & ((-1)^{\kappa+1}\mathbf{B}_h + \mathbf{B}_h^{\kappa+1})\mathbf{S}_h \\ ((-1)^{\kappa+1}\mathbf{I}_h + \mathbf{B}_h^{\kappa})\mathbf{S}_h & ((-1)^{\kappa}\mathbf{B}_h + \mathbf{B}_h^{\kappa})\mathbf{S}_h \end{bmatrix}. \tag{3.31}$$

Plugging (3.31) into (3.30) yields

$$\begin{aligned} \begin{bmatrix} y^{n+1} \\ y^n \end{bmatrix} &= \frac{1}{2}\begin{bmatrix} ((-1)^{n-1}\mathbf{I}_h + \mathbf{B}_h^{n})\mathbf{S}_h & ((-1)^{n}\mathbf{B}_h + \mathbf{B}_h^{n})\mathbf{S}_h \\ ((-1)^{n}\mathbf{I}_h + \mathbf{B}_h^{n-1})\mathbf{S}_h & ((-1)^{n-1}\mathbf{B}_h + \mathbf{B}_h^{n-1})\mathbf{S}_h \end{bmatrix}\begin{bmatrix} y^2 \\ y^1 \end{bmatrix} \\ &+ \frac{1}{2}\sum_{l=2}^{n}\begin{bmatrix} ((-1)^{n-l}\mathbf{I}_h + \mathbf{B}_h^{n-l+1})\mathbf{S}_h & ((-1)^{n-l+1}\mathbf{B}_h + \mathbf{B}_h^{n-l+1})\mathbf{S}_h \\ ((-1)^{n-l+1}\mathbf{I}_h + \mathbf{B}_h^{n-l})\mathbf{S}_h & ((-1)^{n-l}\mathbf{B}_h + \mathbf{B}_h^{n-l})\mathbf{S}_h \end{bmatrix}\begin{bmatrix} F^{l+1} \\ 0 \end{bmatrix}, \end{aligned} \tag{3.32}$$

which gives for $i = n, n+1$,

$$y^i = \frac{1}{2}\left[(-1)^i \mathbf{I}_h + \mathbf{B}_h^{i-1}\right]\mathbf{S}_h y^2 + \frac{1}{2}\left[(-1)^{i-1}\mathbf{B}_h + \mathbf{B}_h^{i-1}\right]\mathbf{S}_h y^1 + \frac{1}{2}\sum_{l=2}^{n}\left[(-1)^{i-l+1}\mathbf{I}_h + \mathbf{B}_h^{i-l}\right]\Gamma^{l+1}, \tag{3.33}$$

which together with Lemma 3.5 yields (3.27). □

For error analysis purposes, we assume that the exact solutions u, Φ and Ψ in (2.6) hold the following regularity

$$\begin{aligned} &u, u_t \in L^\infty(0,T;\mathbf{H}^{k+1}(\Omega)), \qquad \Psi, \Psi_t, \Phi, \Phi_t \in L^\infty(0,T;H^{k+1}(\Omega)),\\ &u_{tt}, \Psi_{tt} \in L^\infty(0,T;\mathbf{H}^2(\Omega)), \qquad \Psi_{ttt} \in L^\infty(0,T;\mathbf{L}^2(\Omega)), \qquad u_{ttt}, u_{tttt} \in L^\infty(0,T;\mathbf{L}^2(\Omega)). \end{aligned} \tag{3.34}$$

In addition, we also assume that the external potential $V(x) \in L^\infty(\Omega)$.

In view of the regularity assumptions in (3.34) for the exact solution u, Ψ and Φ, and Lemma 3.1, we have for any $n \geq 0$,

$$\begin{aligned} &\|u^n\|_\infty \leq C_u, \qquad \|\Psi^{n-1/2}\|_\infty \leq C_\Psi, \qquad \|\Phi^{n-1/2}\|_\infty \leq C_\Phi,\\ &\|\mathrm{R}_h u^n\|_\infty \leq D_u, \qquad \|\mathrm{R}_h \Psi^{n-1/2}\|_\infty \leq D_\Psi, \qquad \|\mathrm{R}_h \Phi^{n-1/2}\|_\infty \leq D_\Phi, \end{aligned} \tag{3.35}$$

where the constants

$$\begin{aligned} &C_u = \sup_{0\leq n\leq N} \|u^n\|_\infty, \qquad C_\Psi = \sup_{0\leq n\leq N}\|\Psi^{n-1/2}\|_\infty, \qquad C_\Phi = \sup_{0\leq n\leq N}\|\Phi^{n-1/2}\|_\infty,\\ &D_u = \sup_{0\leq n\leq N}\|\mathrm{R}_h u^n\|_\infty, \qquad D_\Psi = \sup_{0\leq n\leq N}\|\mathrm{R}_h\Psi^{n-1/2}\|_\infty, \qquad D_\Phi = \sup_{0\leq n\leq N}\|\mathrm{R}_h\Phi^{n-1/2}\|_\infty. \end{aligned}$$

Recall that the exact solution of (2.6) satisfies

$$\left(\Psi^{n+1/2} + \Psi^{n-1/2}, v\right) = \left(S_1^n, v\right) + \left(2|u^n|^2, v\right), \tag{3.36a}$$

$$\mathbf{i}\left\langle D_\tau u^{n+1}, \omega\right\rangle = A_0\left(\overline{u}^{n+1/2}, \omega\right) + \left\langle\left(\Phi^{n+1/2} + V(x) + \Psi^{n+1/2}\right)\overline{u}^{n+1/2}, \omega\right\rangle + \langle R_1^{n+1}, \omega\rangle, \tag{3.36b}$$

$$A_1\left(\Phi^{n+1/2}, \chi\right) = \mu\left(\Psi^{n+1/2} - c, \chi\right), \tag{3.36c}$$

for any $v, \chi \in H_0^1(\Omega)$ and $\omega \in \mathbf{H}_0^1(\Omega)$, where the consistency errors

$$S_1^n = \Psi^{n+1/2} + \Psi^{n-1/2} - 2\Psi^n,$$

and

$$R_1^{n+1} = -\mathbf{i}(u_t^{n+1/2} - D_\tau u^{n+1}) + \Delta(\overline{u}^{n+1/2} - u^{n+1/2}) + (\Phi^{n+1/2} + V(x) + \Psi^{n+1/2})(u^{n+1/2} - \overline{u}^{n+1/2}). \tag{3.37}$$

We define the errors e_u^{n+1}, $e_\Psi^{n+1/2}$ and $e_\Phi^{n+1/2}$ with $0 \le n \le N-1$ as

$$e_u^{n+1} = u^{n+1} - u_h^{n+1}, \quad e_\Psi^{n+1/2} = \Psi^{n+1/2} - \Psi_h^{n+1/2}, \quad e_\Phi^{n+1/2} = \Phi^{n+1/2} - \Phi_h^{n+1/2}.$$

Taking $v = v_h$, $\omega = \omega_h$ and $\chi = \chi_h$ in (3.36), and subtracting (2.21) from (3.36) yield

$$(e_\Psi^{n+1/2} + e_\Psi^{n-1/2}, v_h) = (S_1^n, v_h) + (T_1^n, v_h), \tag{3.38a}$$

$$\mathbf{i}\langle D_\tau e_u^{n+1}, \omega_h\rangle = A_0(\overline{e}_u^{n+1/2}, \omega_h) + \langle G_1^{n+1}, \omega_h\rangle + \langle R_1^{n+1}, \omega_h\rangle, \tag{3.38b}$$

$$A_1(e_\Phi^{n+1/2}, \chi_h) = \mu(e_\Psi^{n+1/2}, \chi_h), \tag{3.38c}$$

where

$$T_1^n = 2|u^n|^2 - 2|u_h^n|^2,$$

and

$$G_1^{n+1} = (\Phi^{n+1/2}\overline{u}^{n+1/2} - \Phi_h^{n+1/2}\overline{u}_h^{n+1/2}) + V(x)(\overline{u}^{n+1/2} - \overline{u}_h^{n+1/2}) + (\Psi^{n+1/2}\overline{u}^{n+1/2} - \Psi_h^{n+1/2}\overline{u}_h^{n+1/2}). \tag{3.39}$$

By using the projection operator R_h, the errors e_u^{n+1}, $e_\Psi^{n+1/2}$ and $e_\Phi^{n+1/2}$ can be split as

$$e_u^{n+1} = (u^{n+1} - \mathrm{R}_h u^{n+1}) + (\mathrm{R}_h u^{n+1} - u_h^{n+1}) = \xi_u^{n+1} + \eta_u^{n+1}, \tag{3.40}$$

$$e_\Psi^{n+1/2} = (\Psi^{n+1/2} - \mathrm{R}_h\Psi^{n+1/2}) + (\mathrm{R}_h\Psi^{n+1/2} - \Psi_h^{n+1/2}) = \xi_\Psi^{n+1/2} + \eta_\Psi^{n+1/2}, \tag{3.41}$$

$$e_\Phi^{n+1/2} = (\Phi^{n+1/2} - \mathrm{R}_h\Phi^{n+1/2}) + (\mathrm{R}_h\Phi^{n+1/2} - \Phi_h^{n+1/2}) = \xi_\Phi^{n+1/2} + \eta_\Phi^{n+1/2}. \tag{3.42}$$

Thus, the equivalent form of the error equations (3.38) are presented as

$$(\eta_\Psi^{n+1/2} + \eta_\Psi^{n-1/2}, v_h) = (S_2^n, v_h) + (T_1^n, v_h), \tag{3.43a}$$

$$\mathbf{i}\langle D_\tau \eta_u^{n+1}, \omega_h\rangle = A_0(\overline{\eta}_u^{n+1/2}, \omega_h) + \langle G_1^{n+1}, \omega_h\rangle + \langle R_2^{n+1}, \omega_h\rangle, \tag{3.43b}$$

$$A_1(\eta_\Phi^{n+1/2}, \chi_h) = \mu(\eta_\Psi^{n+1/2}, \chi_h) + \mu(R_3^{n+1/2}, \chi_h), \tag{3.43c}$$

where

$$S_2^n := S_1^n - (\xi_\Psi^{n+1/2} + \xi_\Psi^{n-1/2}), \quad R_2^{n+1} := R_1^{n+1} - \mathbf{i}D_\tau \xi_u^{n+1}, \quad R_3^{n+1/2} := \xi_\Psi^{n+1/2},$$

and we have used (3.2) to get rid of the terms $A_0(\overline{\xi}_u^{n+1/2}, \omega_h)$ and $A_1(\xi_\Phi^{n+1/2}, \chi_h)$. By using the projection error (3.3) and the mean value theorem, it holds

$$\|D_\tau \xi_u^{n+1}\| = \left\|D_\tau u^{n+1} - R_h D_\tau u^{n+1}\right\| \leq Ch^{k+1}\left\|D_\tau u^{n+1}\right\|_{k+1} \leq Ch^{k+1}\left\|u_t(x,t^*)\right\|_{k+1}, \tag{3.44}$$

where $t^* \in (t_n, t_{n+1})$. Then applying the Taylor expansion and the properties of the interpolation operator, for any $n \geq 0$, gives the estimates

$$\|S_2^n\| \leq C(\tau^2 + h^{k+1}), \tag{3.45}$$

$$\|R_2^{n+1}\| \leq C(\tau^2 + h^{k+1}), \tag{3.46}$$

$$\|R_3^{n+1/2}\| \leq Ch^{k+1}. \tag{3.47}$$

Then we obtain the following error estimates.

