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A mass- and energy-preserving numerical scheme for solving coupled Gross–Pitaevskii equations in high dimensions

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Abstract

This article is concerned with numerical study of a coupled system of Gross–Pitaevskii equations which describes the spin-orbit-coupled Bose–Einstein condensates. Due to the fact that this system possesses the total mass and energy conservation property and often appears in high dimensions, it brings a significant burden in designing and analyzing a suitable numerical scheme for solving the coupled Gross–Pitaevskii equations (CGPEs). In this article, an implicit finite difference scheme is proposed to solve the CGPEs, which is proved to be uniquely solvable, mass- and energy-conservative in the discrete sense. In particular, it is proved in a rigorous way that, without any grid-ratio restriction, the scheme is stable and convergent at the rate of $O(h^2+\tau^2)$ with time step τ and mesh size h in the maximum norm, while previous works often require certain restriction on the grid ratio and only give the error estimates in the discrete L^2 norm or H^1 norm which could not imply the maximum error estimate. Numerical results are carried out to underline the error estimate and conservation laws, and investigate several dynamics of the CGPEs.

KEYWORDS

coupled Gross–Pitaevskii equations, finite difference method, mass and energy conservation, point-wise error estimate, solvability

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1 | INTRODUCTION

In this article, we consider the following d-dimensional (d=1,2,3) coupled Gross–Pitaevskii equations (CGPEs):

$$i\partial_t\psi_1 = \left[-\frac{1}{2}\Delta + V_1(\mathbf{x}) + ik_0\partial_x + \frac{\alpha}{2} + \sum_{l=1}^{2}\beta_{1l}|\psi_l|^2\right]\psi_1 + \frac{\lambda}{2}\psi_2, \quad t>0, \tag{1.1}$$

$$i\partial_t\psi_2 = \left[-\frac{1}{2}\Delta + V_2(\mathbf{x}) - ik_0\partial_x - \frac{\alpha}{2} + \sum_{l=1}^{2}\beta_{2l}|\psi_l|^2\right]\psi_2 + \frac{\lambda}{2}\psi_1, \quad t>0, \tag{1.2}$$

where

$$V_1(\mathbf{x}) = V_2(\mathbf{x}) = \begin{cases} \frac{1}{2}\gamma_1^2x^2, & d=1,\\ \frac{1}{2}(\gamma_1^2x^2+\gamma_2^2y^2), & d=2,\\ \frac{1}{2}(\gamma_1^2x^2+\gamma_2^2y^2+\gamma_3^2z^2), & d=3,\end{cases}$$

$i=\sqrt{-1}$, and γ_d $(d=1,2,3)$, k_0, α, β_{lm} $(l,m=1,2)$, λ are given real constants, $\Psi := (\psi_1,\psi_2)^\top$ are the unknown complex-valued wave function. The Equations (1.1) and (1.2) are the dimensionless form (see [7]) of the CGPEs derived in describing the spin-orbit (SO) coupled Bose–Einstein condensate (BEC) (see [21–22,24–28,43–44]).

It is seen from [7] that the dimensionless CGPEs (1.1) and (1.2) preserve the total mass,

$$M(\Psi(\cdot,t)) := ||\Psi(\cdot,t)||^2 = \int_{\mathbb{R}^d}\left(|\psi_1(\mathbf{x},t)|^2 + |\psi_2(\mathbf{x},t)|^2\right)d\mathbf{x} \equiv M(\Psi(\cdot,0)),\ t>0, \tag{1.3}$$

and energy,

$$\begin{aligned} E(\Psi(\cdot,t)) \ :=& \int_{\mathbb{R}^d}\left[\sum_{l=1}^{2}\left(\frac{1}{2}|\nabla\psi_l|^2 + V_l(\mathbf{x})|\psi_l|^2\right) + \frac{\alpha}{2}(|\psi_1|^2-|\psi_2|^2) + \lambda\mathrm{Re}(\psi_1\overline{\psi_2})\right.\\ &\left. - k_0\mathrm{Im}(\overline{\psi_1}\partial_x\psi_1 - \overline{\psi_2}\partial_x\psi_2) + \sum_{l=1}^{2}\sum_{j=1}^{2}\frac{\beta_{lj}}{2}|\psi_l|^2|\psi_j|^2\right]d\mathbf{x} \equiv E(\psi_0),\ t\geq 0, \end{aligned} \tag{1.4}$$

where $\bar{s}$, $\mathrm{Re}(s)$ and $\mathrm{Im}(s)$ represent the conjugate, the real part and imaginary part of s, respectively.

From mathematical points of view, extensive results have been carried out in the literature to study the Gross–Pitaevskii equation (GPE) arising in modeling the BEC, see [1, 3-11, 14, 15, 19, 20, 35, 38-40] and references therein. However, few numerical method was proposed in literature for solving the CGPEs (1.1) and (1.2). In [7], Bao and Cai analytically and numerically studied the ground states and dynamics of two-component SO-coupled BECs modeled by the CGPEs. In computing the dynamics of the CPGEs, a time-splitting Fourier pseudo-spectral method is proposed in [7]. Their numerical results demonstrate the efficiency and accuracy of the numerical methods and show the rich phenomenon in the SO-coupled BECs. Antoine, Besse and Rispoli built and validated some explicit high-order schemes in [4] for simulating the dynamics of the CPGEs and other nonlinear Schrödinger (NLS) equations or GPEs. Their method is based on the combination of high-order implicit-explicit schemes in time and Fourier pseudo-spectral approximations in space. To the best of our knowledge, though there exists many finite difference schemes are proposed to solve the CGPEs without the first-order derivative terms (see [3, 5, 31-34, 36]), there is no finite difference method is proposed and analyzed in literature for solving the CGPEs (1.1) and (1.2). Due to the high efficiency and ease in implementing, finite difference method is very popular in numerically solving the NLS-type equations.

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However, to give a clear and optimal grid-ratio condition of the finite difference method is a very important and challenging issue.

There are tremendous literatures on establishing unconditional and optimal error estimates of implicit finite difference schemes for solving the one-dimensional NLS-type equations (see [14,15,41] and references therein). The key tools used in building the error bounds are strongly dependent on the conservation properties and the one-dimensional Sobolev embedding inequalities, so they cannot be generalized directly to high-dimensional cases. However, the CGPEs are expressed in d dimensions for $d = 1, 2, 3$ depending on the values taken by the trapping frequencies in the x-, y-, and z-directions. In [6], under a weak constraint on the grid ratio, Bao and Cai applied the standard energy method together with the cut-off function technique [2,16,17,30] to build the error estimates of two finite difference schemes of the GPE with an angular momentum rotation term. In [39], the authors established the point-wise optimal error estimates of finite difference methods for solving the coupled GPEs under a weak constraint on the grid ratio. In [38], the authors proposed an mass- and energy-preserving, fourth-order compact finite difference scheme for a two-dimensional NLS equation and established the optimal L^2-error estimate of the scheme without any grid-ratio restriction, but their result still requires that the initial value is sufficiently small. It is known that the maximum error estimate of numerical methods is preferable in numerical analysis, while in two or three dimensional cases the L^2- and the H^1-error estimate does not imply the maximum one.

From the stability and long-time computation point of view, a numerical scheme possessing the conservative properties in the discrete sense is preferable and more popular than the non-conservative ones which may lead to non-physical "blow-up." In fact, more and more interests are attracted in designing and analyzing conservative numerical schemes in solving those partial differential equations inheriting conservative or dissipative properties (see [13, 18, 29, 38, 40, 42] and references therein). Hence, the purpose of this article lies in constructing and analyzing a mass- and energy-preserving finite difference scheme for the high-dimensional CGPEs. The main contribution of the present work is to establish the optimal H^2-error estimates implying consequently the point-wise error estimates of the derived scheme without any time-step restriction depending on the grid size in space.

The remainder of this article is arranged as follows. In Section 2, a Crank-Nicolson finite difference (CNFD) scheme is proposed for the CGPEs. In Section 3, the optimal H^2-error estimates of the proposed scheme are established without any grid-ratio constraint. In Section 4, some numerical results are reported to test the theoretical analysis.

2 | FINITE DIFFERENCE SCHEME

For simplicity, similar as the processing in [7], we here only consider the numerical method in two dimensions, that is, $d = 2$ and $\Omega = (x_L, x_R) \times (y_L, y_R)$ in (1.1) and (1.2). Extension to three-dimensional case is straightforward, and the convergence result remains valid with little modification. That is, we consider the CGPEs

$$i\partial_t\psi_1 = \left[-\frac{1}{2}\Delta + V_1(x,y) + ik_0\partial_x + \frac{\alpha}{2} + \sum_{l=1}^{2}\beta_{1l}|\psi_l|^2\right]\psi_1 + \frac{\lambda}{2}\psi_2, \quad (x,y)\in\Omega,\ t>0, \tag{2.1}$$

$$i\partial_t\psi_2 = \left[-\frac{1}{2}\Delta + V_2(x,y) - ik_0\partial_x - \frac{\alpha}{2} + \sum_{l=1}^{2}\beta_{2l}|\psi_l|^2\right]\psi_2 + \frac{\lambda}{2}\psi_1, \quad (x,y)\in\Omega,\ t>0, \tag{2.2}$$

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with homogeneous Dirichlet boundary conditions

$$\psi_1(x,y,t) = 0, \quad \psi_2(x,y,t) = 0, \quad (x,y) \in \partial\Omega, \quad t > 0, \tag{2.3}$$

and initial conditions

$$\psi_1(x,y,0) = \varphi_1(x,y), \quad \psi_2(x,y,0) = \varphi_2(x,y), \quad (x,y) \in \overline{\Omega}. \tag{2.4}$$