THEOREM Suppose that u, Ψ and Φ satisfy the regularity conditions (3.34). If $\tau \leq Ch$, then there exists constant $\tau_0 > 0$ and $h_0 > 0$ such that when time step $\tau < \tau_0$ and mesh size $h < h_0$, the solution of the relaxation Crank–Nicolson finite element scheme (2.21) satisfies

$$\max_{0\leq n\leq N}\left\|e_u^n\right\| \leq C\left(\tau^2 + h^{k+1}\right), \tag{3.48}$$

$$\max_{0\leq n\leq N-1}\left\|e_\Psi^{n+1/2}\right\| \leq C\left(\tau^2 + h^{k+1}\right), \tag{3.49}$$

$$\max_{0\leq n\leq N-1}\left\|e_\Phi^{n+1/2}\right\| \leq C(\tau^2 + h^{k+1}). \tag{3.50}$$

Proof. We prove the results using the method of mathematical induction.
Step 1. In this step, we prove the following estimates.

$$\|e_\Psi^{1/2}\| \leq C(\tau^2 + h^{k+1}), \tag{3.51}$$

$$\|e_\Phi^{1/2}\| \leq C(\tau^2 + h^{k+1}), \tag{3.52}$$

$$\|e_u^1\| \leq C\left(\tau^2 + h^{k+1}\right), \tag{3.53}$$

$$\|D_\tau \eta_u^1\| \le C\left(\tau^2 + h^{k+1}\right). \tag{3.54}$$

For $n=0$, taking $v_h = \eta_\Psi^{1/2} - \eta_\Psi^{-1/2}$ in (3.43a) gives

$$\begin{aligned}\|\eta_\Psi^{1/2}\|^2 - \|\eta_\Psi^{-1/2}\|^2 &= \left(S_2^0, \eta_\Psi^{1/2} - \eta_\Psi^{-1/2}\right) + \left(T_1^0, \eta_\Psi^{1/2} - \eta_\Psi^{-1/2}\right)\\ &\le 2\|S_2^0\|^2 + \frac{1}{2}\|\eta_\Psi^{1/2}\|^2 + \frac{1}{2}\|\eta_\Psi^{-1/2}\|^2 + 2\|T_1^0\|^2. \end{aligned}\tag{3.55}$$

Note that the following inequalities hold

$$\begin{aligned}\|T_1^0\| \le 2\||u_0|^2 - |u_h^0|^2\| \le 2\|u_0 + u_h^0\|_\infty \|u_0 - u_h^0\| \le Ch^{k+1},\\ \|\eta_\Psi^{-1/2}\| \le \|e_\Psi^{-1/2}\| + \|\xi_\Psi^{-1/2}\| \le Ch^{k+1},\end{aligned}\tag{3.56}$$

which together with (3.45) when plugging into (3.55) yields

$$\|\eta_\Psi^{1/2}\|^2 \le 3\|\eta_\Psi^{-1/2}\|^2 + 4\|S_2^0\|^2 + 4\|T_1^0\|^2 \le C(\tau^2 + h^{k+1})^2. \tag{3.57}$$

By (3.57) and the projection error (3.3) for $\|\xi_\Psi^{1/2}\|$,

$$\|e_\Psi^{1/2}\| \le \|\eta_\Psi^{1/2}\| + \|\xi_\Psi^{1/2}\| \le C(\tau^2 + h^{k+1}). \tag{3.58}$$

By applying the Lemma 3.4 to the (3.38c) with $n=0$, we conclude the following error estimate

$$\|e_\Phi^{1/2}\| \le C\|e_\Psi^{1/2}\| + Ch^{k+1} \le C(\tau^2 + h^{k+1}). \tag{3.59}$$

In view of $\tau \le Ch$, (3.35), (3.57), (3.59), and the inverse inequality (3.4), there exist $h_1 > 0$ such that when $h < h_1$,

$$\|\Psi_h^{1/2}\|_\infty \le \|\mathrm{R}_h \Psi^{1/2}\|_\infty + \|\eta_\Psi^{1/2}\|_\infty \le \|\mathrm{R}_h \Psi^{1/2}\|_\infty + Ch^{-1}\|\eta_\Psi^{1/2}\| \le D_\Psi + C_\Psi h \le D_\Psi + 1, \tag{3.60}$$

$$\|\Phi_h^{1/2}\|_\infty \le \|\mathrm{R}_h \Phi^{1/2}\|_\infty + Ch^{-1}\|\eta_\Phi^{1/2}\| \le D_\Phi + C_\Psi h \le D_\Phi + 1. \tag{3.61}$$

Taking $\omega_h = \overline{\eta}_u^{1/2}$ in (3.43b) with $n=0$ gives

$$\mathbf{i}\left\langle D_\tau \eta_u^1, \overline{\eta}_u^{1/2}\right\rangle = A_0\left(\overline{\eta}_u^{1/2}, \overline{\eta}_u^{1/2}\right) + \left\langle G_1^1, \overline{\eta}_u^{1/2}\right\rangle + \left\langle R_2^1, \overline{\eta}_u^{1/2}\right\rangle,$$

where the imaginary part yields

$$
\begin{aligned}
\frac{1}{2\tau}\left(\|\eta_u^1\|^2-\|\eta_u^0\|^2\right) &= \operatorname{Im}\left\langle G_1^1+R_2^1,\overline{\eta}_u^{1/2}\right\rangle \\
&\le \left\|G_1^1+R_2^1\right\|\left\|\overline{\eta}_u^{1/2}\right\| \\
&\le \frac{1}{2}\left\|G_1^1+R_2^1\right\|^2+\frac{1}{2}\left\|\overline{\eta}_u^{1/2}\right\|^2 \\
&= \frac{1}{2}\left(\left\|G_1^1\right\|^2+\left\|R_2^1\right\|^2+2\left\|G_1^1\right\|\left\|R_2^1\right\|\right)+\frac{1}{8}\left\|\eta_u^1+\eta_u^0\right\|^2 \\
&\le \left\|G_1^1\right\|^2+\left\|R_2^1\right\|^2+\frac{1}{4}\left(\|\eta_u^1\|^2+\|\eta_u^0\|^2\right).
\end{aligned} \tag{3.62}
$$

By employing (3.35), (3.58)–(3.61),

$$
\begin{aligned}
\left\|G_1^1\right\| &\le \|\overline{u}^{1/2}\|_\infty\left(\|e_\Phi^{1/2}\|+\|e_\Psi^{1/2}\|\right)+\left(\|\Phi_h^{1/2}\|_\infty+\|V(x)\|_\infty+\|\Psi_h^{1/2}\|_\infty\right)\|\overline{e}_u^{1/2}\| \\
&\le C\left(\|\eta_u^1\|+\|\eta_u^0\|\right)+C\left(\tau^2+h^{k+1}\right).
\end{aligned} \tag{3.63}
$$

Plugging (3.46) and (3.63) into (3.62) gives

$$
\frac{1}{2\tau}\left(\|\eta_u^1\|^2-\|\eta_u^0\|^2\right)\le C_1\left(\|\eta_u^1\|^2+\|\eta_u^0\|^2\right)+C(\tau^2+h^{k+1})^2. \tag{3.64}
$$

Since the initial value $\eta_u^0=0$, (3.64) leads to

$$
\left\|\eta_u^1\right\|\le C\tau(\tau^2+h^{k+1}), \tag{3.65}
$$

as long as $\tau<\tau_1:=1/(2C_1)$. Since $0<\tau<1$, we then conclude that

$$
\left\|e_u^1\right\|\le\|\xi_u^1\|+\|\eta_u^1\|\le C(\tau^2+h^{k+1}).
$$

Again, using $\eta_u^0=0$ and (3.65) gives

$$
\|D_\tau\eta_u^1\|=\frac{1}{\tau}\left\|\eta_u^1\right\|\le C(\tau^2+h^{k+1}). \tag{3.66}
$$

Based on (3.4), (3.35) and (3.65), there exists h_2 such that when $h<h_2$,

$$
\|u_h^1\|_\infty\le\|\mathrm{R}_hu^1\|_\infty+\|\mathrm{R}_hu^1-u_h^1\|_\infty\le\|\mathrm{R}_hu^1\|_\infty+Ch^{-1}\|\eta_u^1\|\le D_u+C_uh\le D_u+1. \tag{3.67}
$$

Step 2. In this step, we prove the following estimates

$$\left\|e_u^2\right\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.68}$$

$$\left\|D_\tau \eta_u^2\right\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.69}$$

$$\max_{1\le n\le 2}\left\|e_\Psi^{n+1/2}\right\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.70}$$

$$\max_{1\le n\le 2}\left\|e_\Phi^{n+1/2}\right\| \le C(\tau^2 + h^{k+1}). \tag{3.71}$$

Taking the difference between t_1 and t_0 of (3.43a) with $n = 1$ leads to

$$\left(\eta_\Psi^{3/2} - \eta_\Psi^{-1/2}, v_h\right) = \left(S_2^1 - S_2^0, v_h\right) + \left(T_1^1 - T_1^0, v_h\right). \tag{3.72}$$

By Lemma 3.3 and (3.67), it follows that

$$\begin{aligned}
\|T_1^1 - T_1^0\| &= 2\left\||u^1|^2 - |u_h^1|^2 - |u^0|^2 + |u_h^0|^2\right\| \\
&\le 2\|u^1 - u^0\|_\infty \|u^1 - u_h^1\| \\
&\quad + \left(\|u_h^1\|_\infty + \|u_h^0\|_\infty + \|u^1 - u^0\|_\infty\right)\left\|u_h^0 - u_h^1 - u^0 + u^1\right\| \\
&\le C\|u^1 - u^0\|_\infty\|e_u^1\| + C\|e_u^1 - e_u^0\| + C\|u^1 - u^0\|_\infty\|e_u^1 - e_u^0\| \\
&\le C\|e_u^1 - e_u^0\| + C\|u^1 - u^0\|_\infty\left(\|e_u^1 - e_u^0\| + \|e_u^1\|\right) \\
&\le C\|e_u^1 - e_u^0\| + C\tau\|e_u^1 - e_u^0\| + C\tau\|e_u^1\| \le C\|e_u^1 - e_u^0\| + C\tau\|e_u^1\| \\
&\le C\tau\|D_\tau\eta_u^1\| + C\tau\|\eta_u^1\| + C\tau h^{k+1}.
\end{aligned} \tag{3.73}$$

Note that

$$\begin{aligned}
\|S_2^1 - S_2^0\| &= \left\|\left(S_1^1 - (\xi_\Psi^{3/2} + \xi_\Psi^{1/2})\right) - \left(S_1^0 - (\xi_\Psi^{1/2} + \xi_\Psi^{-1/2})\right)\right\| \\
&\le \left\|S_1^1 - S_1^0\right\| + \left\|\xi_\Psi^{3/2} - \xi_\Psi^{-1/2}\right\|.
\end{aligned} \tag{3.74}$$

By using the Taylor expression at t_1 and the regularity assumption (3.34),

$$\begin{aligned}
\left\|S_1^1 - S_1^0\right\| = \left\|\Psi^{3/2} - 2\Psi^1 + 2\Psi^0 - \Psi^{-1/2}\right\| \le \Bigg\|\frac{1}{2}\int_{t_1}^{t_{3/2}}(t_{3/2} - t)^2\Psi_{ttt}(x,t)\,\mathrm{d}t \\
+ \int_{t_1}^{t_0}(t_0 - t)^2\Psi_{ttt}(x,t)\,\mathrm{d}t - \frac{1}{2}\int_{t_1}^{t_{-1/2}}(t_{-1/2} - t)^2\Psi_{ttt}(x,t)\,\mathrm{d}t\Bigg\| \le C\tau^3.
\end{aligned} \tag{3.75}$$

By using the mean value theorem,

$$\|\xi_\Psi^{3/2} - \xi_\Psi^{-1/2}\| = 2\tau \left\| \left(\frac{\Psi^{3/2} - \Psi^{-1/2}}{2\tau}\right) - \mathrm{R}_h \left(\frac{\Psi^{3/2} - \Psi^{-1/2}}{2\tau}\right) \right\|$$
$$\leq C\tau h^{k+1} \left\| \frac{\Psi^{3/2} - \Psi^{-1/2}}{2\tau} \right\|_{k+1} \leq C\tau h^{k+1} \left\| \Psi_t(x, t^*) \right\|_{k+1}, \tag{3.76}$$

where $t^* \in (t_{-1/2}, t_{3/2})$. Plugging (3.75) and (3.76) into (3.74) leads to

$$\left\| S_2^1 - S_2^0 \right\| \leq C\tau(\tau^2 + h^{k+1}). \tag{3.77}$$

Then, taking $v_h = \eta_\Psi^{3/2} + \eta_\Psi^{-1/2}$ in (3.72) yields

$$\|\eta_\Psi^{3/2}\|^2 - \|\eta_\Psi^{-1/2}\|^2 \leq \left(\|S_2^1 - S_2^0\| + \|T_1^1 - T_1^0\| \right) \|\eta_\Psi^{3/2} + \eta_\Psi^{-1/2}\|.$$

By (3.56), (3.65), (3.66), (3.73) and (3.77), the following inequality holds

$$\|\eta_\Psi^{3/2}\| \leq \|\eta_\Psi^{-1/2}\| + \|S_2^1 - S_2^0\| + \|T_1^1 - T_1^0\|$$
$$\leq C\tau \|D_\tau \eta_u^1\| + C\tau \|\eta_u^1\| + C\tau(\tau^2 + h^{k+1}) \leq C(\tau^2 + h^{k+1}), \tag{3.78}$$

which together with the projection error (3.3) for $\|\xi_\Psi^{3/2}\|$ yields

$$\|e_\Psi^{3/2}\| \leq \|\eta_\Psi^{3/2}\| + \|\xi_\Psi^{3/2}\| \leq C(\tau^2 + h^{k+1}). \tag{3.79}$$

By applying the Lemma 3.4 to the (3.38c) with $n = 1$, we also obtain the following error estimate

$$\|e_\Phi^{3/2}\| \leq C\|e_\Psi^{3/2}\| + Ch^{k+1} \leq C(\tau^2 + h^{k+1}). \tag{3.80}$$

By using the inverse inequality (3.4), (3.35) and (3.78), there exist $h_3 > 0$ such that when $h < h_3$,

$$\|\Psi_h^{3/2}\|_\infty \leq \|\mathrm{R}_h \Psi^{3/2}\|_\infty + \|\eta_\Psi^{3/2}\|_\infty \leq \|\mathrm{R}_h \Psi^{3/2}\|_\infty + Ch^{-1}\|\eta_\Psi^{3/2}\| \leq D_\Psi + C_\Psi h \leq D_\Psi + 1, \tag{3.81}$$

$$\|\Phi_h^{3/2}\|_\infty \leq \|\mathrm{R}_h \Phi^{3/2}\|_\infty + Ch^{-1}\|\eta_\Phi^{3/2}\| \leq D_\Phi + C_\Psi h \leq D_\Phi + 1. \tag{3.82}$$

Taking $\omega_h = \overline{\eta}_u^{3/2}$ in (3.43b) with $n = 1$ gives

$$\mathbf{i}\left\langle D_\tau \eta_u^2, \overline{\eta}_u^{3/2} \right\rangle = A_0 \left(\overline{\eta}_u^{3/2}, \overline{\eta}_u^{3/2} \right) + \left\langle G_1^2, \overline{\eta}_u^{3/2} \right\rangle + \left\langle R_2^2, \overline{\eta}_u^{3/2} \right\rangle,$$

where the imaginary part yields

$$\begin{aligned}\frac{1}{2\tau}\left(\|\eta_u^2\|^2-\|\eta_u^1\|^2\right) &= \mathrm{Im}\left\langle G_1^2+R_2^2,\overline{\eta}_u^{3/2}\right\rangle\\ &\le \left\|G_1^2+R_2^2\right\|\left\|\overline{\eta}_u^{3/2}\right\|\\ &\le \frac{1}{2}\left\|G_1^2+R_2^2\right\|^2+\frac{1}{2}\left\|\overline{\eta}_u^{3/2}\right\|^2\\ &= \frac{1}{2}\left(\left\|G_1^2\right\|^2+\left\|R_2^2\right\|^2+2\left\|G_1^2\right\|\left\|R_2^2\right\|\right)+\frac{1}{8}\left\|\eta_u^2+\eta_u^1\right\|^2\\ &\le \left\|G_1^2\right\|^2+\left\|R_2^2\right\|^2+\frac{1}{4}\left(\|\eta_u^2\|^2+\|\eta_u^1\|^2\right). \end{aligned} \tag{3.83}$$

By applying (3.35), (3.79)–(3.82), we have

$$\begin{aligned}\left\|G_1^2\right\| &\le \|\overline{u}^{3/2}\|_\infty\left(\|e_\Phi^{3/2}\|+\|e_\Psi^{3/2}\|\right)+\left(\|\Phi_h^{3/2}\|_\infty+\|V(x)\|_\infty+\|\Psi_h^{3/2}\|_\infty\right)\|\overline{e}_u^{3/2}\|\\ &\le C\left(\|\eta_u^2\|+\|\eta_u^1\|\right)+C\left(\tau^2+h^{k+1}\right). \end{aligned} \tag{3.84}$$

Plugging (3.46) and (3.84) into (3.83) gives

$$\frac{1}{2\tau}\left(\|\eta_u^2\|^2-\|\eta_u^1\|^2\right)\le C_2\left(\|\eta_u^2\|^2+\|\eta_u^1\|^2\right)+C(\tau^2+h^{k+1})^2. \tag{3.85}$$

In view of (3.65), (3.85) leads to

$$\left\|\eta_u^2\right\|\le C\tau(\tau^2+h^{k+1}), \tag{3.86}$$

as long as $\tau<\tau_2:=1/(2C_2)$. Since $0<\tau<1$, we then conclude that

$$\left\|e_u^2\right\|\le\|\xi_u^2\|+\|\eta_u^2\|\le C(\tau^2+h^{k+1}).$$

By using the triangle inequality and (3.86) gives

$$\|D_\tau\eta_u^2\|=\frac{1}{\tau}\left\|\eta_u^2-\eta_u^1\right\|\le\frac{1}{\tau}\left(\left\|\eta_u^2\right\|+\left\|\eta_u^1\right\|\right)\le C(\tau^2+h^{k+1}). \tag{3.87}$$

With (3.4), (3.35) and (3.86), there exists $h_4>0$ such that when $h<h_4$,

$$\|u_h^2\|_\infty\le\|\mathrm{R}_hu^2\|_\infty+\|\mathrm{R}_hu^2-u_h^2\|_\infty\le\|\mathrm{R}_hu^2\|_\infty+Ch^{-1}\|\eta_u^2\|\le D_u+1. \tag{3.88}$$

Next, we take the difference between t_2 and t_1 of (3.43a) with $n = 2$ and $v_h = \eta_\Psi^{5/2} + \eta_\Psi^{1/2}$, which yields

$$\|\eta_\Psi^{5/2}\|^2 - \|\eta_\Psi^{1/2}\|^2 \le \left(\|S_2^2 - S_2^1\| + \|T_1^2 - T_1^1\|\right)\|\eta_\Psi^{5/2} + \eta_\Psi^{1/2}\|.$$

Similar to (3.73)–(3.77), by applying Lemma 3.6, (3.66), (3.67), (3.87) and (3.88), we have

$$\begin{aligned}\|S_2^2 - S_2^1\| &= \left\|\left(S_1^2 - (\xi_\Psi^{5/2} + \xi_\Psi^{3/2})\right) - \left(S_1^1 - (\xi_\Psi^{3/2} + \xi_\Psi^{1/2})\right)\right\| \\ &\le \left\|S_1^2 - S_1^1\right\| + \left\|\xi_\Psi^{5/2} - \xi_\Psi^{1/2}\right\| \\ &\le C\tau(\tau^2 + h^{k+1}),\end{aligned} \tag{3.89}$$

and

$$\|T_1^2 - T_1^1\| \le C\tau\|D_\tau\eta_u^2\| + C\tau\|D_\tau\eta_u^1\| + C\tau\|\eta_u^2\| + C\tau h^{k+1} \le C(\tau^2 + h^{k+1}). \tag{3.90}$$

By combining with (3.57), (3.89) and (3.90), we have

$$\|\eta_\Psi^{5/2}\| \le \|\eta_\Psi^{1/2}\| + \|S_2^2 - S_2^1\| + \|T_1^2 - T_1^1\| \le C(\tau^2 + h^{k+1}). \tag{3.91}$$

With the projection estimate (3.3), we get

$$\|e_\Psi^{5/2}\| \le \|\eta_\Psi^{5/2}\| + \|\xi_\Psi^{5/2}\| \le C(\tau^2 + h^{k+1}). \tag{3.92}$$

Applying the Lemma 3.4 to the (3.38c) with $n = 2$, it holds

$$\|e_\Phi^{5/2}\| \le C\|e_\Psi^{5/2}\| + Ch^{k+1} \le C(\tau^2 + h^{k+1}). \tag{3.93}$$

Step 3. We assume that the estimates in (3.48)–(3.50) hold for $0 \le n \le m$ with $m \ge 2$ as follows

$$\max_{0\le n\le m}\left\|e_u^n\right\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.94}$$

$$\max_{1\le n\le m}\left\|D_\tau\eta_u^n\right\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.95}$$

$$\max_{0\le n\le m}\left\|e_\Psi^{n+1/2}\right\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.96}$$

$$\max_{0\le n\le m}\left\|e_\Phi^{n+1/2}\right\| \le C(\tau^2 + h^{k+1}). \tag{3.97}$$

By using (3.35) and the inverse inequality (3.4), there exists $h_5 > 0$ such that when $h < h_5$, it holds for $0 \le n \le m$,

$$\|u_h^n\|_\infty \le \|\mathrm{R}_h u^n\|_\infty + 1 \le D_u + 1, \tag{3.98}$$

$$\|\Psi_h^{n+1/2}\|_\infty \le \|\mathrm{R}_h \Psi^{n+1/2}\|_\infty + 1 \le D_\Psi + 1, \tag{3.99}$$

$$\|\Phi_h^{n+1/2}\|_\infty \le \|\mathrm{R}_h \Phi^{n+1/2}\|_\infty + 1 \le D_\Phi + 1. \tag{3.100}$$

Next, we establish that the estimates (3.94)–(3.97) also hold for $n = m + 1$. Taking the difference between (3.43b) at t_{m+1} and t_{m-1} that gives

$$\begin{aligned}
\mathbf{i}\langle D_\tau \eta_u^{m+1} - D_\tau \eta_u^{m-1}, \omega_h\rangle &= A_0(\overline{\eta}_u^{m+1/2} - \overline{\eta}_u^{m-3/2}, \omega_h) \\
&\quad + \langle G_1^{m+1} - G_1^{m-1}, \omega_h\rangle + \langle R_2^{m+1} - R_2^{m-1}, \omega_h\rangle \\
&= \frac{\tau}{2} A_0(D_\tau \eta_u^{m+1} + 2D_\tau \eta_u^m + D_\tau \eta_u^{m-1}, \omega_h) \\
&\quad + \langle G_1^{m+1} - G_1^{m-1}, \omega_h\rangle + \langle R_2^{m+1} - R_2^{m-1}, \omega_h\rangle,
\end{aligned}$$

which can be written pointwisely as

$$D_\tau \eta_u^{m+1} - D_\tau \eta_u^{m-1} = \mathbf{i}\frac{\tau}{2}\Delta_h \left(D_\tau \eta_u^{m+1} + 2D_\tau \eta_u^m + D_\tau \eta_u^{m-1}\right) + \Gamma_1^{m+1} + \Gamma_2^{m+1}, \tag{3.101}$$

where $\Gamma_1^{m+1} := -\mathbf{i}P_h(R_2^{m+1} - R_2^{m-1})$, $\Gamma_2^{m+1} := -\mathbf{i}P_h(G_1^{m+1} - G_1^{m-1})$ and $P_h : \mathbf{L}^2(\Omega) \to V_h^c$ denotes the L^2 projection. By applying $\mathbf{S}_h^{-1}$ to (3.101) and using the operators introduced in (3.20), (3.21) and (3.25), it follows

$$D_\tau \eta_u^{m+1} = (\mathbf{B}_h - \mathbf{I}_h) D_\tau \eta_u^m + \mathbf{B}_h D_\tau \eta_u^{m-1} + \mathbf{S}_h^{-1} \sum_{j=1}^{2} \Gamma_j^{m+1}. \tag{3.102}$$

Applying Lemma 3.6 to (3.102) gives

$$\|D_\tau \eta_u^{m+1}\| + \|D_\tau \eta_u^m\| \le 2\left\|\mathbf{S}_h(D_\tau \eta_u^2)\right\| + 2\left\|\mathbf{S}_h(D_\tau \eta_u^1)\right\| + 2\sum_{n=2}^{m}\left(\|\Gamma_1^{n+1}\| + \|\Gamma_2^{n+1}\|\right). \tag{3.103}$$

Step 4. In this step, we use the standard integral remainder of Taylor expansion to estimate $\|\Gamma_1^{n+1}\|$ and $\|\Gamma_2^{n+1}\|$ in (3.103) based on the regularity assumption in (3.34). By definition,

$$\|\Gamma_1^{n+1}\| \le \|R_2^{n+1} - R_2^{n-1}\| \le \|R_1^{n+1} - R_1^{n-1}\| + \|D_\tau \xi_u^{n+1} - D_\tau \xi_u^{n-1}\|, \tag{3.104}$$

$$\|\varGamma_2^{n+1}\| \leq \|G_1^{n+1} - G_1^{n-1}\|. \tag{3.105}$$

We first estimate $\|\varGamma_1^{n+1}\|$. From (3.37), we obtain

$$\begin{aligned}\|R_1^{n+1} - R_1^n\| \leq & \left\|(u_t^{n+1/2} - D_\tau u^{n+1}) - (u_t^{n-1/2} - D_\tau u^n)\right\| \\ & + \left\|\varDelta(\overline{u}^{n+1/2} - u^{n+1/2} - \overline{u}^{n-1/2} + u^{n-1/2})\right\| \\ & + \Big\|(\varPhi^{n+1/2} + V(x) + \varPsi^{n+1/2})(u^{n+1/2} - \overline{u}^{n+1/2}) \\ & \quad - (\varPhi^{n-1/2} + V(x) + \varPsi^{n-1/2})(u^{n-1/2} - \overline{u}^{n-1/2})\Big\|. \end{aligned} \tag{3.106}$$