For a positive integer N, choose time-step $\tau = T/N$ and denote time steps $t_n = n\tau$, $n = 0, 1, 2, \dots, N$, where $0 < T < T_{\max}$ with $T_{\max}$ the maximal existing time of the solution; choose mesh sizes $h_1 = (x_R - x_L)/J$, $h_2 = (y_R - y_L)/K$ with two positive integers J and K, and denote $h = \max\{h_1, h_2\}$. Introduce two index sets

$$\mathcal{T}_h = \{(j,k) | \, j = 1, 2, \dots, J-1, \ k = 1, 2, \dots, K-1\},$$
$$\mathring{\mathcal{T}}_h = \{(j,k) | \, j = 0, 1, 2, \dots, J, \ k = 0, 1, 2, \dots, K\}, \quad \Gamma_h = \mathring{\mathcal{T}}_h \setminus \mathcal{T}_h,$$

three grid point sets

$$\overline{\Omega}_h = \{(x_j, y_k) = (x_L + jh_1, y_L + kh_2) | \, (j,k) \in \mathring{\mathcal{T}}_h\}, \quad \Omega_h = \overline{\Omega}_h \cap \Omega, \quad \partial\Omega_h = \overline{\Omega}_h \cap \partial\Omega,$$

and a space of grid functions

$$X_h = \{w = \{w_{j,k}\}, \ (j,k) \in \mathring{\mathcal{T}}_h, | \, w_{j,k} = 0, \ \text{if } (j,k) \in \Gamma_h\}.$$

Let $({\psi_1}_{j,k}^n, {\psi_2}_{j,k}^n)^\top$ and $({\phi_1}_{j,k}^n, {\phi_2}_{j,k}^n)^\top$ be the numerical approximation and the exact value of $(\psi_1, \psi_2)^\top$ at the point (x_j, y_k, t_n) for $(j,k) \in \mathring{\mathcal{T}}_h, n = 0, 1, 2, \dots, N$, respectively. As usual, for a grid function $v^n \in X_h$ for $n = 0, 1, 2, \dots, N$, we introduce the following finite difference quotient operators,

$$\delta_t^+ v_{j,k}^n = \frac{1}{\tau}\left(v_{j,k}^{n+1} - v_{j,k}^n\right), \quad \delta_x^+ v_{j,k}^n = \frac{1}{h_1}\left(v_{j+1,k}^n - v_{j,k}^n\right),$$
$$\delta_x v_{j,k}^n = \frac{1}{2h_1}\left(v_{j+1,k}^n - v_{j-1,k}^n\right), \quad \delta_x^2 v_{j,k}^n = \frac{1}{h_1^2}\left(v_{j-1,k}^n - 2v_{j,k}^n + v_{j+1,k}^n\right).$$

Difference quotient operators $\delta_y^+ v_{j,k}^n, \delta_y^2 v_{j,k}^n$ can be introduced similarly. Besides, we introduce the discrete vision of the gradient operator and Laplacian operator as follows

$$\nabla_h v_{j,k}^n = \left(\delta_x^+ v_{j,k}^n, \delta_y^+ v_{j,k}^n\right)^\top, \quad \Delta_h v_{j,k}^n = \delta_x^2 v_{j,k}^n + \delta_y^2 v_{j,k}^n.$$

Define discrete inner products and discrete norms over X_h as

$$\langle u, v\rangle = h_1 h_2 \sum_{j=1}^{J-1}\sum_{k=1}^{K-1} u_{j,k}\overline{v}_{j,k}, \quad \langle u, v\rangle_0 = h_1 h_2 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} u_{j,k}\overline{v}_{j,k},$$

$$||u|| = \sqrt{\langle u, u\rangle}, \quad ||u||_\infty = \max_{(j,k)\in\mathcal{T}_h} |u_{j,k}|, \quad ||u||_p = \sqrt[p]{h_1 h_2 \sum_{j=1}^{J-1}\sum_{k=1}^{K-1} |u_{j,k}|^p},$$

$$|u|_1 = \sqrt{\langle \nabla_h u, \nabla_h u\rangle_0} = \sqrt{\langle \delta_x^+ u, \delta_x^+ u\rangle_0 + \langle \delta_y^+ u, \delta_y^+ u\rangle_0}, \quad |u|_2 = \sqrt{\langle \Delta_h u, \Delta_h u\rangle},$$

$$|||u|||_1 = \sqrt{||u||^2 + |u|_1^2}, \quad |||u|||_2 = \sqrt{||u||^2 + |u|_1^2 + |u|_2^2}.$$

Here, for the grid function $u \in X_h$, $|u|_k$ and $|||u|||_k$ $(k = 1, 2)$ are semi-norms and norms of u, respectively. Corresponding to the standard Sobolev spaces, we here use $H^k(\Omega_h)$ to denote the space of complex-valued or real-valued discrete functions with norm $|||\cdot|||_k$, $(k = 1, 2)$, and use $H_0^1(\Omega_h)$ to denote a subspace of $H^1(\Omega_h)$ satisfying the homogeneous Dirichlet boundary conditions.

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For simplicity of notations, in the following of the article, we use C to denote a generic positive constant which may depend on the exact solution and the given data but is independent of all the discrete parameters. Furthermore, we use the notation $w \lesssim v$ to present $|w| \le Cv$, and use $w \gtrsim v$ to present $w \ge C|v|$.

By using the centered finite difference discretization, we give the following CNFD scheme:

$$\begin{aligned} i\delta_t^+ \psi_{1\,j,k}^{\,n} = &\frac{1}{2}\left[-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2} + \frac{\beta_{11}}{2}\left(|\psi_{1\,j,k}^{\,n}|^2 + |\psi_{1\,j,k}^{\,n+1}|^2\right)\right.\\ &\left.+\frac{\beta_{12}}{2}\left(|\psi_{2\,j,k}^{\,n}|^2 + |\psi_{2\,j,k}^{\,n+1}|^2\right)\right]\left(\psi_{1\,j,k}^{\,n} + \psi_{1\,j,k}^{\,n+1}\right) + \frac{\lambda}{4}\left(\psi_{2\,j,k}^{\,n} + \psi_{2\,j,k}^{\,n+1}\right),\\ &(j,k) \in \mathcal{T}_h, \quad n = 0,1,2,\dots,N-1, \end{aligned} \tag{2.5}$$

$$\begin{aligned} i\delta_t^+ \psi_{2\,j,k}^{\,n} = &\frac{1}{2}\left[-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2} + \frac{\beta_{21}}{2}\left(|\psi_{1\,j,k}^{\,n}|^2 + |\psi_{1\,j,k}^{\,n+1}|^2\right)\right.\\ &\left.+\frac{\beta_{22}}{2}\left(|\psi_{2\,j,k}^{\,n}|^2 + |\psi_{2\,j,k}^{\,n+1}|^2\right)\right]\left(\psi_{2\,j,k}^{\,n} + \psi_{2\,j,k}^{\,n+1}\right) + \frac{\lambda}{4}\left(\psi_{1\,j,k}^{\,n} + \psi_{1\,j,k}^{\,n+1}\right),\\ &(j,k) \in \mathcal{T}_h, \quad n = 0,1,2,\dots,N-1, \end{aligned} \tag{2.6}$$

$$\psi_{1\,j,k}^{\,0} = \varphi_1(x_j, y_k), \quad \psi_{2\,j,k}^{\,0} = \varphi_2(x_j, y_k), \quad (j,k) \in \mathring{\mathcal{T}}_h, \tag{2.7}$$

$$\psi_{1\,j,k}^{\,n} = 0, \quad \psi_{2\,j,k}^{\,n} = 0, \quad (j,k) \in \Gamma_h, \ \ n = 1,2,\dots,N, \tag{2.8}$$

where $V_{1_{j,k}} = V_1(x_j, y_k)$, $V_{2_{j,k}} = V_2(x_j, y_k)$.

2.1 | Conservative properties

In the next of the article, the following lemma will be used frequently.

Lemma 2.1. *For any two grid functions $u^n, v^n \in H^2(\Omega_h) \bigcap H_0^1(\Omega_h)$, $n = 0, 1, \dots, N$, we have*

$$\operatorname{Im}\left\langle i\delta_t^+ u^n, u^{n+1} + u^n\right\rangle = \frac{1}{\tau}(||u^{n+1}||^2 - ||u^n||^2), \tag{2.9}$$

$$\langle \Delta_h u^n, v^n\rangle = -\langle \nabla_h u^n, \nabla_h v^n\rangle_0, \tag{2.10}$$

$$\operatorname{Re}\left\langle \Delta_h(u^{n+1} + u^n), \delta_t^+ u^n\right\rangle = -\frac{1}{\tau}\left(|u^{n+1}|_1^2 - |u^n|_1^2\right), \tag{2.11}$$

$$\operatorname{Re}\left\langle \Delta_h(u^{n-1} + u^{n+1}), \delta_t u^n\right\rangle = -\frac{1}{2\tau}\left(|u^{n+1}|_1^2 - |u^{n-1}|_1^2\right), \tag{2.12}$$

$$\operatorname{Re}\left\langle \Delta_h(u^{n+1} + u^n), \delta_t^+ \Delta_h u^n\right\rangle = \frac{1}{\tau}\left(|u^{n+1}|_2^2 - |u^n|_2^2\right), \tag{2.13}$$

$$\operatorname{Re}\left\langle \Delta_h(u^{n-1} + u^{n+1}), \delta_t \Delta_h u^n\right\rangle = \frac{1}{2\tau}\left(|u^{n+1}|_2^2 - |u^{n-1}|_2^2\right), \tag{2.14}$$

$$\operatorname{Re}\left\langle \delta_t^2 u^n, \delta_t u^n\right\rangle = \frac{1}{2\tau}\left(||\delta_t^+ u^n||^2 - ||\delta_t^+ u^{n-1}||^2\right). \tag{2.15}$$

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Proof. The results are directly computed from the standard summation by parts formula, and we omit the details here for brevity. ■

Like the fact that the initial-boundary value problem conserves the total mass and energy, the CNFD scheme is expected to possesses the similar conservative properties in the discrete sense.

Lemma 2.2. *The CNFD scheme (2.5)–(2.8) preserves the total mass and energy in the discrete sense, that is,*

$$M^n := ||\psi_1^n||^2 + ||\psi_2^n||^2 \equiv M^0, \quad n = 0, 1, 2, \dots, N, \tag{2.16}$$

$$\begin{aligned}
E^n :=& \frac{1}{2}(|\psi_1^n|_1^2 + |\psi_2^n|_1^2) + h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\left(V_{1_{j,k}}|\psi_{1}{}_{j,k}^n|^2 + V_{2_{j,k}}|\psi_{2}{}_{j,k}^n|^2\right)\\
&+\frac{\alpha}{2}\left(||\psi_1^n||^2 - ||\psi_2^n||^2\right) - h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\left[k_0\mathrm{Im}(\overline{\psi_1}{}_{j,k}^n\delta_x\psi_1{}_{j,k}^n - \overline{\psi_2}{}_{j,k}^n\delta_x\psi_2{}_{j,k}^n)\right]\\
&+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\left[\lambda\cdot\mathrm{Re}(\psi_1{}_{j,k}^n\overline{\psi_2}{}_{j,k}^n) + \frac{\beta_{11}}{2}|\psi_1{}_{j,k}^n|^4 + \frac{\beta_{22}}{2}|\psi_2{}_{j,k}^n|^4 + \beta_{12}|\psi_1{}_{j,k}^n|^2|\psi_2{}_{j,k}^n|^2\right]\\
\equiv& E^0, \quad n = 0, 1, 2, \dots, N.
\end{aligned}\tag{2.17}$$

Proof. Computing the inner product of (2.5) with $\psi_1^n + \psi_1^{n+1}$ and taking the imaginary part give

$$\frac{1}{\tau}(||\psi_1^{n+1}||^2 - ||\psi_1^n||^2) = \frac{\lambda}{4}h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\mathrm{Im}\left[\left(\psi_2{}_{j,k}^n + \psi_2{}_{j,k}^{n+1}\right)\left(\overline{\psi}_1{}_{j,k}^n + \overline{\psi}_1{}_{j,k}^{n+1}\right)\right] \tag{2.18}$$

for $n = 0, 1, 2, \dots, N-1$, where Lemma 2.1 was used. Computing the inner product of (2.6) with $\psi_2^n + \psi_2^{n+1}$ and taking the imaginary part give

$$\frac{1}{\tau}(||\psi_2^{n+1}||^2 - ||\psi_2^n||^2) = \frac{\lambda}{4}h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\mathrm{Im}\left[\left(\psi_1{}_{j,k}^n + \psi_1{}_{j,k}^{n+1}\right)\left(\overline{\psi}_2{}_{j,k}^n + \overline{\psi}_2{}_{j,k}^{n+1}\right)\right] \tag{2.19}$$

for $n = 0, 1, 2, \dots, N-1$. Adding (2.19) to (2.18) and noticing that

$$\mathrm{Im}\left[\left(\psi_2{}_{j,k}^n + \psi_2{}_{j,k}^{n+1}\right)\left(\overline{\psi}_1{}_{j,k}^n + \overline{\psi}_1{}_{j,k}^{n+1}\right) + \left(\psi_1{}_{j,k}^n + \psi_1{}_{j,k}^{n+1}\right)\left(\overline{\psi}_2{}_{j,k}^n + \overline{\psi}_2{}_{j,k}^{n+1}\right)\right] = 0, \tag{2.20}$$

one can obtain

$$\frac{1}{\tau}(||\psi_1^{n+1}||^2 + ||\psi_2^{n+1}||^2 - ||\psi_1^n||^2 - ||\psi_2^n||^2) = 0, \quad n = 0, 1, 2, \dots, N-1, \tag{2.21}$$

that is,

$$M^{n+1} - M^n = 0, \quad n = 0, 1, 2, \dots, N-1, \tag{2.22}$$

this immediately gives (2.16).

Computing the inner product of (2.5) with $2(\psi_1^{n+1} - \psi_1^n)$ and taking the real part give

$$\begin{aligned}
&\frac{1}{2}(|\psi_1^{n+1}|_1^2 - |\psi_1^n|_1^2) + h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}V_{1_{j,k}}\left(|\psi_1{}_{j,k}^{n+1}|^2 - |\psi_1{}_{j,k}^n|^2\right)\\
&\quad+\frac{\alpha}{2}\left(||\psi_1^{n+1}||^2 - ||\psi_1^n||^2\right) - h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\mathrm{Im}\left[k_0(\overline{\psi_1}{}_{j,k}^{n+1}\delta_x\psi_1{}_{j,k}^{n+1} - \overline{\psi_1}{}_{j,k}^n\delta_x\psi_1{}_{j,k}^n)\right]
\end{aligned}$$

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$$+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\left[\frac{\beta_{11}}{2}(|\psi_{1j,k}^{n+1}|^4-|\psi_{1j,k}^{n}|^4)+\frac{\beta_{12}}{2}(|\psi_{2j,k}^{n+1}|^2+|\psi_{2j,k}^{n}|^2)(|\psi_{1j,k}^{n+1}|^2-|\psi_{1j,k}^{n}|^2)\right]$$

$$+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\frac{\lambda}{2}\mathrm{Re}\left[(\psi_{2j,k}^{n+1}+\psi_{2j,k}^{n})(\overline{\psi_1}_{j,k}^{n+1}-\overline{\psi_1}_{j,k}^{n})\right]=0,\quad n=0,1,2,\ \dots\ ,N. \tag{2.23}$$

where Lemma 2.1 was used. Computing the inner product of (2.6) with $2(\psi_2^{n+1}-\psi_2^n)$ and taking the real part give

$$\frac{1}{2}(|\psi_2^{n+1}|_1^2-|\psi_2^n|_1^2)+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}V_{2_{j,k}}\left(|\psi_{2j,k}^{n+1}|^2-|\psi_{2j,k}^{n}|^2\right)$$

$$-\frac{\alpha}{2}\left(||\psi_2^{n+1}||^2-||\psi_2^n||^2\right)+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\mathrm{Im}\left[k_0\left(\overline{\psi_2}_{j,k}^{n+1}\delta_x\psi_{2j,k}^{n+1}-\overline{\psi_2}_{j,k}^{n}\delta_x\psi_{2j,k}^{n}\right)\right]$$

$$+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\left[\frac{\beta_{11}}{2}(|\psi_{2j,k}^{n+1}|^4-|\psi_{2j,k}^{n}|^4)+\frac{\beta_{12}}{2}(|\psi_{1j,k}^{n+1}|^2+|\psi_{1j,k}^{n}|^2)(|\psi_{2j,k}^{n+1}|^2-|\psi_{2j,k}^{n}|^2)\right]$$

$$+h_1h_2\sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\frac{\lambda}{2}\mathrm{Re}\left[(\psi_{1j,k}^{n+1}+\psi_{1jk}^{n})(\overline{\psi_2}_{j,k}^{n+1}-\overline{\psi_2}_{j,k}^{n})\right]=0,\quad n=0,1,2,\ \dots\ ,N. \tag{2.24}$$

Noting that

$$\begin{aligned}&\mathrm{Re}\left[(\psi_{2j,k}^{n+1}+\psi_{2j,k}^{n})(\overline{\psi_1}_{j,k}^{n+1}-\overline{\psi_1}_{j,k}^{n})+(\psi_{1j,k}^{n+1}+\psi_{1j,k}^{n})(\overline{\psi_2}_{j,k}^{n+1}-\overline{\psi_2}_{j,k}^{n})\right]\\&\quad=2\mathrm{Re}\left(\psi_{1j,k}^{n+1}\overline{\psi_2}_{j,k}^{n+1}-\psi_{1j,k}^{n}\overline{\psi_2}_{j,k}^{n}\right),\quad (j,k)\in\mathcal{T}_h,\quad n=0,1,2,\ \dots\ ,N-1,\end{aligned} \tag{2.25}$$

and

$$\begin{aligned}&(|\psi_{2j,k}^{n+1}|^2+|\psi_{2j,k}^{n}|^2)(|\psi_{1j,k}^{n+1}|^2-|\psi_{1j,k}^{n}|^2)+(|\psi_{1j,k}^{n+1}|^2+|\psi_{1j,k}^{n}|^2)(|\psi_{2j,k}^{n+1}|^2-|\psi_{2j,k}^{n}|^2)\\&\quad=2|\psi_{1j,k}^{n+1}|^2|\psi_{2j,k}^{n+1}|^2-2|\psi_{1j,k}^{n}|^2|\psi_{2j,k}^{n}|^2,\quad (j,k)\in\mathcal{T}_h,\quad n=0,1,2,\ \dots\ ,N-1,\end{aligned} \tag{2.26}$$

we obtain by adding (2.24) to (2.23) that

$$E^{n+1}-E^n=0,\quad n=0,1,2,\ \dots\ ,N-1, \tag{2.27}$$

which immediately gives (2.17). This completes the proof. ■

2.2 | Solvability

For proving the solvability of the proposed scheme, we need the following fixed point theorem.

Lemma 2.3 ([12]). *Let $(H,\langle\cdot,\cdot\rangle)$ be a finite-dimensional inner product space, $||\cdot||$ be the associated norm, and $g: H\to H$ be continuous. Assume, moreover, that*

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

Then, there exists a $z^*\in H$ such that $g(z^*)=0$ and $||z^*||\le\alpha$.

On the solvability of the CNFD scheme, we have

Lemma 2.4 (Solvability). *For any initial data $(\psi_1^0,\psi_2^0)\in X_h\times X_h$, there exists a solution $(\psi_1^{n+1},\psi_2^{n+1})\in X_h\times X_h$ for each of the CNFD scheme for $n=0,\ \dots\ ,N-1$.*

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Proof. For a fixed $n \in \{0, 1, \dots, N-1\}$, the CNFD scheme (2.5) and (2.6) can be rewritten as

$$\psi_{1_{j,k}}^{n+\frac{1}{2}} - \psi_{1_{j,k}}^{n} + \frac{2i}{\tau}\left[-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2} + \frac{\beta_{11}}{2}\left(|\psi_{1_{j,k}}^{n}|^2 + |2\psi_{1_{j,k}}^{n+\frac{1}{2}} - \psi_{1_{j,k}}^{n}|^2\right)\right.$$
$$\left.+\frac{\beta_{12}}{2}\left(|\psi_{2_{j,k}}^{n}|^2 + |2\psi_{2_{j,k}}^{n+\frac{1}{2}} - \psi_{2_{j,k}}^{n}|^2\right)\right]\psi_{1_{j,k}}^{n+\frac{1}{2}} + \frac{i\lambda}{\tau}\psi_{2_{j,k}}^{n+\frac{1}{2}} = 0, \quad (j,k) \in \mathcal{T}_h, \tag{2.28}$$

$$\psi_{2_{j,k}}^{n+\frac{1}{2}} - \psi_{2_{j,k}}^{n} + \frac{2i}{\tau}\left[-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2} + \frac{\beta_{21}}{2}\left(|\psi_{1_{j,k}}^{n}|^2 + |2\psi_{1_{j,k}}^{n+\frac{1}{2}} - \psi_{1_{j,k}}^{n}|^2\right)\right.$$
$$\left.+\frac{\beta_{22}}{2}\left(|\psi_{2_{j,k}}^{n}|^2 + |2\psi_{2_{j,k}}^{n+\frac{1}{2}} - \psi_{2_{j,k}}^{n}|^2\right)\right]\psi_{2_{j,k}}^{n+\frac{1}{2}} + \frac{i\lambda}{\tau}\psi_{1_{j,k}}^{n+\frac{1}{2}} = 0, \quad (j,k) \in \mathcal{T}_h. \tag{2.29}$$