Next, we apply the Taylor expression to each term in (3.106) at t_n. For the first term, it follows

$$\begin{aligned} & \left\|(u_t^{n+1/2} - D_\tau u^{n+1}) - (u_t^{n-1/2} - D_\tau u^n)\right\| \\ & = \left\|u_t^{n+1/2} - u_t^{n-1/2} - \frac{1}{\tau}\left(u^{n+1} - 2u^n + u^{n-1}\right)\right\| \\ & \leq \Big\|\frac{1}{2!}\int_{t_n}^{t_{n+1/2}} (t_{n+1/2} - t)^2 u_{tttt}(t)\,\mathrm{d}t - \frac{1}{2!}\int_{t_n}^{t_{n-1/2}} (t_{n-1/2} - t)^2 u_{tttt}(t)\,\mathrm{d}t \\ & \quad - \frac{1}{3!} \times \frac{1}{\tau}\int_{t_n}^{t_{n+1}} (t_{n+1} - t)^3 u_{tttt}(t)\,\mathrm{d}t - \frac{1}{3!} \times \frac{1}{\tau}\int_{t_n}^{t_{n-1}} (t_{n-1} - t)^3 u_{tttt}(t)\,\mathrm{d}t\Big\| \\ & \leq \Big\|\frac{\tau^3}{16}\int_0^1 (1-s)^2\, u_{tttt}\left(t_n + \frac{\tau}{2}s\right)\,\mathrm{d}s + \frac{\tau^3}{16}\int_0^1 (1-s)^2\, u_{tttt}\left(t_n - \frac{\tau}{2}s\right)\,\mathrm{d}s \\ & \quad - \frac{\tau^3}{6}\int_0^1 (1-s)^3 u_{tttt}(t_n + \tau s)\,\mathrm{d}s - \frac{\tau^3}{6}\int_0^1 (1-s)^3 u_{tttt}(t_n - \tau s)\,\mathrm{d}s\Big\| \leq C\tau^3. \end{aligned} \tag{3.107}$$

For the second term, it holds

$$\begin{aligned} & \left\|\varDelta(\overline{u}^{n+1/2} - u^{n+1/2} - \overline{u}^{n-1/2} + u^{n-1/2})\right\| \\ & \leq \Big\|\frac{1}{2} \times \frac{1}{2!}\int_{t_n}^{t_{n+1}} (t_{n+1} - t)^2 u_{ttt}(t)\,\mathrm{d}t - \frac{1}{2!}\int_{t_n}^{t_{n+1/2}} (t_{n+1/2} - t)^2 u_{ttt}(t)\,\mathrm{d}t \\ & \quad + \frac{1}{2} \times \frac{1}{2!}\int_{t_n}^{t_{n-1}} (t_{n-1} - t)^2 u_{ttt}(t)\,\mathrm{d}t + \frac{1}{2!}\int_{t_n}^{t_{n-1/2}} (t_{n-1/2} - t)^2 u_{ttt}(t)\,\mathrm{d}t\Big\|_{H^2} \leq C\tau^3. \end{aligned} \tag{3.108}$$

For the third item, it follows

$$\begin{aligned}&\left\|(\Phi^{n+1/2}+V+\Psi^{n+1/2})(u^{n+1/2}-\overline{u}^{n+1/2})-(\Phi^{n-1/2}+V+\Psi^{n-1/2})(u^{n-1/2}-\overline{u}^{n-1/2})\right\|\\&\quad\le\left\|\Phi^{n+1/2}+V(x)+\Psi^{n+1/2}\right\|_\infty\left\|u^{n+1/2}-\overline{u}^{n+1/2}-u^{n-1/2}+\overline{u}^{n-1/2}\right\|\\&\quad+\left\|(\Phi^{n+1/2}-\Phi^{n-1/2})+(\Psi^{n+1/2}-\Psi^{n-1/2})\right\|_\infty\left\|u^{n-1/2}-\overline{u}^{n-1/2}\right\|.\end{aligned}\tag{3.109}$$

Similar to (3.108), it holds

$$\left\|u^{n-1/2}-\overline{u}^{n-1/2}\right\|\le C\tau^2,\tag{3.110}$$

$$\left\|u^{n+1/2}-\overline{u}^{n+1/2}-u^{n-1/2}+\overline{u}^{n-1/2}\right\|\le C\tau^3.\tag{3.111}$$

In addition, Taylor's theorem and the regularity assumption (3.34) imply

$$\left\|(\Phi^{n+1/2}-\Phi^{n-1/2})+(\Psi^{n+1/2}-\Psi^{n-1/2})\right\|_\infty=\left\|\int_{t_{n-1/2}}^{t_{n+1/2}}\Phi_t(s)\,\mathrm{d}s+\int_{t_{n-1/2}}^{t_{n+1/2}}\Psi_t(s)\,\mathrm{d}s\right\|_\infty\le C\tau.\tag{3.112}$$

Therefore, using (3.107)–(3.112) and the regularity assumption (3.35), we conclude

$$\left\|R_1^{n+1}-R_1^n\right\|\le C\tau^3.\tag{3.113}$$

Moreover, by using the projection error estimate (3.3), it follows

$$\begin{aligned}\|D_\tau\xi_u^{n+1}-D_\tau\xi_u^{n-1}\|&=\left\|\mathrm{R}_h\left(\frac{u^{n+1}-u^n-u^{n-1}+u^{n-2}}{\tau}\right)-\frac{u^{n+1}-u^n-u^{n-1}+u^{n-2}}{\tau}\right\|\\&\le C\frac{1}{\tau}\int_0^\tau\left(\int_{t_{n-2}+s}^{t_n+s}\left\|\mathrm{R}_hu_{tt}(t)-u_{tt}(t)\right\|\,\mathrm{d}t\right)\mathrm{d}s\le C\tau h^{k+1},\end{aligned}\tag{3.114}$$

where we have used

$$u^{n+1}-u^n-u^{n-1}+u^{n-2}=\int_0^\tau\left(\int_{t_{n-2}+s}^{t_n+s}u_{tt}(t)\,\mathrm{d}t\right)\mathrm{d}s.\tag{3.115}$$

(3.113) and (3.114) together with (3.104) imply

$$\|\Gamma_1^{n+1}\|\le\|R_1^{n+1}-R_1^n\|+\|R_1^n-R_1^{n-1}\|+\|D_\tau\xi_u^{n+1}-D_\tau\xi_u^{n-1}\|\le C\tau(\tau^2+h^{k+1}).\tag{3.116}$$

Next, we estimate $\|\Gamma_2^{n+1}\|$. From (3.39), it follows

$$\begin{aligned}\left\|G_1^{n+1}-G_1^{n-1}\right\| \le & \left\|(\Psi^{n+1/2}\overline{u}^{n+1/2}-\Psi_h^{n+1/2}\overline{u}_h^{n+1/2})-(\Psi^{n-3/2}\overline{u}^{n-3/2}-\Psi_h^{n-3/2}\overline{u}_h^{n-3/2})\right\| \\ & +\|V(x)\|_\infty\left\|(\overline{u}^{n+1/2}-\overline{u}_h^{n+1/2})-(\overline{u}^{n-3/2}-\overline{u}_h^{n-3/2})\right\| \\ & +\left\|(\Phi^{n+1/2}\overline{u}^{n+1/2}-\Phi_h^{n+1/2}\overline{u}_h^{n+1/2})-(\Phi^{n-3/2}\overline{u}^{n-3/2}-\Phi_h^{n-3/2}\overline{u}_h^{n-3/2})\right\|.\end{aligned} \tag{3.117}$$

For the first term in (3.117),

$$\begin{aligned}&\left\|(\Psi^{n+1/2}\overline{u}^{n+1/2}-\Psi_h^{n+1/2}\overline{u}_h^{n+1/2})-(\Psi^{n-3/2}\overline{u}^{n-3/2}-\Psi_h^{n-3/2}\overline{u}_h^{n-3/2})\right\| \\ \le & \left\|(\Psi^{n+1/2}-\Psi^{n-3/2})(\overline{u}^{n-3/2}-\overline{u}_h^{n-3/2})\right\|+\left\|(\Psi^{n+1/2}-\Psi_h^{n+1/2})(\overline{u}^{n+1/2}-\overline{u}^{n-3/2})\right\| \\ & +\left\|\overline{u}_h^{n-3/2}(\Psi^{n+1/2}-\Psi^{n-3/2}-\Psi_h^{n+1/2}+\Psi_h^{n-3/2})\right\| \\ & +\left\|\Psi_h^{n+1/2}\left(\overline{u}^{n+1/2}-\overline{u}^{n-3/2}-\overline{u}_h^{n+1/2}+\overline{u}_h^{n-3/2}\right)\right\| := K_1+K_2+K_3+K_4.\end{aligned} \tag{3.118}$$

By the Taylor expansion, the split (3.40), (3.41) and the projection errors, it is easy to obtain

$$K_1 \le \frac{C\tau}{2}\left\|u^{n-1}+u^{n-2}-u_h^{n-1}-u_h^{n-2}\right\| \le C\tau\left(\|\eta_u^{n-1}\|+\|\eta_u^{n-2}\|\right)+C\tau h^{k+1}, \tag{3.119}$$

$$K_2 \le \left\|\Psi^{n+1/2}-\Psi_h^{n+1/2}\right\|\left\|\frac{(u^{n+1}+u^n)-(u^{n-1}+u^{n-2})}{2}\right\| \le C\tau\left(\tau^2+h^{k+1}\right), \tag{3.120}$$

where we have used (3.96). By (3.98), and using the mean value theorem, it holds

$$\begin{aligned}K_3 \le & C\|e_\Psi^{n+1/2}-e_\Psi^{n-3/2}\| \le C\|\eta_\Psi^{n+1/2}-\eta_\Psi^{n-3/2}\|+C\tau\left\|\frac{\xi_\Psi^{n+1/2}-\xi_\Psi^{n-3/2}}{\tau}\right\| \\ \le & C\|\eta_\Psi^{n+1/2}-\eta_\Psi^{n-3/2}\|+C\tau h^{k+1}.\end{aligned} \tag{3.121}$$

Then, taking the difference of (3.43a) between two time levels and using (3.41) yields

$$(\eta_\Psi^{n+1/2}-\eta_\Psi^{n-3/2},v_h)=(S_2^n-S_2^{n-1},v_h)+(T_1^n-T_1^{n-1},v_h). \tag{3.122}$$

Similar to (3.73) and (3.77), it follows

$$\|T_1^n-T_1^{n-1}\| \le C\tau\|D_\tau\eta_u^n\|+C\tau\|\eta_u^n\|+C\tau h^{k+1}, \tag{3.123}$$

$$\left\| S_2^n - S_2^{n-1} \right\| \le C\tau(\tau^2 + h^{k+1}). \tag{3.124}$$

By setting $v_h = \eta_\Psi^{n+1/2} - \eta_\Psi^{n-3/2}$ in (3.122), applying Cauchy–Schwartz inequality, and using (3.123) and (3.124),

$$\|\eta_\Psi^{n+1/2} - \eta_\Psi^{n-3/2}\| \quad \le \|S_2^n - S_2^{n-1}\| + \|T_1^n - T_1^{n-1}\| \le C\tau \left(\|D_\tau \eta_u^n\| + \|\eta_u^n\|\right) + C\tau(\tau^2 + h^{k+1}). \tag{3.125}$$

Plugging (3.125) into (3.121) gives

$$K_3 \le C\tau \left(\|D_\tau \eta_u^n\| + \|\eta_u^n\|\right) + C\tau(\tau^2 + h^{k+1}). \tag{3.126}$$

By (3.44) and (3.99), K_4 in (3.118) gives

$$\begin{aligned} K_4 \le & C \left\| (\overline{u}^{n+1/2} - \overline{u}_h^{n+1/2}) - (\overline{u}^{n-3/2} - \overline{u}_h^{n-3/2}) \right\| \\ \le & C\tau \left\| D_\tau e_u^{n+1} + 2D_\tau e_u^n + D_\tau e_u^{n-1} \right\| \\ \le & C\tau \left(\left\| D_\tau \eta_u^{n+1} \right\| + \left\| D_\tau \eta_u^n \right\| + \left\| D_\tau \eta_u^{n-1} \right\| \right) + C\tau h^{k+1}. \end{aligned} \tag{3.127}$$

Plugging (3.119), (3.120), (3.126) and (3.127) into (3.118) implies

$$\begin{aligned} & \left\| (\Psi^{n+1/2}\overline{u}^{n+1/2} - \Psi_h^{n+1/2}\overline{u}_h^{n+1/2}) - (\Psi^{n-3/2}\overline{u}^{n-3/2} - \Psi_h^{n-3/2}\overline{u}_h^{n-3/2}) \right\| \\ & \le C\tau \left(\|D_\tau \eta_u^{n+1}\| + \|D_\tau \eta_u^n\| + \|D_\tau \eta_u^{n-1}\| + \|\eta_u^n\| + \|\eta_u^{n-1}\| + \|\eta_u^{n-2}\| \right) + C\tau(\tau^2 + h^{k+1}). \end{aligned} \tag{3.128}$$