This gives us a hint to define a mapping $\mathcal{G} = (\mathcal{G}_1, \mathcal{G}_2)$: $(\mu, \nu) \in X_h \times X_h \to (\mathcal{G}_1(\mu, \nu), \mathcal{G}_2(\mu, \nu)) \in X_h \times X_h$ as

$$\mathcal{G}_1(\mu,\nu)_{jk} = \mu_{jk} - \psi_{1_{j,k}}^{n} + \frac{2i}{\tau}\left[-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2} + \frac{\beta_{11}}{2}\left(|\psi_{1_{j,k}}^{n}|^2 + |2\mu_{jk} - \psi_{1_{j,k}}^{n}|^2\right)\right.$$
$$\left.+\frac{\beta_{12}}{2}\left(|\psi_{2_{j,k}}^{n}|^2 + |2\nu_{jk} - \psi_{2_{j,k}}^{n}|^2\right)\right]\mu_{jk} + \frac{i\lambda}{\tau}\nu_{jk}, \quad (j,k) \in \mathcal{T}_h, \tag{2.30}$$

$$\mathcal{G}_2(\mu,\nu)_{jk} = \nu_{jk} - \psi_{2_{j,k}}^{n} + \frac{2i}{\tau}\left[-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2} + \frac{\beta_{21}}{2}\left(|\psi_{1_{j,k}}^{n}|^2 + |2\mu_{jk} - \psi_{1_{j,k}}^{n}|^2\right)\right.$$
$$\left.+\frac{\beta_{22}}{2}\left(|\psi_{2_{j,k}}^{n}|^2 + |2\nu_{jk} - \psi_{2_{j,k}}^{n}|^2\right)\right]\nu_{jk} + \frac{i\lambda}{\tau}\mu_{jk}, \quad (j,k) \in \mathcal{T}_h. \tag{2.31}$$

Taking the inner product of $\mathcal{G}$ and (μ, ν), that is, multiplying (2.30) and (2.31) with μ and ν, respectively, and summing them up, then taking real parts we obtain

$$\begin{aligned} \mathrm{Re}\,\langle \mathcal{G}(\mu,\nu), (\mu,\nu)\rangle &= Re\,\langle \mathcal{G}_1(\mu,\nu), \mu\rangle + Re\,\langle \mathcal{G}_2(\mu,\nu), \nu\rangle \\ &= ||(\mu,\nu)||^2 - \langle (\psi_1^n, \psi_2^n), (\mu,\nu)\rangle \geq ||(\mu,\nu)|| \cdot \left(||(\mu,\nu)|| - ||(\psi_1^n, \psi_2^n)||\right). \end{aligned} \tag{2.32}$$

Let $\alpha = ||(\psi_1^n, \psi_2^n)|| + 1$ in Lemma 2.3, and we observe that there exists a solution $(\mu^*, \nu^*) \in X_h \times X_h$ satisfying $\mathcal{G}(\mu^*, \nu^*) = 0$. Then $(\psi_1^{n+1}, \psi_2^{n+1}) = 2(\mu^*, \nu^*) - (\psi_1^n, \psi_2^n)$ satisfies the scheme (2.5) and (2.6). This completes the proof. ∎

3 | ERROR ESTIMATE OF THE CNFD SCHEME

In this section, we establish the optimal H^2-error estimate of the CNFD scheme without imposing any restriction on the grid ratio. To do this, we need some assumptions and useful lemmas.

(A) Assumption on the external trapping potential $V_m = V_m(x, y)$ for $m = 1, 2$:

$$V_m \in C(\Omega), \quad m = 1, 2;$$

(B) Assumption on the exact solution $\psi_m = \psi_m(x, y, t)$ for $m = 1, 2$:

$$\psi_m \in C^4([0,T]; L^\infty(\Omega)) \cap C^3([0,T]; W^{2,\infty}(\Omega)) \cap C^1([0,T]; W^{4,\infty}(\Omega) \cap H_0^1(\Omega)), \quad m = 1, 2.$$

Lemma 3.1 ([45]). *For any grid function $u \in H^2(\Omega_h)$, there is the following inequality in two dimensions,*

$$||u||_\infty \leq C||u||^{\frac{1}{2}}(||u|| + |u|_2)^{\frac{1}{2}}. \tag{3.1}$$

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In the following, for a function $f = f(x,y,t)$ over $\overline{\Omega} \times [0,T]$, we denote

$$||f||_{L^\infty} := \sup_{t\in[0,T]} \sup_{(x,y)\in\overline{\Omega}} |f(x,y,t)|.$$

Define the local truncation errors of the CNFD scheme $\eta_l^n \in X_h$ for $l = 1,2,\ n = 0,1,2,\dots,N-1$ as

$$\begin{aligned}\eta_{1\,j,k}^{\,n} &:= i\delta_t^+ \phi_{1\,j,k}^{\,n} - \frac{1}{2}\left[-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2} + \frac{\beta_{11}}{2}\left(|\phi_{1\,j,k}^{\,n}|^2 + |\phi_{1\,j,k}^{\,n+1}|^2\right)\right.\\ &\left.+\frac{\beta_{12}}{2}\left(|\phi_{2\,j,k}^{\,n}|^2 + |\phi_{2\,j,k}^{\,n+1}|^2\right)\right]\left(\phi_{1\,j,k}^{\,n} + \phi_{1\,j,k}^{\,n+1}\right) - \frac{\lambda}{4}\left(\phi_{2\,j,k}^{\,n} + \phi_{2\,j,k}^{\,n+1}\right),\\ &(j,k) \in \mathcal{T}_h,\quad n = 0,1,2,\dots,N-1,\end{aligned} \tag{3.2}$$

$$\begin{aligned}\eta_{2\,j,k}^{\,n} &:= i\delta_t^+ \phi_{2\,j,k}^{\,n} - \frac{1}{2}\left[-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2} + \frac{\beta_{21}}{2}\left(|\phi_{1\,j,k}^{\,n}|^2 + |\phi_{1\,j,k}^{\,n+1}|^2\right)\right.\\ &\left.+\frac{\beta_{22}}{2}\left(|\phi_{2\,j,k}^{\,n}|^2 + |\phi_{2\,j,k}^{\,n+1}|^2\right)\right]\left(\phi_{2\,j,k}^{\,n} + \phi_{2\,j,k}^{\,n+1}\right) - \frac{\lambda}{4}\left(\phi_{1\,j,k}^{\,n} + \phi_{1\,j,k}^{\,n+1}\right),\\ &(j,k) \in \mathcal{T}_h,\quad n = 0,1,2,\dots,N-1.\end{aligned} \tag{3.3}$$

By using Taylor's expansion and the boundary conditions, one can obtain the following lemma.

Lemma 3.2 (local truncation error). *Under assumptions (A) and (B), we have the following estimates for the local truncation errors*:

$$|\eta_{l\,j,k}^{\,n}| \lesssim \tau^2 + h^2,\quad l = 1,2,\quad (j,k) \in \mathcal{T}_h,\quad n = 0,1,2,\dots,N-1, \tag{3.4}$$

$$|\delta_t^+ \eta_{l\,j,k}^{\,n}| \lesssim \tau^2 + h^2,\ \ l = 1,2,\quad (j,k) \in \mathcal{T}_h,\quad n = 0,1,2,\dots,N-2. \tag{3.5}$$

Choose a smooth function $\rho \in C^1(\mathbb{R})$ such that $\rho(s) = 1$ when $|s| \le 1$, $\rho(s) = 0$ when $|s| \ge 2$, and $0 \le \rho(s) \le 1$ for $s \in \mathbb{R}$, for example,

$$\rho(s) = \begin{cases} 1, & |s| \in [0,1],\\ 1 - (|s|-1)^2 + 2(|s|-1)^2(|s|-2), & |s| \in [1,2],\\ 0, & |s| \in [2,\infty).\end{cases}$$

Lemma 3.3 (*cut-off* function). *By assumption (B), we can define $M_0 = ||\psi||_{L^\infty(\Omega\times[0,T])}$, and choose a positive number $B = M_0 + 1$. For $s \ge 0$, define*

$$f_B(s) = s\rho(\sqrt{s}/B). \tag{3.6}$$

Then $f_B(s)$ is global Lipschitz and

$$|f_B(s_1) - f_B(s_2)| \le C_B\left|\sqrt{s_1} - \sqrt{s_2}\right|,\quad \forall s_1, s_2 \ge 0, \tag{3.7}$$

where $C_B = 4B\left(1 + \max_{\xi\in[1,2]} |\rho'(\xi)|\right)$.