Similar to K_4 in (3.127), the second term in (3.117) yields

$$\left\| \overline{e}_u^{n+1/2} - \overline{e}_u^{n-3/2} \right\| \le C\tau \left(\left\| D_\tau \eta_u^{n+1} \right\| + \left\| D_\tau \eta_u^n \right\| + \left\| D_\tau \eta_u^{n-1} \right\| \right) + C\tau h^{k+1}. \tag{3.129}$$

Similar to (3.118), the estimate of the third term in (3.117) is given by

$$\begin{aligned} & \left\| (\Phi^{n+1/2}\overline{u}^{n+1/2} - \Phi_h^{n+1/2}\overline{u}_h^{n+1/2}) - (\Phi^{n-3/2}\overline{u}^{n-3/2} - \Phi_h^{n-3/2}\overline{u}_h^{n-3/2}) \right\| \\ & \le C\tau(\tau^2 + h^{k+1}) + C\tau \left(\|D_\tau \eta_u^{n+1}\| + \|D_\tau \eta_u^n\| + \|D_\tau \eta_u^{n-1}\| + \|\eta_u^n\| + \|\eta_u^{n-1}\| + \|\eta_u^{n-2}\| \right). \end{aligned} \tag{3.130}$$

Thereby, by (3.128), (3.129) and (3.130), it holds

$$\|\Gamma_2^{n+1}\| \leq \left\|G_1^{n+1} - G_1^{n-1}\right\| \leq C\tau\left(\|\eta_u^n\| + \|\eta_u^{n-1}\| + \|\eta_u^{n-2}\|\right) \\ + C\tau\left(\|D_\tau\eta_u^{n+1}\| + \|D_\tau\eta_u^n\| + \|D_\tau\eta_u^{n-1}\|\right) + C\tau(\tau^2 + h^{k+1}). \tag{3.131}$$

Step 5. In this step, we show that the estimates (3.94) and (3.95) hold for $n = m+1$, that is

$$\left\|e_u^{m+1}\right\| \leq C\left(\tau^2 + h^{k+1}\right), \tag{3.132}$$

$$\left\|D_\tau\eta_u^{m+1}\right\| \leq C\left(\tau^2 + h^{k+1}\right). \tag{3.133}$$

Taking $n = 0$ in (3.43b) and using (3.19) and $\eta_u^0 = 0$ yield

$$\frac{1}{\tau}\langle \mathbf{S}_h\eta_u^1, \omega_h\rangle = -\mathbf{i}\langle G_1^1, \omega_h\rangle - \mathbf{i}\langle R_2^1, \omega_h\rangle, \tag{3.134}$$

which by taking $\omega_h = \mathbf{S}_h\eta_u^1$ in (3.134) and using the estimates (3.46), (3.63) and (3.65) yields

$$\|\mathbf{S}_h\eta_u^1\| \leq \tau\left(\|G_1^1\| + \|R_2^1\|\right) \leq C\tau(\tau^2 + h^{k+1}). \tag{3.135}$$

Using $\eta_u^0 = 0$ again gives

$$\|\mathbf{S}_h(D_\tau\eta_u^1)\| = \frac{1}{\tau}\|\mathbf{S}_h\eta_u^1\| \leq C(\tau^2 + h^{k+1}). \tag{3.136}$$

Moreover, it also holds

$$\|\mathbf{S}_h\eta_u^2\| \leq \|\mathbf{T}_h\eta_u^1\| + C\tau\left(\|G_1^2\| + \|R_2^2\|\right) \leq \|(2\mathbf{I}_h - \mathbf{S}_h)\eta_u^1\| + C\tau\left(\|G_1^2\| + \|R_2^2\|\right) \\ \leq 2\|\eta_u^1\| + \|\mathbf{S}_h\eta_u^1\| + C\tau(\tau^2 + h^{k+1}), \tag{3.137}$$

where we have used (3.46), (3.65), (3.80), (3.135) and

$$\left\|G_1^2\right\| \leq \|\overline{u}^{3/2}\|_\infty\left(\|e_\Phi^{3/2}\| + \|e_\Psi^{3/2}\|\right) + \left(\|\Phi_h^{3/2}\|_\infty + \|V(x)\|_\infty + \|\Psi_h^{3/2}\|_\infty\right)\|\overline{e}_u^{3/2}\| \\ \leq C\left(\|\eta_u^2\| + \|\eta_u^1\|\right) + C\left(\tau^2 + h^{k+1}\right). \tag{3.138}$$

Similar to (3.64), by using (3.46) and (3.138), it holds

$$\begin{aligned}\frac{1}{2\tau}\left(\|\eta_u^2\|^2-\|\eta_u^1\|^2\right)&=\mathrm{Im}\left\langle G_1^2+R_2^2,\overline{\eta}_u^{3/2}\right\rangle\le\left\|G_1^2+R_2^2\right\|\left\|\overline{\eta}_u^{3/2}\right\|\\&\le\frac{1}{2}\left\|G_1^2+R_2^2\right\|^2+\frac{1}{2}\left\|\overline{\eta}_u^{3/2}\right\|^2\\&\le\frac{1}{2}\left(\left\|G_1^2\right\|^2+\left\|R_2^2\right\|^2+2\left\|G_1^2\right\|\left\|R_2^2\right\|\right)+\frac{1}{8}\left\|\eta_u^2+\eta_u^1\right\|^2\\&\le\left\|G_1^2\right\|^2+\left\|R_2^2\right\|^2+\frac{1}{4}\left(\|\eta_u^2\|^2+\|\eta_u^1\|^2\right)\\&\le C\left(\|\eta_u^2\|^2+\|\eta_u^1\|^2\right)+C(\tau^2+h^{k+1})^2.\end{aligned}\tag{3.139}$$

As long as $\tau<\tau_3:=\min\{\tau_1,1/(2C)\}$, plugging (3.65) into (3.139) implies

$$\|\eta_u^2\|\le C\tau(\tau^2+h^{k+1}).\tag{3.140}$$

Then, it holds

$$\|\mathbf{S}_h\eta_u^2\|\le C\tau(\tau^2+h^{k+1}).\tag{3.141}$$

By using (3.135) and (3.141),

$$\|\mathbf{S}_h(D_\tau\eta_u^2)\|\le\frac{1}{\tau}\left(\|\mathbf{S}_h\eta_u^2\|+\|\mathbf{S}_h\eta_u^1\|\right)\le C(\tau^2+h^{k+1}).\tag{3.142}$$

Plugging (3.116), (3.131), (3.136) and (3.142) into (3.103) and using initial estimates in Step 1 yield

$$\|D_\tau\eta_u^{m+1}\|+\|D_\tau\eta_u^m\|\le C\tau\sum_{n=1}^{m}\left(\|\eta_u^n\|+\|D_\tau\eta_u^{n+1}\|+\|D_\tau\eta_u^n\|\right)+C(\tau^2+h^{k+1}).\tag{3.143}$$

Setting $\omega_h=\overline{\eta}_u^{n+1/2}$ in (3.43b), and taking its imaginary part give

$$\begin{aligned}\frac{1}{2\tau}\left(\|\eta_u^{n+1}\|^2-\|\eta_u^n\|^2\right)&=\mathrm{Im}\left\langle G_1^{n+1},\overline{\eta}_u^{n+1/2}\right\rangle+\mathrm{Im}\left\langle R_2^{n+1},\overline{\eta}_u^{n+1/2}\right\rangle\\&\le\frac{1}{2}\left\|G_1^{n+1}\right\|\|\eta_u^{n+1}+\eta_u^n\|+\frac{1}{2}\left\|R_2^{n+1}\right\|\|\eta_u^{n+1}+\eta_u^n\|.\end{aligned}\tag{3.144}$$

Similar to (3.63), we have

$$\begin{aligned}\|G_1^{n+1}\|\le&\left(\|\Phi_h^{n+1/2}\|_\infty+\|V(x)\|_\infty+\|\Psi_h^{n+1/2}\|_\infty\right)\|\overline{e}_u^{n+1/2}\|\\&+\|\overline{u}^{n+1/2}\|_\infty\left(\|e_\Phi^{n+1/2}\|+\|e_\Psi^{n+1/2}\|\right)\le C\left(\|\eta_u^{n+1}\|+\|\eta_u^n\|\right)+C(\tau^2+h^{k+1}),\end{aligned}\tag{3.145}$$

where we have used the boundedness (3.99) and (3.100), and the estimates (3.96) and (3.97).

Applying (3.46) and (3.145) upon simplification, (3.144) gives

$$\|\eta_u^{n+1}\| - \|\eta_u^n\| \le \tau \left\|G_1^{n+1}\right\| + \tau \left\|R_2^{n+1}\right\| \le C\tau \left(\|\eta_u^{n+1}\| + \|\eta_u^n\|\right) + C\tau \left(\tau^2 + h^{k+1}\right), \tag{3.146}$$

which upon summing up (3.146) from $n = 1$ to m leads to

$$\|\eta_u^{m+1}\| \le \|\eta_u^1\| + C\left(\tau^2 + h^{k+1}\right) + C\tau \sum_{n=1}^{m} \left(\|\eta_u^{n+1}\| + \|\eta_u^n\|\right). \tag{3.147}$$

The summation of (3.143) and (3.147) yields

$$\|\eta_u^{m+1}\| + \|D_\tau \eta_u^{m+1}\| + \|D_\tau \eta_u^m\| \le C\tau \sum_{n=1}^{m} \left(\|\eta_u^{n+1}\| + \|D_\tau \eta_u^{n+1}\| + \|D_\tau \eta_u^n\|\right) + C(\tau^2 + h^{k+1}). \tag{3.148}$$

By Gronwall's inequality in Lemma 3.2, there exists $\tau_4 > 0$independent of m such that when $\tau < \tau_4$,

$$\|\eta_u^{m+1}\| + \|D_\tau \eta_u^{m+1}\| + \|D_\tau \eta_u^m\| \le C\left(\tau^2 + h^{k+1}\right), \tag{3.149}$$

where C depends on T and is independent of m. The estimate (3.149), together with the projection error, implies the estimates (3.132) and (3.133).

Step 6. Last, we show that (3.96) and (3.97) also hold for $n = m + 1$. By (3.4), (3.35), (3.147), and $\tau \le Ch$, there exist $h_6 > 0$, depending on T, but independent of m such that when $h < h_6$,

$$\|u_h^{m+1}\|_\infty \le \|\mathrm{R}_h u^{m+1}\|_\infty + Ch^{-1}\|\eta_u^{m+1}\| \le D_u + C_u h \le D_u + 1.$$

Setting $v_h = \eta_\Psi^{n+1/2} + \eta_\Psi^{n-3/2}$ in (3.122) gives

$$\|\eta_\Psi^{n+1/2}\| - \|\eta_\Psi^{n-3/2}\| \le \|S_2^n - S_2^{n-1}\| + \|T_1^n - T_1^{n-1}\| \le C\tau\left(\|D_\tau \eta_u^n\| + \|\eta_u^n\|\right) + C\tau(\tau^2 + h^{k+1}). \tag{3.150}$$

Summing up (3.150) from $n = 1$ to $n = m + 1$ gives

$$\|\eta_\Psi^{m+3/2}\| \le C\tau \sum_{n=1}^{m+1} \left(\|D_\tau \eta_u^n\| + \|\eta_u^n\|\right) + C(\tau^2 + h^{k+1}) \le C(\tau^2 + h^{k+1}), \tag{3.151}$$

where we have used (3.56), (3.57), (3.94), (3.95) and (3.96) with $n = m$. The estimate (3.151) together with the projection error implies

$$\|e_\Psi^{m+3/2}\| \le \|\xi_\Psi^{m+3/2}\| + \|\eta_\Psi^{m+3/2}\| \le C\left(\tau^2 + h^{k+1}\right). \tag{3.152}$$

Lemma 3.4, (3.152) and (3.38c) further give

$$\|e_{\Phi}^{m+3/2}\| \le C\|e_{\Psi}^{m+3/2}\| + Ch^{k+1} \le C(\tau^2 + h^{k+1}).$$

Therefore, the estimates (3.94)–(3.97) hold for $n = m+1$, if $\tau_0 = \max\{\tau_i\}_{i=1}^4$ and $h_0 = \min\{h_j\}_{j=1}^6$, which depend on T, but are independent of N. This completes the proof. □

4. Extension

The model equation (1.1) without the self-repulsion term $|u|^2u$ and the external potential will degenerate to the SP equation with constant coefficients (Athanassoulis *et al.*, 2023)

$$\mathbf{i}u_t = -\alpha\Delta u + \beta\Phi u, \quad (x,t) \in \Omega \times (0,T], \tag{4.1a}$$

$$\Delta\Phi = |u|^2 - c, \quad x \in \Omega, \tag{4.1b}$$

$$u(x,0) = u_0(x), \quad x \in \Omega, \tag{4.1c}$$

$$u(x,t) = 0 \quad \text{and} \quad \Phi(x) = 0, \quad x \in \partial\Omega, \tag{4.1d}$$

where the parameter $\alpha > 0$, $\beta \in \mathbb{R}$.

Introducing an auxiliary variable Ψ, the system (4.1) can be equivalently expressed as

$$\begin{cases} \Psi = |u|^2, \\ \mathbf{i}u_t = -\alpha\Delta u + \beta\Phi u, \\ \Delta\Phi = \Psi - c. \end{cases} \tag{4.2}$$

Then, the proposed relaxation FEM (2.21) for the nonlinear SP equation (1.1) reduces to the Besse-style relaxation Crank–Nicolson FEM (Athanassoulis *et al.*, 2023),

$$\left(\Psi_h^{n+1/2} + \Psi_h^{n-1/2}, v_h\right) = \left(2|u_h^n|^2, v_h\right), \quad \forall v_h \in V_h, \tag{4.3a}$$

$$\mathbf{i}\left\langle D_\tau u_h^{n+1}, \omega_h\right\rangle = \alpha A_0\left(\overline{u}_h^{n+1/2}, \omega_h\right) + \beta\left\langle \Phi_h^{n+1/2}\overline{u}_h^{n+1/2}, \omega_h\right\rangle, \quad \forall \omega_h \in V_h^c, \tag{4.3b}$$

$$A_1\left(\Phi_h^{n+1/2}, \chi_h\right) = -\left((\Psi_h^{n+1/2} - c), \chi_h\right), \quad \forall \chi_h \in V_h. \tag{4.3c}$$

The following results hold for the scheme above.

LEMMA 4.1. (Athanassoulis *et al.*, 2023) For any $\tau > 0$, the relaxation Crank–Nicolson FEM (4.3) satisfies the discrete conservation for both mass and modified energy with $0 \leq n \leq N-1$, respectively

$$M_h^{n+1} = M_h^0, \tag{4.4}$$

$$E_h^{n+1} = E_h^0, \tag{4.5}$$

where the mass $M_h^{n+1} = \int_\Omega |u_h^{n+1}|^2 \mathrm{d}x$, and the modified energy

$$E_h^{n+1} = \alpha A(u_h^{n+1}, u_h^{n+1}) + \frac{\beta}{2} A(\Phi_h^{n+3/2}, \Phi_h^{n+1/2}).$$

Following the convergence analysis of the proposed scheme (2.21) for the nonlinear SP equation (1.1), we can extend the current error estimates to the scheme (4.3) for the SP equation (4.1). More specifically, we derive the following results.

THEOREM 4.1. Suppose that u, Ψ and Φ satisfy the regularity conditions (3.34). If $\tau \leq Ch$, then there exists a constant $\tau_0 > 0$ and $h_0 > 0$ such that when time step $\tau < \tau_0$ and mesh size $h < h_0$, the solutions of the relaxation Crank–Nicolson finite element scheme (4.3) satisfy the following estimates

$$\max_{0 \leq n \leq N-1} \left\| e_u^{n+1} \right\| \leq C\left(\tau^2 + h^{k+1}\right), \tag{4.6}$$

$$\max_{0 \leq n \leq N-1} \left\| e_\Psi^{n+1/2} \right\| \leq C\left(\tau^2 + h^{k+1}\right), \tag{4.7}$$

$$\max_{0 \leq n \leq N-1} \left\| e_\Phi^{n+1/2} \right\| \leq C(\tau^2 + h^{k+1}). \tag{4.8}$$

The proof is similar to that of Theorem 3.2, thus we omit it here.

REMARK 4.2. The proposed method and the error analysis also have the potential to be applied to other types of equations, such as the Gross–Pitaevskii–Poisson equation (Verma *et al.*, 2021) and the Gross–Pitaevskii–Poisson system (Sakaguchi & Malomed, 2020). The Gross–Pitaevskii–Poisson equation incorporates a nonlocal mean density and additionally conserves the momentum, adding complexity beyond (1.1), while the Gross–Pitaevskii–Poisson system involves the interaction between positive and negative bosonic ions. We leave these explorations for future work.

5. Numerical experiments

In this section, we present numerical experiments to validate our theoretical analysis. This includes an examination of the convergence rates and the conservation properties of the relaxation Crank–Nicolson FEM. All numerical examples are implemented using the FEALPy package (Wei & Huang, 2017-2025).

Table 1 *Time discretization errors with $T = 0.1$ and $V(x_1, x_2) = V_2(x_1, x_2)$*

τ	1.0e-02	5.0e-03	2.5e-03
$\|u_h^{T/\tau} - u_h^{T/(2\tau)}\|$	6.3247e-03	1.5870e-03	3.9710e-04
Order	–	1.99	2.00

Table 2 *Spatial discretization errors with $T = 0.1$ and $V(x_1, x_2) = V_2(x_1, x_2)$*

$\mathbb{Q}^k$	$\|u_{50} - u_{100}\|$	Order	$\|u_{100} - u_{200}\|$	Order	$\|u_{200} - u_{400}\|$	Order
$k = 1$	1.8851e-02	–	4.7363e-03	1.99	1.1856e-03	2.00
$k = 2$	6.4115e-04	–	8.0828e-05	2.99	1.0144e-05	2.99

We consider the two-dimensional SP equation on $\Omega = [-8, 8]^2$,

$$\begin{aligned} \mathbf{i}u_t(x_1, x_2, t) &= -\frac{1}{2}\Delta u + \Phi(x_1, x_2, t)u + V(x_1, x_2)u + |u|^2 u, \quad (x_1, x_2) \in \Omega, \\ -\Delta\Phi(x_1, x_2, t) &= |u|^2 - 1, \quad (x_1, x_2) \in \Omega, \\ u(x_1, x_2, t) &= 0, \quad (x_1, x_2) \in \partial\Omega, \\ \Phi(x_1, x_2, t) &= 0, \quad (x_1, x_2) \in \partial\Omega, \\ u(x_1, x_2, 0) = u_0(x_1, x_2) &= \frac{1}{\sqrt{2\pi}} e^{\frac{-x_1^2 + x_2^2}{4}} (x_1 + \mathbf{i}x_2), \quad (x_1, x_2) \in \Omega. \end{aligned} \tag{5.1}$$

Here, we consider three different external potentials $V(x_1, x_2) = V_i(x_1, x_2)$, $i = 0, 1, 2$ with $V_0(x_1, x_2) = 0$, $V_1(x_1, x_2) = \frac{x_1^2 + x_2^2}{2}$ and $V_2(x_1, x_2) = \frac{x_1^2 - x_2^2}{2}$.

Test case 1. To validate the accuracy and convergence rate of the relaxation Crank–Nicolson FEM, we take the $\mathbb{Q}^k$ polynomials with $k = 1, 2$. As the exact solution is unavailable, we compute the time discretization errors as $\|u_h^{T/\tau} - u_h^{T/(2\tau)}\|$, where $u_h^{T/\tau}$ is finite element solution at $t = T$ with time step τ. Table 1 reports the time discretization error in L^2 norm and the order of accuracy, utilising a sufficiently small fixed spatial mesh size. Based on the obtained results, it is evident that the proposed method exhibits second-order accuracy in time.

Test case 2. In Table 2, we compute the spatial discretization errors $\|u_{NC} - u_{2NC}\|$ between the two-level approximations at final time $T = 0.1$ with a sufficiently small fixed time step, where u_{NC} denotes the numerical solution on $NC \times NC$ meshes. It is observed that the proposed method demonstrates $(k+1)$th order accuracy in space.

Test case 3. Subsequently, we apply the proposed method using a mesh with $NC = 80$ for spatial discretization and a time step of $\tau = 2 \times 10^{-3}$, based on $\mathbb{Q}^2$ polynomials, to verify the performance of our numerical scheme in preserving mass and energy conservation properties. For $0 \leq n \leq N - 1$, we define the mass change and energy change as follows:

$$\text{Mass Change} = \left| \frac{M_h(t_n) - M_h(0)}{M_h(0)} \right|, \quad \text{Energy Change} = \left| \frac{E_h(t_n) - E_h(0)}{E_h(0)} \right|. \tag{5.2}$$

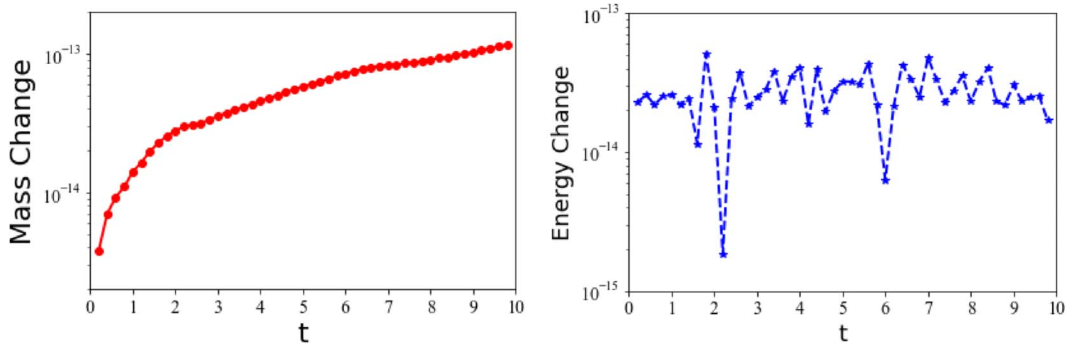


FIG. 1. Evolution of the mass and modified energy with $V(x_1, x_2) = V_0(x_1, x_2)$.

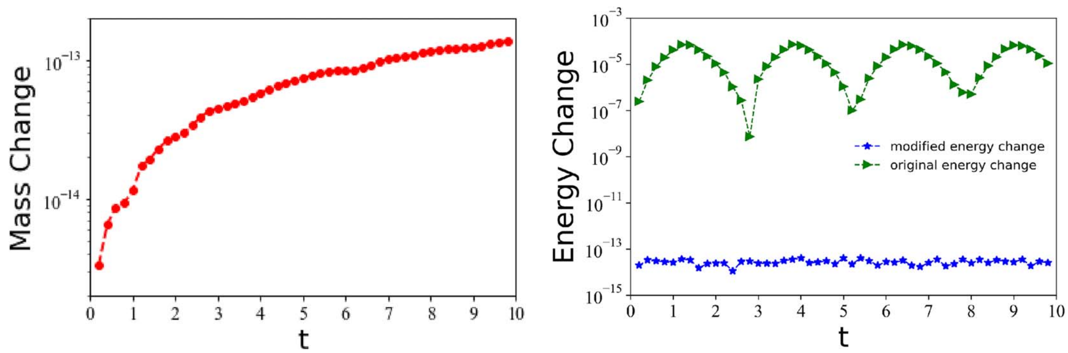


FIG. 2. Evolution of the mass and energy with $V(x_1, x_2) = V_1(x_1, x_2)$.

The discrete mass and energy, as defined in Lemma 2.2, are computed for $V(x_1, x_2) = V_i(x_1, x_2)$, with $i = 0, 1, 2$, and the changes in mass and energy are illustrated in Figs 1–3, respectively. Although the case with $V(x_1, x_2) = V_2(x_1, x_2)$ shows a relatively larger energy error compared with other cases, as seen in Fig. 3, the results suggest that both mass and modified energy are well preserved at the discrete level for all cases.