Proof. We do different analysis for different situations. If $\|s_1\|_{L^\infty} \ge 4B^2$ and $\|s_2\|_{L^\infty} \ge 4B^2$, the inequality (3.7) is obvious. If $\|s_1\|_{L^\infty} < 4B^2$ and $\|s_2\|_{L^\infty} \ge 4B^2$, we have

$$\begin{aligned}|f_B(s_1) - f_B(s_2)| &= \left|s_1\rho(\sqrt{s_1}/B) - s_2\rho(\sqrt{s_2}/B)\right| = \left|s_1\left(\rho(\sqrt{s_1}/B) - \rho(\sqrt{s_2}/B)\right)\right|\\ &= \left|s_1\rho'(\xi)\left(\sqrt{s_1}/B - \sqrt{s_2}/B\right)\right| \le 4B\max_{\xi\in[1,2]}\left|\rho'(\xi)\right|\left|\sqrt{s_1} - \sqrt{s_2}\right|.\end{aligned} \tag{3.8}$$

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Similarly, the result also holds for the case $\|s_1\|_{L^\infty} \geq 4B^2$ and $\|s_2\|_{L^\infty} < 4B^2$. If $\|s_1\|_{L^\infty} < 4B^2$ and $\|s_2\|_{L^\infty} < 4B^2$, we have

$$
\begin{aligned}
|f_B(s_1) - f_B(s_2)| &= \left|s_1\rho(\sqrt{s_1}/B) - s_2\rho(\sqrt{s_2}/B)\right| \\
&\leq \left|(s_1 - s_2)\rho(\sqrt{s_1}/B)\right| + \left|s_2\left(\rho(\sqrt{s_1}/B) - \rho(\sqrt{s_2}/B)\right)\right| \\
&\leq |s_1 - s_2| + \left|s_2\rho'(\xi)\left(\sqrt{s_1}/B - \sqrt{s_2}/B\right)\right| \\
&\leq 4B\left(1 + \max_{\xi\in[1,2]}|\rho'(\xi)|\right)\left|\sqrt{s_1} - \sqrt{s_2}\right|. \qquad (3.9)
\end{aligned}
$$

This completes the proof. ■

Define "error" functions $e_l^n \in X_h$ for $l = 1, 2$ and $n = 0, 1, 2, \dots, N$ as

$$e_{ljk}^n = \phi_{ljk}^n - \psi_{ljk}^n, \quad (j,k) \in \mathring{\mathcal{T}}_h, \qquad (3.10)$$

then we have

Theorem 3.1. *Under assumptions (A) and (B), there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \leq h_0$ and $0 < \tau \leq \tau_0$, we have the following optimal error estimate for the CNFD scheme*:

$$\|e_l^n\| \lesssim h^2 + \tau^2, \quad |e_l^n|_2 \lesssim 1, \quad \|e_l^n\|_\infty \lesssim 1, \quad l = 1, 2, \ \ n = 1, 2, 3, \dots, N. \qquad (3.11)$$

Proof. For simplicity and clarity, we split our proof into four steps.

Step 1. Construction of an alternative scheme by using the *cut-off* function to truncate the nonlinearity into a global Lipschitz function with compact support.

Choose $\hat{\psi}_l^0 = \psi_l^0$ and define $\hat{\psi}_l^n \in X_h$ for $l = 1, 2$ and $n = 0, 1, 2, \dots, N$ as the solution of the following finite difference equations,

$$
\begin{aligned}
i\delta_t^+\hat{\psi}_{1j,k}^n = \frac{1}{2}\Big[&-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2} + \frac{\beta_{11}}{2}\left(f_B(|\hat{\psi}_{1j,k}^n|^2) + f_B(|\hat{\psi}_{1j,k}^{n+1}|^2)\right) \\
&+\frac{\beta_{12}}{2}\left(f_B(|\hat{\psi}_{2j,k}^n|^2) + f_B(|\hat{\psi}_{2j,k}^{n+1}|^2)\right)\Big]\left(\hat{\psi}_{1j,k}^n + \hat{\psi}_{1j,k}^{n+1}\right) + \frac{\lambda}{4}\left(\hat{\psi}_{2j,k}^n + \hat{\psi}_{2j,k}^{n+1}\right), \\
&(j,k) \in \mathcal{T}_h, \ \ n = 0, 1, 2, \dots, N-1, \qquad (3.12)
\end{aligned}
$$

$$
\begin{aligned}
i\delta_t^+\hat{\psi}_{2j,k}^n = \frac{1}{2}\Big[&-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2} + \frac{\beta_{21}}{2}\left(f_B(|\hat{\psi}_{1j,k}^n|^2) + f_B(|\hat{\psi}_{1j,k}^{n+1}|^2)\right) \\
&+\frac{\beta_{22}}{2}\left(f_B(|\hat{\psi}_{2j,k}^n|^2) + f_B(|\hat{\psi}_{2j,k}^{n+1}|^2)\right)\Big]\left(\hat{\psi}_{2j,k}^n + \hat{\psi}_{2j,k}^{n+1}\right) + \frac{\lambda}{4}\left(\hat{\psi}_{1j,k}^n + \hat{\psi}_{1j,k}^{n+1}\right), \\
&(j,k) \in \mathcal{T}_h, \ \ n = 0, 1, 2, \dots, N-1. \qquad (3.13)
\end{aligned}
$$

Define grid functions $\hat{\eta}_l^n \in X_h$ for $l = 1, 2$ as

$$
\begin{aligned}
\hat{\eta}_{1j,k}^n = i\delta_t^+\phi_{1j,k}^n - \frac{1}{2}\Big[&-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2} + \frac{\beta_{11}}{2}\left(f_B(|\phi_{1j,k}^n|^2) + f_B(|\phi_{1j,k}^{n+1}|^2)\right) \\
&+\frac{\beta_{12}}{2}\left(f_B(|\phi_{2j,k}^n|^2) + f_B(|\phi_{2j,k}^{n+1}|^2)\right)\Big]\left(\phi_{1j,k}^n + \phi_{1j,k}^{n+1}\right) - \frac{\lambda}{4}\left(\phi_{2j,k}^n + \phi_{2j,k}^{n+1}\right), \\
&(j,k) \in \mathcal{T}_h, \ \ n = 0, 1, 2, \dots, N-1, \qquad (3.14)
\end{aligned}
$$

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$$\hat{\eta}_{2j,k}^{\ n} = i\delta_t^+ \phi_{2j,k}^{\ n} - \frac{1}{2}\left[-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2} + \frac{\beta_{21}}{2}\left(f_B(|\phi_{1j,k}^{\ n}|^2) + f_B(|\phi_{1j,k}^{\ n+1}|^2)\right)\right.$$
$$\left. + \frac{\beta_{22}}{2}\left(f_B(|\phi_{2j,k}^{\ n}|^2) + f_B(|\phi_{2j,k}^{\ n+1}|^2)\right)\right]\left(\phi_{2j,k}^{\ n} + \phi_{2j,k}^{\ n+1}\right) - \frac{\lambda}{4}\left(\phi_{1j,k}^{\ n} + \phi_{1j,k}^{\ n+1}\right),$$
$$(j,k) \in \mathcal{T}_h, \quad n = 0,1,2,\ \dots\ ,N-1. \tag{3.15}$$

Noticing the fact

$$f_B(|\phi_{lj,k}^{\ n}|^2) = |\phi_{lj,k}^{\ n}|^2, \quad (j,k) \in \mathcal{T}_h, \quad l = 1,2, \quad n = 0,1,2,\ \dots\ ,N-1,$$

we know from (3.2) and (3.3) that $\hat{\eta}_1^{\ n}$ and $\hat{\eta}_2^{\ n}$ just are η_1^n and η_2^n, respectively, the local truncation errors of the finite difference scheme (2.5) and (2.6). Hence, the finite difference equations (3.12) and (3.13) can be viewed as another finite difference scheme of the CGPEs (2.1) and (2.2), and consequently $\hat{\psi}_{lj,k}^{\ n}$ can be viewed as another approximation of $\psi_l(x_j, y_k, t_n)$ for $l = 1,2$.

Step 2. Error estimate of the alternative scheme by using the standard energy method.

Define "error" functions $\hat{e}_l^{\ n} \in X_h$ for $l = 1,2,\ n = 0,1,2,\ \dots\ ,N$ as

$$\hat{e}_{lj,k}^{\ n} = \phi_{lj,k}^{\ n} - \hat{\psi}_{lj,k}^{\ n}. \tag{3.16}$$

Subtracting (3.12) and (3.13) from (3.14) and (3.15), respectively, we obtain "error" equations as follows,

$$i\delta_t^+ \hat{e}_{1j,k}^{\ n} - \frac{1}{2}\left(-\frac{1}{2}\Delta_h + V_{1_{j,k}} + ik_0\delta_x + \frac{\alpha}{2}\right)\left(\hat{e}_{1j,k}^{\ n} + \hat{e}_{1j,k}^{\ n+1}\right)$$
$$- \frac{\lambda}{4}\left(\hat{e}_{2j,k}^{\ n} + \hat{e}_{2j,k}^{\ n+1}\right) - \hat{\xi}_{1j,k}^{\ n+1} = \eta_{1j,k}^{\ n}, \quad (j,k) \in \mathcal{T}_h, \quad n = 0,1,2,\ \dots\ ,N-1, \tag{3.17}$$

$$i\delta_t^+ \hat{e}_{2j,k}^{\ n} - \frac{1}{2}\left(-\frac{1}{2}\Delta_h + V_{2_{j,k}} - ik_0\delta_x - \frac{\alpha}{2}\right)\left(\hat{e}_{2jk}^{\ n} + \hat{e}_{2j,k}^{\ n+1}\right)$$
$$- \frac{\lambda}{4}\left(\hat{e}_{1j,k}^{\ n} + \hat{e}_{1j,k}^{\ n+1}\right) - \hat{\xi}_{2j,k}^{\ n+1} = \eta_{2j,k}^{\ n}, \quad (j,k) \in \mathcal{T}_h, \quad n = 0,1,2,\ \dots\ ,N-1, \tag{3.18}$$

where $\hat{\xi}_1^{\ n+1}, \hat{\xi}_2^{\ n+1} \in X_h$ for $n = 0,1,2,\ \dots\ ,N-1$ are defined as