For cases of $V(x_1, x_2) = V_1(x_1, x_2)$ and $V(x_1, x_2) = V_2(x_1, x_2)$, we also compute a direct approximation of the original energy in (1.3) at t_n, defined as

$$\tilde{E}_h^n := \int_\Omega \left(\frac{1}{2} |\nabla u_h^n|^2 + \frac{1}{2\mu} |\nabla \bar{\Phi}_h^n|^2 + V(x)|u_h^n|^2 + \frac{1}{2}|u_h^n|^4 \right) \mathrm{d}x, \quad 0 \le n \le N, \tag{5.3}$$

where

$$\bar{\Phi}_h^n = \frac{\Phi_h^{n+1/2} + \Phi_h^{n-1/2}}{2}.$$

For both cases, the changes in the approximated original energy $\tilde{E}_h^n$, defined similarly to the energy change in (5.2), are also shown in Figs 2 and 3. Although the changes in the directly approximated

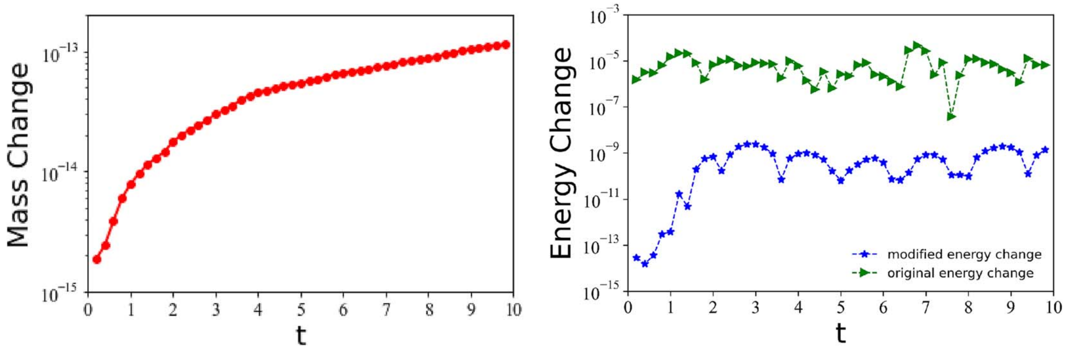
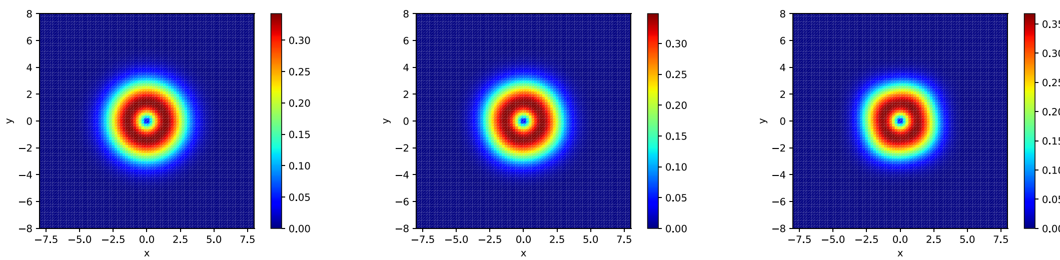
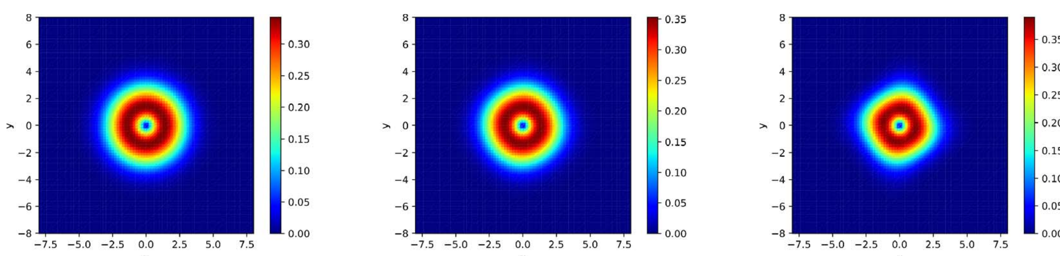


FIG. 3. Evolution of the mass and energy with $V(x_1, x_2) = V_2(x_1, x_2)$.



(a) $t = 0$ (b) $t = 5$ (c) $t = 10$

FIG. 4. The patterns evolution of the wave function $|u(x_1, x_2, t)|$ with $V(x_1, x_2) = V_0(x_1, x_2)$.



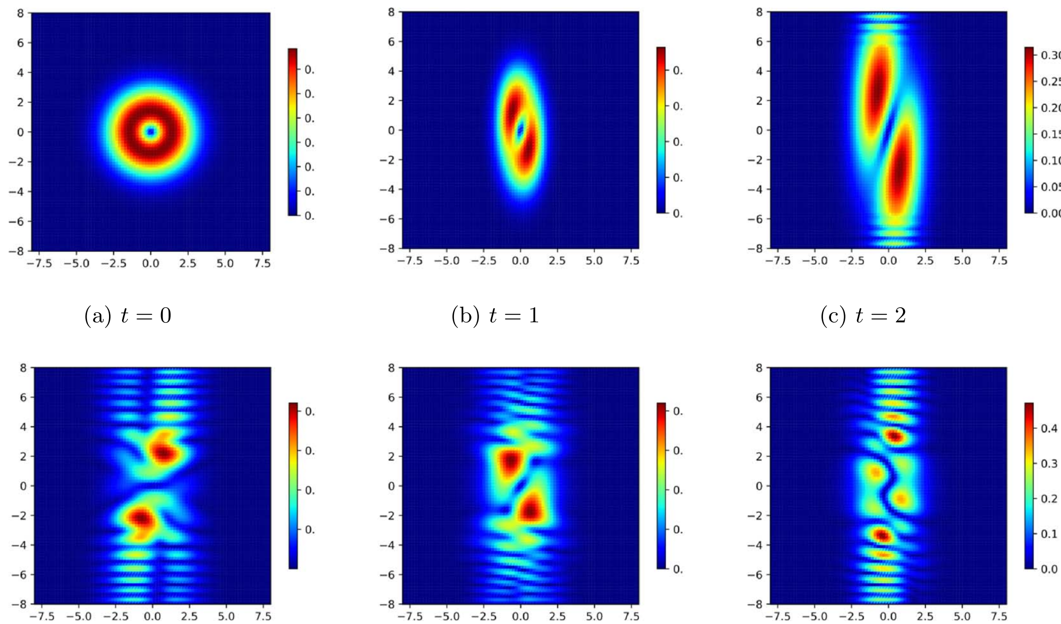
(a) $t = 0$ (b) $t = 5$ (c) $t = 10$

FIG. 5. The patterns evolution of the wave function $|u(x_1, x_2, t)|$ with $V(x_1, x_2) = V_1(x_1, x_2)$.

original energy are relatively larger than those of the modified energy, the original energy remains well preserved in both cases.

Test case 4. We present the evolution of the solution in Figs 4–6 for the external potentials $V(x_1, x_2) = V_i(x_1, x_2)$, $i = 0, 1, 2$, respectively, using a mesh with $NC = 80$ and a time step of $\tau = 1 \times 10^{-3}$, based on $\mathbb{Q}^2$ polynomials.

We first conduct numerical tests for the case with a zero potential, i.e., $V(x_1, x_2) = V_0(x_1, x_2)$. Figure 4 shows the patterns of the wave function $|u(x, y, t)|$ at time $t = 0, 5, 10$, from which we can



(a) $t = 0$ (b) $t = 1$ (c) $t = 2$

(d) $t = 5$ (e) $t = 7.5$ (f) $t = 10$

FIG. 6. The patterns evolution of the wave function $|u(x_1, x_2, t)|$ with $V(x_1, x_2) = V_2(x_1, x_2)$.

find that the pattern of the initial solution has evolved, but not significantly, and the pattern evolves around the center of the pattern.

Next, we introduce different external potentials under the same conditions to observe the resulting changes in the solution. This allows us to evaluate the performance of the proposed numerical method by comparing our results with similar findings in the literature.

We present the evolution of the solution in Fig. 5 with potential $V(x_1, x_2) = V_1(x_1, x_2)$ at times $t = 0$, $t = 5$ and $t = 10$. With the external potential V_1, the solution exhibits a pattern similar to that seen with zero potential. Notably, the pattern with V_0 at $t = 10$ (see Fig. 4(c)) and the pattern with V_1 at $t = 5$ (see Fig. 5(b)) are quite similar. This suggests that the external potential V_1 accelerates the evolution of patterns, particularly around the center of the pattern, compared to the zero potential case. Additionally, similar patterns of evolution to those in Fig. 5 were also observed in (Wang *et al.*, 2018).

We also introduce a different external potential $V(x_1, x_2) = V_2(x_1, x_2)$ for problem (5.1). The evolution of patterns is presented in Fig. 6 at different times from $t = 0$ to $t = 10$. Under the influence of the external potential V_2, the patterns are driven away from the center, and similar patterns were also observed in (Yi & Liu, 2022).

Test case 5. We compare the performance of the proposed relaxation Crank–Nicolson finite element algorithm (2.21), or Algorithm 2.1, with the IM from (Yi & Liu, 2022) by solving the SP problem (5.1) with $V(x_1, x_2) = V_2(x_1, x_2)$.

First, we compare the performance of Algorithm 2.1 with that of the IM using DG discretization (IM-DG) from (Yi & Liu, 2022). The parameters are set as follows: time step $\tau = 0.001$, mesh size $NC \times NC = 80 \times 80$ and $\mathbb{Q}^2$ polynomials. In the DG discretization, the penalty parameters are $\beta_0 = 10$

TABLE 3 *The computational time with $T = 10$ and $V(x_1, x_2) = V_2(x_1, x_2)$*

Algorithm 2.1 (linear, no iteration)	IM-DG (Tols $= 10^{-1}$)	IM-DG (Tols $= 10^{-6}$)
33411.52s	195226.01s	407897.47s

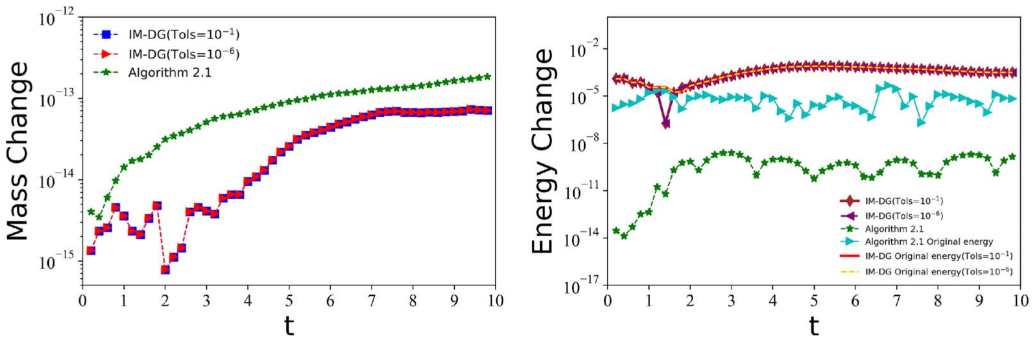
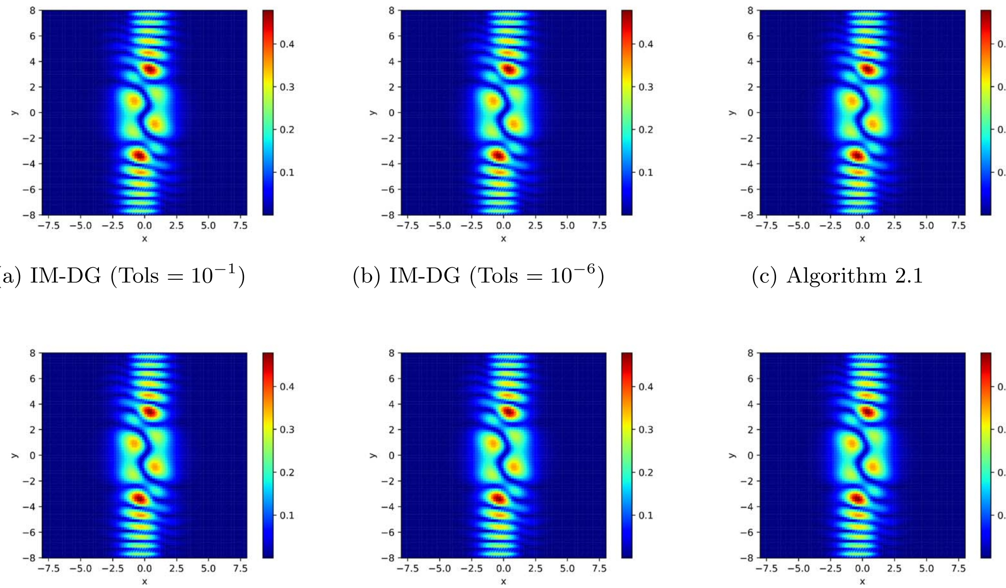


FIG. 7. The patterns evolution of the mass and energy for Algorithm 2.1 and IM-DG with $\tau = 0.001$.

and $\beta_1 = 1/12$. For the IM-DG method, the iteration is terminated when the prescribed tolerance (Tols $= 10^{-1}$ or 10^{-6}) is reached. The corresponding solution patterns at $t = 10$ are shown in Fig. 8(a,b), and they are comparable to that of Algorithm 2.1 as shown in Fig. 6(f). The corresponding CPU times of Algorithm 2.1 and IM-DG is reported in Table 3, showing that Algorithm 2.1 is significantly more efficient, while the IM-DG method requires substantially more computational time. The evolution of mass, modified energy, and original energy is presented in Fig. 7. Both methods conserve mass well. Algorithm 2.1 preserves the modified energy with high accuracy, and the original energy is also conserved, though with a slightly larger error. In contrast, the IM-DG method exhibits noticeably larger relative errors in conserving both the modified and original energies compared to Algorithm 2.1.