$$\begin{aligned}
\hat{\xi}_{1j,k}^{\ n+1} &= \frac{1}{2}\left[\frac{\beta_{11}}{2}\left(|\phi_{1j,k}^{\ n}|^2 + |\phi_{1j,k}^{\ n+1}|^2\right) + \frac{\beta_{12}}{2}\left(|\phi_{2j,k}^{\ n}|^2 + |\phi_{2j,k}^{\ n+1}|^2\right)\right]\left(\phi_{1j,k}^{\ n} + \phi_{1j,k}^{\ n+1}\right) \\
&\quad - \frac{1}{2}\left[\frac{\beta_{11}}{2}\left(f_B(|\hat{\psi}_{1j,k}^{\ n}|^2) + f_B(|\hat{\psi}_{1j,k}^{\ n+1}|^2)\right) + \frac{\beta_{12}}{2}\left(f_B(|\hat{\psi}_{2j,k}^{\ n}|^2) + f_B(|\hat{\psi}_{2j,k}^{\ n+1}|^2)\right)\right] \\
&\quad \times \left(\hat{\psi}_{1jk}^{\ n} + \hat{\psi}_{1j,k}^{\ n+1}\right) \\
&= \frac{1}{2}\left[\frac{\beta_{11}}{2}\left(f_B(|\phi_{1j,k}^{\ n}|^2) - f_B(|\hat{\psi}_{1j,k}^{\ n}|^2) + f_B(|\phi_{1j,k}^{\ n+1}|^2) - f_B(|\hat{\psi}_{1j,k}^{\ n+1}|^2)\right)\right. \\
&\quad \left. + \frac{\beta_{12}}{2}\left(f_B(|\phi_{2j,k}^{\ n}|^2) - f_B(|\hat{\psi}_{2j,k}^{\ n}|^2) + f_B(|\phi_{2j,k}^{\ n+1}|^2) - f_B(|\hat{\psi}_{2j,k}^{\ n+1}|^2)\right)\right]\left(\phi_{1j,k}^{\ n} + \phi_{1j,k}^{\ n+1}\right) \\
&\quad + \frac{1}{2}\left[\frac{\beta_{11}}{2}\left(f_B(|\hat{\psi}_{1j,k}^{\ n}|^2) + f_B(|\hat{\psi}_{1j,k}^{\ n+1}|^2)\right) + \frac{\beta_{12}}{2}\left(f_B(|\hat{\psi}_{2j,k}^{\ n}|^2) + f_B(|\hat{\psi}_{2j,k}^{\ n+1}|^2)\right)\right] \\
&\quad \times \left(\hat{e}_{1j,k}^{\ n} + \hat{e}_{1j,k}^{\ n+1}\right), \quad (j,k) \in \mathcal{T}_h,
\end{aligned} \tag{3.19}$$

$$\begin{aligned}
\hat{\xi}_{2j,k}^{\ n+1} &= \frac{1}{2}\left[\frac{\beta_{21}}{2}\left(|\phi_{1j,k}^{\ n}|^2 + |\phi_{1j,k}^{\ n+1}|^2\right) + \frac{\beta_{22}}{2}\left(|\phi_{2j,k}^{\ n}|^2 + |\phi_{2j,k}^{\ n+1}|^2\right)\right]\left(\phi_{2j,k}^{\ n} + \phi_{2j,k}^{\ n+1}\right) \\
&\quad - \frac{1}{2}\left[\frac{\beta_{21}}{2}\left(f_B(|\hat{\psi}_{1j,k}^{\ n}|^2) + f_B(|\hat{\psi}_{1j,k}^{\ n+1}|^2)\right) + \frac{\beta_{22}}{2}\left(f_B(|\hat{\psi}_{2j,k}^{\ n}|^2) + f_B(|\hat{\psi}_{2j,k}^{\ n+1}|^2)\right)\right]
\end{aligned}$$

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$$\times\left(\hat{\psi}_{2_{j,k}}^{\,n}+\hat{\psi}_{2_{j,k}}^{\,n+1}\right)$$
$$=\frac{1}{2}\left[\frac{\beta_{21}}{2}\left(f_B(|\phi_{1_{j,k}}^{\,n}|^2)-f_B(|\hat{\psi}_{1_{j,k}}^{\,n}|^2)+f_B(|\phi_{1_{j,k}}^{\,n+1}|^2)-f_B(|\hat{\psi}_{1_{j,k}}^{\,n+1}|^2)\right)\right.$$
$$\left.+\frac{\beta_{22}}{2}\left(f_B(|\phi_{2_{j,k}}^{\,n}|^2)-f_B(|\hat{\psi}_{2_{j,k}}^{\,n}|^2)+f_B(|\phi_{2_{j,k}}^{\,n+1}|^2)-f_B(|\hat{\psi}_{2_{j,k}}^{\,n+1}|^2)\right)\right]\left(\phi_{2_{j,k}}^{\,n}+\phi_{2_{j,k}}^{\,n+1}\right)$$
$$+\frac{1}{2}\left[\frac{\beta_{21}}{2}\left(f_B(|\hat{\psi}_{1_{j,k}}^{\,n}|^2)+f_B(|\hat{\psi}_{1_{j,k}}^{\,n+1}|^2)\right)+\frac{\beta_{22}}{2}\left(f_B(|\hat{\psi}_{2_{j,k}}^{\,n}|^2)+f_B(|\hat{\psi}_{2_{j,k}}^{\,n+1}|^2)\right)\right]$$
$$\times\left(\hat{e}_{2_{j,k}}^{\,n}+\hat{e}_{2_{j,k}}^{\,n+1}\right),\quad (j,k)\in\mathcal{T}_h. \tag{3.20}$$

These together with (3.7) and the definition of f_B give

$$|\hat{\xi}_{1_{j,k}}^{\,n+1}|\le C(|\hat{e}_{1_{j,k}}^{\,n}|+|\hat{e}_{1_{j,k}}^{\,n+1}|+|\hat{e}_{2_{j,k}}^{\,n}|+|\hat{e}_{2_{j,k}}^{\,n+1}|), \tag{3.21}$$

$$|\hat{\xi}_{2_{j,k}}^{\,n+1}|\le C(|\hat{e}_{1_{j,k}}^{\,n}|+|\hat{e}_{1_{j,k}}^{\,n+1}|+|\hat{e}_{2_{j,k}}^{\,n}|+|\hat{e}_{2_{j,k}}^{\,n+1}|). \tag{3.22}$$

Computing the inner product of (3.17) and (3.18) with $\hat{e}_1{}^n+\hat{e}_1{}^{n+1}$ and $\hat{e}_2{}^n+\hat{e}_2{}^{n+1}$, respectively, then taking the imaginary part of the results, we obtain

$$\frac{1}{\tau}\left(||\hat{e}_1{}^{n+1}||^2-||\hat{e}_1{}^n||^2\right)-\frac{\lambda}{4}\mathrm{Im}\left\langle\hat{e}_2{}^n+\hat{e}_2{}^{n+1},\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle$$
$$-\mathrm{Im}\left\langle\hat{\xi}_1{}^{n+1},\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle=\mathrm{Im}\left\langle\eta_1^n,\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle,\quad n=0,1,2,\ \dots\ ,N-1, \tag{3.23}$$

$$\frac{1}{\tau}\left(||\hat{e}_2{}^{n+1}||^2-||\hat{e}_2{}^n||^2\right)-\frac{\lambda}{4}\mathrm{Im}\left\langle\hat{e}_1{}^n+\hat{e}_1{}^{n+1},\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle$$
$$-\mathrm{Im}\left\langle\hat{\xi}_2{}^{n+1},\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle=\mathrm{Im}\left\langle\eta_2^n,\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle,\quad n=0,1,2,\ \dots\ ,N-1. \tag{3.24}$$

Adding (3.24) to (3.23) and using the equality

$$\mathrm{Im}\left\langle\hat{e}_2{}^n+\hat{e}_2{}^{n+1},\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle+\mathrm{Im}\left\langle\hat{e}_1{}^n+\hat{e}_1{}^{n+1},\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle=0 \tag{3.25}$$

yield

$$||\hat{e}_1{}^{n+1}||^2+||\hat{e}_2{}^{n+1}||^2-||\hat{e}_1{}^n||^2-||\hat{e}_2{}^n||^2$$
$$=\tau\mathrm{Im}\left\langle\hat{\xi}_1{}^{n+1},\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle+\tau\mathrm{Im}\left\langle\hat{\xi}_2{}^{n+1},\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle$$
$$+\tau\mathrm{Im}\left\langle\eta_1^n,\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle+\tau\mathrm{Im}\left\langle\eta_2^n,\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle \tag{3.26}$$

for $n=0,1,2,\ \dots\ ,N-1$. By using Cauchy's inequality, Lemma 3.2 and (3.21) and (3.22), one can obtain

$$\left|\mathrm{Im}\left\langle\hat{\xi}_1{}^{n+1},\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle\right|\le\frac{1}{2}||\hat{\xi}_1{}^{n+1}||^2+||\hat{e}_1{}^n||^2+||\hat{e}_1{}^{n+1}||^2$$
$$\le C(||\hat{e}_1{}^n||^2+||\hat{e}_1{}^{n+1}||^2+||\hat{e}_2{}^n||^2+||\hat{e}_2{}^{n+1}||^2), \tag{3.27}$$

$$\left|\mathrm{Im}\left\langle\hat{\xi}_2{}^{n+1},\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle\right|\le C(||\hat{e}_1{}^n||^2+||\hat{e}_1{}^{n+1}||^2+||\hat{e}_2{}^n||^2+||\hat{e}_2{}^{n+1}||^2), \tag{3.28}$$

$$\left|\mathrm{Im}\left\langle\eta_1^n,\hat{e}_1{}^n+\hat{e}_1{}^{n+1}\right\rangle\right|\le\frac{1}{2}||\eta_1^n||^2+||\hat{e}_1{}^n||^2+||\hat{e}_1{}^{n+1}||^2$$
$$\le C(h^2+\tau^2)^2+C(||\hat{e}_1{}^n||^2+||\hat{e}_1{}^{n+1}||^2), \tag{3.29}$$

$$\left|\mathrm{Im}\left\langle\eta_2^n,\hat{e}_2{}^n+\hat{e}_2{}^{n+1}\right\rangle\right|\le C(h^2+\tau^2)^2+C(||\hat{e}_2{}^n||^2+||\hat{e}_2{}^{n+1}||^2). \tag{3.30}$$

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Plugging (3.27)–(3.30) into (3.26) gives

$$
\begin{aligned}
&||\hat{e}_1{}^{n+1}||^2 + ||\hat{e}_2{}^{n+1}||^2 - ||\hat{e}_1{}^{n}||^2 - ||\hat{e}_2{}^{n}||^2 \\
&\quad \le C\tau\left[\left(h^2+\tau^2\right)^2 + ||\hat{e}_1{}^{n+1}||^2 + ||\hat{e}_2{}^{n+1}||^2 - ||\hat{e}_1{}^{n}||^2 - ||\hat{e}_2{}^{n}||^2\right], \quad 0 \le n < N. \qquad (3.31)
\end{aligned}
$$

By using Gronwall's inequality, we obtain from (3.31) that, if τ is small enough, there is

$$
||\hat{e}_1{}^{n}|| + ||\hat{e}_2{}^{n}|| \le C(\tau^2 + h^2), \quad n = 1, 2, \dots, N. \qquad (3.32)
$$

Step 3. Equivalence of the two schemes for sufficiently small h and τ.

By using a lifting technique (see [40]), we obtain from (3.17) that

$$
\begin{aligned}
|\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|_2 &= ||4i\delta_t^+\hat{e}_1{}^{n} - 2V_1\left(\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}\right) - 2ik_0\delta_x\left(\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}\right) \\
&\quad - \alpha\left(\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}\right) - \lambda\left(\hat{e}_2{}^{n} + \hat{e}_2{}^{n+1}\right) - 4\hat{\xi}_1{}^{n+1} - 4\eta_1^n|| \\
&\le C(||\delta_t^+\hat{e}_1{}^{n}|| + ||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|| + ||\hat{e}_2{}^{n} + \hat{e}_2{}^{n+1}|| + ||\delta_x(\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1})|| \\
&\quad + ||\hat{\xi}_1{}^{n+1}|| + ||\eta_1^n||), \quad n = 0, 1, 2, \dots, N-1. \qquad (3.33)
\end{aligned}
$$

For the estimate of the first term on the right hand side of (3.33), by using (3.32), we have

$$
||\delta_t^+\hat{e}_1{}^{n}|| \le \tau^{-1}(||\hat{e}_1{}^{n+1}|| + ||\hat{e}_1{}^{n}||) \le C\tau^{-1}(h^2 + \tau^2). \qquad (3.34)
$$

For the estimates of the second term and the third term on the right hand side of (3.33), by using (3.32), we have

$$
||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|| \le ||\hat{e}_1{}^{n}|| + ||\hat{e}_1{}^{n+1}|| \le C(h^2 + \tau^2), \qquad (3.35)
$$

$$
||\hat{e}_2{}^{n} + \hat{e}_2{}^{n+1}|| \le ||\hat{e}_2{}^{n}|| + ||\hat{e}_2{}^{n+1}|| \le C(h^2 + \tau^2). \qquad (3.36)
$$

For the estimate of the fourth term on the right hand side of (3.33), we have

$$
\begin{aligned}
C||\delta_x(\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1})|| &\le C|\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|_1 \le C|\hat{e}_1{}^{n} + \hat{e}^{n+1}|_2^{\frac{1}{2}}||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}||^{\frac{1}{2}} \\
&\le \frac{1}{2}|\hat{e}_1{}^{n} + \hat{e}^{n+1}|_2 + C||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|| \le \frac{1}{2}|\hat{e}_1{}^{n} + \hat{e}^{n+1}|_2 + C(h^2 + \tau^2). \\
&\qquad (3.37)
\end{aligned}
$$

For the estimates of the last two terms on the right hand side of (3.33), by using (3.21), (3.22), (3.32) and Lemma 3.2, we obtain

$$
||\hat{\xi}_1{}^{n+1}|| + ||\eta_1^n|| \le C(h^2 + \tau^2). \qquad (3.38)
$$

Plugging (3.34)–(3.38) into (3.33) yields

$$
|\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|_2 \le C\tau^{-1}(h^2 + \tau^2), \quad n = 0, 1, 2, \dots, N-1. \qquad (3.39)
$$

This, together with Lemma 3.1 and (3.32), gives

$$
\begin{aligned}
||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}||_\infty &\le ||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}||^{\frac{1}{2}}(||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|| + |\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}|_2)^{\frac{1}{2}} \\
&\le C\tau^{-\frac{1}{2}}(h^2 + \tau^2), \quad n = 0, 1, 2, \dots, N-1. \qquad (3.40)
\end{aligned}
$$

By using Minkowski's inequality and (3.40), one can obtain

$$
||\hat{e}_1{}^{n+1}||_\infty - ||\hat{e}_1{}^{n}||_\infty \le ||\hat{e}_1{}^{n} + \hat{e}_1{}^{n+1}||_\infty \le C\tau^{-\frac{1}{2}}(h^2 + \tau^2), \quad n = 0, 1, 2, \dots, N-1. \qquad (3.41)
$$

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Summing (3.41) for n from 0 to m, then replacing m by n, we obtain

$$||\hat{e_1}^{n+1}||_\infty \le C(n+1)\tau^{-\frac{1}{2}}(h^2+\tau^2) \le C\tau^{-\frac{3}{2}}(h^2+\tau^2) = C(\tau^{-\frac{3}{2}}h^2+\tau^{\frac{1}{2}}), \quad n=0,1,2,\ldots,N-1. \tag{3.42}$$

This tells us that, if τ is small enough and $\frac{\tau}{h} \ge 1$, there is

$$||\hat{e_1}^n||_\infty \le 1, \quad n=1,2,\ldots,N. \tag{3.43}$$

On the other hand, by using Lemma 3.1 and the inverse Sobolev's inequality, we have

$$||\hat{e_1}^n||_\infty \le ||\hat{e_1}^n||^{\frac{1}{2}}(||\hat{e_1}^n||+|\hat{e_1}^n|_2)^{\frac{1}{2}} \le ||\hat{e_1}^n||^{\frac{1}{2}}(||\hat{e_1}^n||+h^{-2}||\hat{e_1}^n||)^{\frac{1}{2}} \le Ch^{-1}(h^2+\tau^2) = C(h^{-1}\tau^2+h), \quad n=0,1,2,\ldots,N-1. \tag{3.44}$$

This tells us that, if h is small enough and $\frac{\tau}{h} \le 1$, there still is

$$||\hat{e_1}^n||_\infty \le 1, \quad n=0,1,2,\ldots,N. \tag{3.45}$$

Hence, for sufficiently small h and τ, without any restriction on $\frac{\tau}{h}$, it is always true to have

$$||\hat{e_1}^n||_\infty \le 1, \quad n=0,1,2,\ldots,N. \tag{3.46}$$

Hence, if τ and h are small enough, there is

$$||\hat{\psi_1}^n||_\infty \le ||\phi_1^n||_\infty + ||\hat{e_1}^n||_\infty \le M_0+1 = \sqrt{B}, \quad n=1,2,\ldots,N. \tag{3.47}$$

Similarly, when h and τ are small enough, we can obtain

$$||\hat{\psi_2}^n||_\infty \le M_0+1 = \sqrt{B}, \quad n=1,2,\ldots,N. \tag{3.48}$$

Thus, when $h \le h_0$ and $\tau \le \tau_0$ for a small h_0 and a small τ_0, we know from the definition of the function f_B that,

$$f_B(|\hat{\psi}_{ljk}^n|^2) = |\hat{\psi}_{ljk}^n|^2, \quad l=1,2, \quad (j,k)\in \mathring{\mathcal{T}}_h, \quad n=0,1,2,\ldots,N. \tag{3.49}$$

This implies that, when $h \le h_0$ and $\tau \le \tau_0$, the scheme (3.12) and (3.13) is just the scheme (2.5) and (2.6), and consequently we obtain

$$||e_l^n|| \lesssim \tau^2+h^2, \quad ||e_l^n||_\infty \lesssim 1, \quad l=1,2, \quad n=1,2,\ldots,N. \tag{3.50}$$

Step 4. Boundedness of the numerical solution in the discrete H^2 norm.

By using Minkowski's inequality and (3.39), one can obtain

$$|e_1^{n+1}|_2 - |e_1^n|_2 \lesssim \tau^{-1}(h^2+\tau^2), \quad n=0,1,2,\ldots,N-1, \tag{3.51}$$

this gives

$$|e_1^n|_2 \lesssim \tau^{-2}h^2+1, \quad n=1,2,\ldots,N. \tag{3.52}$$

Similarly, there is

$$|e_2^n|_2 \lesssim \tau^{-2}h^2+1, \quad n=1,2,\ldots,N. \tag{3.53}$$

On the other hand, one can obtain that

$$|e_l^n|_2 \lesssim h^{-2}||e_l^n|| \lesssim h^{-2}\tau^2+1, \quad n=1,2,\ldots,N. \tag{3.54}$$

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Hence, for sufficiently small τ and h, we obtain from (3.52) to (3.54) that it is always true to have

$$|e_l^n|_2 \lesssim 1, \quad n = 1, 2, \dots, N. \tag{3.55}$$

This completes the proof. ∎

In order to establish the error estimate of the CNFD scheme in the discrete H^2 norm, we define two difference quotient operators Δ_h^+ and Δ_h^- by $\Delta_h^{\pm} v = (\Delta_h \pm 2ik_0\delta_x)v$ for any $v \in X_h$, and then give some lemmas on the two operators.