Secondly, to eliminate the influence of the DG discretization and to provide a fairer comparison with Algorithm 2.1, we consider a IM-FEM variant, obtained by replacing the DG discretization in IM-DG from (Yi & Liu, 2022) with the FEM. This modification allows a larger time step for IM to produce a comparable final pattern. Specifically, we consider the time step both $\tau = 0.001$ and $\tau = 0.01$, mesh size $NC \times NC = 80 \times 80$, and employ $\mathbb{Q}^2$ polynomials for both Algorithm 2.1 and IM-FEM. In IM-FEM, the iteration is terminated either after two fixed steps or upon reaching the prescribed tolerance (Tols $= 10^{-1}$ or 10^{-6}). The solution patterns at $t = 10$ with time step $\tau = 0.01$ are presented in Fig. 8(c–f), and they are comparable to the pattern obtained by Algorithm 2.1 with time step $\tau = 0.001$, as shown in Fig. 6(f). The corresponding CPU times, reported in Tables 4 and 5, indicate that Algorithm 2.1 is the most efficient, while IM-FEM requires at least twice as much CPU time of Algorithm 2.1. The evolution of mass, modified energy and original energy is presented in Figs 9 and 10. Both methods conserve mass well. Algorithm 2.1 preserves the modified energy with high accuracy, while the original energy is also conserved, albeit with slightly larger errors. In contrast, Figs 9 and 10 demonstrate that IM-FEM requires a smaller time step and smaller iteration tolerance to preserve its modified energy, and it exhibits larger relative errors in conserving the original energy.



(a) IM-DG (Tols $= 10^{-1}$) (b) IM-DG (Tols $= 10^{-6}$) (c) Algorithm 2.1

(d) IM-FEM (Two-step iteration) (e) IM-FEM (Tols $= 10^{-1}$) (f) IM-FEM (Tols $= 10^{-6}$)

FIG. 8. The patterns of the wave function $|u(x_1, x_2, t)|$ at $t = 10$ with $V_2(x_1, x_2)$.

TABLE 4 *The computational time at* $T = 10$ *with* $\tau = 0.001$ *and* $V(x_1, x_2) = V_2(x_1, x_2)$

Algorithm 2.1 (linear, no iteration)	IM-FEM (two-step iteration)	IM-FEM (Tols $= 10^{-1}$)	IM-FEM (Tols $= 10^{-6}$)
33411.52s	64815.95s	91914.44s	92866.31s

TABLE 5 *The computational time at* $T = 10$ *with* $\tau = 0.01$ *and* $V(x_1, x_2) = V_2(x_1, x_2)$

Algorithm 2.1 (linear, no iteration)	IM-FEM (two-step iteration)	IM-FEM (Tols $= 10^{-1}$)	IM-FEM (Tols $= 10^{-6}$)
3488.17s	6397.19s	9334.41s	11717.49s

6. Concluding remarks

A structure-preserving relaxation Crank–Nicolson FEM has been proposed for the SP equation that contains the self-repulsion $|u|^2u$ in the Schrödinger equation and the charge density $|u|^2$ in the Poisson equation, relying on a decoupled system that is equivalent to the original equation. The fully discrete scheme is linear and is easy to implement without resorting to any iteration method. In addition, the finite element approximation is demonstrated to be both mass and modified energy conservative, irrespective of the mesh and time step. Optimal L^2 error estimates are established for the fully discrete scheme with

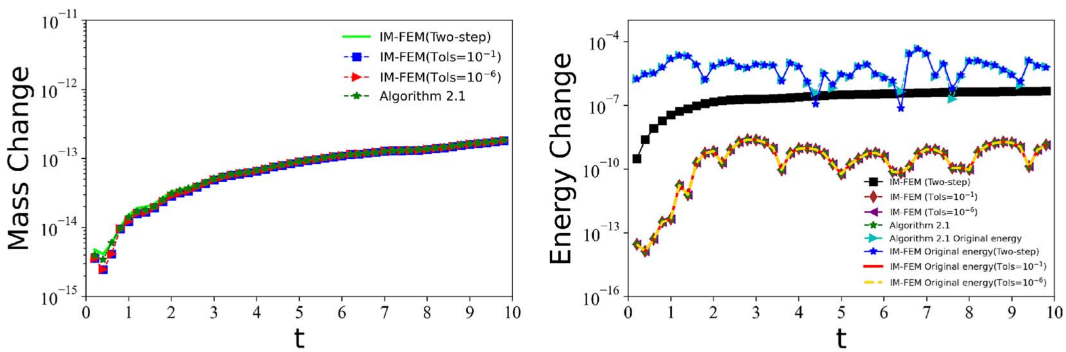


FIG. 9. The patterns evolution of the mass and energy for Algorithm 2.1 and IM-FEM with $\tau = 0.001$.

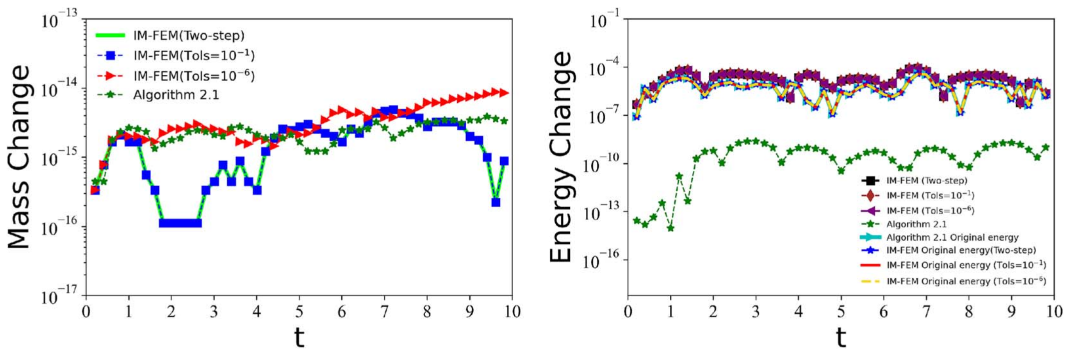


FIG. 10. The patterns evolution of the mass and energy for Algorithm 2.1 and IM-FEM with $\tau = 0.01$.

second order accuracy in time and $(k+1)$th accuracy in space. Numerical tests have been presented to verify the effectiveness and robustness of the proposed method. The proposed relaxation Crank–Nicolson FEM is a very competitive algorithm for solving the SP equation.

The spatial discretization utilised in this paper is the FEM, it is noteworthy that the DG method (Yi & Liu, 2022) can also be a viable alternative, in which the Poisson equation can be solved by the direct DG method (Yin *et al.*, 2014, 2018). The proposed scheme preserves mass and a modified energy. Developing efficient numerical methods that preserve the original energy remains an important and challenging problem, which we leave for future work. In the case of the three-dimensional SP equation, the self-repulsion term is substituted by $|u|^{4/3}u$. Extending the current findings to encompass this scenario could be an intriguing direction for future research, which we intend to pursue.

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Conflicts of interest

The authors declare no conflict of interest.

References

Arriola, E. & Soler, J. (2001) A variational approach to the Schrödinger–Poisson system: asymptotic behaviour, breathers, and stability. *J. Statist. Phys.*, **103**, 1069–1105.

Athanassoulis, A., Katsaounis, T., Kyza, I. & Metcalfe, S. (2023) A novel, structure-preserving, second-order-in-time relaxation scheme for Schrödinger–Poisson systems. *J. Comput. Phys.*, **490**, 112307. https://www.sciencedirect.com/science/article/pii/S0021999123004023

Auzinger, W., Kassebacher, T., Koch, O. & Thalhammer, M. (2017) Convergence of a Strang splitting finite element discretization for the Schrödinger–Poisson equation. *Math. Model. Numer. Anal.*, **51**, 1245–1278.

Bertrand, P., Van Tuan, N., Gros, M., Izrar, B., Feix, M., & Gutierrez, J. (1980) Classical Vlasov plasma description through quantum numerical methods. *J. Plasma Phys.*, **23**, 401–422.

Besse, C. (2004) A relaxation scheme for the nonlinear Schrödinger equation. *SIAM J. Numer. Anal.*, **42**, 934–952.

Besse, C., Descombes, S., Dujardin, G. & Lacroix-Violet, I. (2021) Energy-preserving methods for nonlinear Schrödinger equations. *IMA J. Numer. Anal.*, **41**, 618–653.

Brenner, S. C. & Scott, L. R. (2008) *The Mathematical Theory of Finite Element Methods*, 3rd edn. New York: Springer.

Cai, Y., Rosenkranz, M., Lei, Z. & Bao, W. (2010) Mean-field regime of trapped dipolar Bose-Einstein condensates in one and two dimensions. *Phys. Rev. A*, **82**, 043623.

Castella, F. (1997) L^2 solutions to the Schrödinger–Poisson system: existence, uniqueness, time behavior, and smoothing effects. *Math. Mod. Meth. Appl. Sci.*, **7**, 1051–1083.

Ciarlet, P. G. & Oden, J. T. (1978) The finite element method for elliptic problems. *Elsevier*, **45**, 968–969.

Cotner, E. (2016) Collisional interactions between self-interacting nonrelativistic boson stars: effective potential analysis and numerical simulations. *Phys. Rev. D*, **94**, 063503.

Ehrhardt, M. & Zisowsky, A. (2006) Fast calculation of energy and mass preserving solutions of Schrödinger–Poisson systems on unbounded domains. *J. Comput. Appl. Math.*, **187**, 1–28.

Gong, C., She, M., Yuan, W. & Zhao, D. (2022) SAV Galerkin-Legendre spectral method for the nonlinear Schrödinger-Possion equations. *Electron. Res. Arch.*, **30**, 943–960.

Heywood, J. G. & Rannacher, R. (1990) Finite-element approximation of the nonstationary Navier-stokes problem. Part IV: error analysis for second-order time discretization. *SIAM J. Numer. Anal.*, **27**, 353–384.

Lange, H., Toomire, B. & Zweifel, P. F. (1995) An overview of Schrödinger–Poisson problems. *Rep. Math. Phys.*, **36**, 331–345.

Lange, H. & Zweifel, P. F. (1997) Mixed boundary-value problems for the two-dimensional Schrödinger–Poisson system. *Rep. Math. Phys.*, **39**, 283–297.

Lubich, C. (2008) On splitting methods for Schrödinger–Poisson and cubic nonlinear Schrödinger equations. *Math. Comp.*, **77**, 2141–2153.

Markowich, P., Ringhofer, C. & Schmeiser, C. (1990) *Semiconductor Equations*. Vienna: Springer.

Masaki, S. (2011) Energy solution to a Schrödinger–Poisson system in the two-dimensional whole space. *SIAM J. Math. Anal.*, **43**, 2719–2731.

Paredes, A., Olivieri, D. N. & Michinel, H. (2020) From optics to dark matter: a review on nonlinear Schrödinger–Poisson systems. *Physica D*, **403**, 132301.

Ringhofer, C. & Soler, J. (2000) Discrete Schrödinger–Poisson systems preserving energy and mass. *Appl. Math. Lett.*, **13**, 27–32.

Ruffini, R. & Bonazzola, S. (1969) Systems of self-gravitating particles in general relativity and the concept of an equation of state. *Phys. Rev.*, **187**, 1767–1783.

Sakaguchi, H. & Malomed, B. A. (2020) Gross–Pitaevskii–Poisson model for an ultracold plasma: density waves and solitons. *Phys. Rev. Res.*, **2**, 033188.

Shukla, P. K. & Eliasson, B. (2006) Formation and dynamics of dark solitons and vortices in quantum electron plasmas. *Phys. Rev. Lett.*, **96**, 245001.

Shukla, P. K. & Eliasson, B. (2011) Colloquium: nonlinear collective interactions in quantum plasmas with degenerate electron fluids. *Rev. Modern Phys.*, **83**, 885–906.

Verma, A. K., Pandit, R. & Brachet, M. E. (2021) Formation of compact objects at finite temperatures in a dark-matter-candidate self-gravitating bosonic system. *Phys. Rev. Res.*, **3**, L022016.

Wang, H., Liang, Z. & Liu, R. (2018) A splitting Chebyshev collocation method for Schrödinger–Poisson system. *Comp. Appl. Math.*, **37**, 5034–5057.

Wei, H. & Huang, Y. (2017-2025) *FEALPy: Finite Element Analysis Library in Python* https://github.com/weihuayi/fealpy. Xiangtan University.

Yi, N. & Liu, H. (2022) A mass-and energy-conserved DG method for the Schrödinger–Poisson equation. *Numer. Algorithms*, **89**, 905–930.

Yin, P., Huang, Y. & Liu, H. (2014) An iterative discontinuous Galerkin method for solving the nonlinear Poisson–Boltzmann equation. *Commun. Comput. Phys.*, **16**, 491–515.

Yin, P., Huang, Y. & Liu, H. (2018) Error estimates for the iterative discontinuous Galerkin method to the nonlinear Poisson-Boltzmann equation. *Commun. Comput. Phys.*, **23**, 168–197.

Zhang, Y. (2013) Optimal error estimates of compact finite difference discretizations for the Schrödinger–Poisson system. *Commun. Comput. Phys.*, **13**, 1357–1388.

Zouraris, G. E. (2023) Error estimation of the relaxation finite difference scheme for the nonlinear Schrödinger equation. *SIAM J. Numer. Anal.*, **61**, 365–397.