Lemma 3.4. *For any grid function $u \in H^2(\Omega_h) \bigcap H_0^1(\Omega_h)$, we have*

$$\mathrm{Im}\langle u, \Delta_h^{\pm} u\rangle = 0, \tag{3.56}$$

$$|u|_2 - ||u|| \lesssim ||\Delta_h^{\pm} u|| \lesssim |u|_2 + ||u||, \tag{3.57}$$

$$||\Delta_h^{\mp} u|| - ||u|| \lesssim ||\Delta_h^{\pm} u|| \lesssim ||\Delta_h^{\mp} u|| + ||u||. \tag{3.58}$$

Proof. Direct calculation gives

$$\begin{aligned}\mathrm{Im}\langle u, \Delta_h^{\pm} u\rangle &= \mathrm{Im}\langle u, \Delta_h u \pm 2ik_0\delta_x u\rangle = \mathrm{Im}\langle u, \Delta_h u\rangle \pm \mathrm{Im}\langle u, 2ik_0\delta_x u\rangle \\ &= \mp \mathrm{Re}\langle u, 2k_0\delta_x u\rangle,\end{aligned} \tag{3.59}$$

and

$$\begin{aligned}\langle u, 2k_0\delta_x u\rangle &= -\mathrm{Re}\langle 2k_0\delta_x u, u\rangle, \\ \mathrm{Re}\langle u, 2k_0\delta_x u\rangle &= \mathrm{Re}\langle 2k_0\delta_x u, u\rangle,\end{aligned} \tag{3.60}$$

which give

$$\mathrm{Re}\langle u, 2k_0\delta_x u\rangle = 0. \tag{3.61}$$

Combining (3.59) and (3.61) immediately gives (3.56). Now we split the proof of (3.57) into two parts, that is,

$$\begin{aligned}||\Delta_h^{\pm} u|| &= \|\Delta_h u \pm 2ik_0\delta_x u\| \le |u|_2 + \langle \pm 2ik_0\delta_x u, \pm 2ik_0\delta_x u\rangle^{\frac{1}{2}} \\ &= |u|_2 + 2k_0\langle \delta_x^2 u, -u\rangle^{\frac{1}{2}} \le |u|_2 + 2k_0\|\delta_x^2 u\|^{\frac{1}{2}}\|u\|^{\frac{1}{2}} \\ &\le |u|_2 + 2k_0|u|_2^{\frac{1}{2}}\|u\|^{\frac{1}{2}} \le |u|_2 + k_0(|u|_2 + \|u\|),\end{aligned} \tag{3.62}$$

and

$$\begin{aligned}\|\Delta_h^{\pm} u\| &= \|\Delta_h u \pm 2ik_0\delta_x u\| \ge |u|_2 - \langle \pm 2ik_0\delta_x u, \pm 2ik_0\delta_x u\rangle^{\frac{1}{2}} \\ &= |u|_2 - 2k_0\langle \delta_x^2 u, -u\rangle^{\frac{1}{2}} \ge |u|_2 - 2k_0\|\delta_x^2 u\|^{\frac{1}{2}}\|u\|^{\frac{1}{2}} \\ &\ge |u|_2 - 2k_0|u|_2^{\frac{1}{2}}\|u\|^{\frac{1}{2}} \ge |u|_2 - (\varepsilon|u|_2 + \frac{k_0}{\varepsilon}\|u\|)\end{aligned} \tag{3.63}$$

for any $\varepsilon > 0$. Combining (3.62) and (3.63) gives (3.57), and (3.58) can be directly obtained from (3.57). This completes the proof. ∎

Lemma 3.5. *For a series of grid functions $\{u^n \in H^2(\Omega_h) | n = 0, 1, 2, 3, \dots\}$, we have*

$$\mathrm{Re}\langle \Delta_h^{\pm}(u^{n+1} + u^n), \delta_t^+ \Delta_h^{\pm} u^n\rangle = \frac{1}{\tau}(\|\Delta_h^{\pm} u^{n+1}\|^2 - \|\Delta_h^{\pm} u^n\|^2). \tag{3.64}$$

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Proof. Direct calculation gives

$$
\begin{aligned}
&\mathrm{Re}\langle \Delta_h^{\pm}(u^{n+1}+u^n), \delta_t^+\Delta_h^{\pm}u^n\rangle \\
&= \frac{1}{\tau}\mathrm{Re}\langle \Delta_h^{\pm}(u^{n+1}+u^n), \Delta_h^{\pm}(u^{n+1}-u^n)\rangle \\
&= \frac{1}{\tau}(\|\Delta_h^{\pm}u^{n+1}\|^2 - \|\Delta_h^{\pm}u^n\|^2) + \frac{1}{\tau}\mathrm{Re}(\langle u^n, \Delta_h^{\pm}u^{n+1}\rangle - \overline{\langle u^n, \Delta_h^{\pm}u^{n+1}\rangle}) \\
&= \frac{1}{\tau}(\|\Delta_h^{\pm}u^{n+1}\|^2 - \|\Delta_h^{\pm}u^n\|^2).
\end{aligned}
$$

This completes the proof. ∎

Theorem 3.2. *Under assumptions (A) and (B), there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, we have the following optimal error estimate for the CNFD scheme*

$$
|||e_l^n|||_2 \lesssim h^2+\tau^2, \quad ||e_l^n||_\infty \lesssim h^2+\tau^2, \quad l=1,2, \quad n=1,2,\ldots,N. \tag{3.65}
$$

Proof. Thanks to Theorem 3.1, one can see that the "error" equations of the CNFD scheme is same to the "error" Equations (3.17) and (3.18) with $f_B = f$. By using the operators $\Delta_h^{\pm}$, the "error" equations can be rewritten as

$$
\begin{aligned}
&i\delta_t^+ e_{1_{j,k}}^{\,n} - \frac{1}{2}\left(-\frac{1}{2}\Delta_h^- + V_{1_{j,k}} + \frac{\alpha}{2}\right)\left(e_{1_{j,k}}^{\,n} + e_{1_{j,k}}^{\,n+1}\right) - \frac{\lambda}{4}\left(e_{2_{j,k}}^{\,n} + e_{2_{j,k}}^{\,n+1}\right) - \xi_{1_{j,k}}^{\,n+1} = \eta_{1_{j,k}}^{\,n}, \\
&\qquad (j,k)\in\mathcal{T}_h, \quad n=0,1,2,\ldots,N-1,
\end{aligned}
\tag{3.66}
$$

$$
\begin{aligned}
&i\delta_t^+ e_{2_{j,k}}^{\,n} - \frac{1}{2}\left(-\frac{1}{2}\Delta_h^+ + V_{2_{j,k}} - \frac{\alpha}{2}\right)\left(e_{2_{jk}}^{\,n} + e_{2_{j,k}}^{\,n+1}\right) - \frac{\lambda}{4}\left(e_{1_{j,k}}^{\,n} + e_{1_{j,k}}^{\,n+1}\right) - \xi_{2_{j,k}}^{\,n+1} = \eta_{2_{j,k}}^{\,n}, \\
&\qquad (j,k)\in\mathcal{T}_h, \quad n=0,1,2,\ldots,N-1,
\end{aligned}
\tag{3.67}
$$

where $\xi_{1_{j,k}}^{\,n+1} = \hat{\xi}_{1_{j,k}}^{\,n+1}$ and $\xi_{2_{j,k}}^{\,n+1} = \hat{\xi}_{2_{j,k}}^{\,n+1}$ with $f_B = f$.

Computing the inner product of (3.66) and (3.67) with $\delta_t^+\Delta_h^-\hat{e}_1{}^n$ and $\delta_t^+\Delta_h^+\hat{e}_2{}^n$, respectively, then taking the real parts of the results, we obtain

$$
\begin{aligned}
&\frac{1}{\tau}(||\Delta_h^- e_1^{n+1}||^2 - \|\Delta_h^- e_1^n\|^2) \\
&\quad = 2\mathrm{Re}\langle V_1(\hat{e}_1{}^{n+1} + e_1^n), \delta_t^+\Delta_h^- e_1^n\rangle + \alpha\mathrm{Re}\langle e_1^{n+1} + e_1^n, \delta_t^+\Delta_h^- e_1^n\rangle \\
&\qquad + \lambda\mathrm{Re}\langle e_2^{n+1} + e_2^n, \delta_t^+\Delta_h^- e_1^n\rangle + 4\mathrm{Re}\langle \hat{\xi}_1{}^{n+1}, \delta_t^+\Delta_h^- e_1^n\rangle + 4\mathrm{Re}\langle \eta_1^n, \delta_t^+\Delta_h^- e_1^n\rangle \\
&\quad \lesssim |e_1^n|_2^2 + |e_2^n|_2^2 + h^2 + \tau^2,
\end{aligned}
\tag{3.68}
$$

$$
\begin{aligned}
&\frac{1}{\tau}(||\Delta_h^+ e_2^{n+1}||^2 - \|\Delta_h^+ e_2^n\|^2) \\
&\quad = 2\mathrm{Re}\langle V_2(e_2^{n+1} + e_2^n), \delta_t^+\Delta_h^+ e_2^n\rangle - \alpha\mathrm{Re}\langle e_2^{n+1} + e_2^n, \delta_t^+\Delta_h^+ e_2^n\rangle \\
&\qquad + \lambda\mathrm{Re}\langle e_1^{n+1} + e_1^n, \delta_t^+\Delta_h^+ e_2^n\rangle + 4\mathrm{Re}\langle \xi_2^{n+1}, \delta_t^+\Delta_h^+ e_2^n\rangle + 4\mathrm{Re}\langle \eta_2^n, \delta_t^+\Delta_h^+ e_2^n\rangle \\
&\quad \lesssim |e_1^n|_2^2 + |e_2^n|_2^2 + h^2 + \tau^2,
\end{aligned}
\tag{3.69}
$$

where Lemmas 3.2, 3.4, 3.5, and Theorem 3.1 were used.

Denote

$$
\mathcal{E}^n = ||\Delta_h^- e_1^n||^2 + ||\Delta_h^+ e_2^n||^2, \quad n=0,1,2,\ldots,N, \tag{3.70}
$$

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with C_1 is a sufficiently big constant, then by using Cauchy inequality, Lemma 3.5 and Theorem 3.1 we obtain

$$\begin{aligned}\mathcal{E}^n &\lesssim |e_1^n|_2^2 + |e_2^n|_2^2 + ||e_1^n||^2 + ||e_2^n||^2 \\ &\lesssim |e_1^n|_2^2 + |e_2^n|_2^2 + h^2 + \tau^2, \quad n = 0, 1, 2, \dots, N,\end{aligned} \tag{3.71}$$

and

$$\begin{aligned}\mathcal{E}^n &\gtrsim |e_1^n|_2^2 + |e_2^n|_2^2 - ||e_1^n||^2 - ||e_2^n||^2 \\ &\gtrsim |e_1^n|_2^2 + |e_2^n|_2^2 - h^2 - \tau^2, \quad n = 0, 1, 2, \dots, N.\end{aligned} \tag{3.72}$$

Then, adding (3.68) to (3.69) yields

$$\mathcal{E}^{n+1} - \mathcal{E}^n \lesssim \tau(\mathcal{E}^{n+1} + \mathcal{E}^n) + \tau(h^2 + \tau^2)^2, \quad n = 0, 1, 2, \dots, N-1, \tag{3.73}$$

then by using Gronwall inequality, for sufficiently small τ, we have

$$\mathcal{E}^n \lesssim (h^2 + \tau^2)^2, \quad n = 1, 2, \dots, N, \tag{3.74}$$

this together with (3.70) gives

$$|e_1^n|_2 + |e_2^n|_2 \lesssim h^2 + \tau^2, \quad n = 1, 2, \dots, N. \tag{3.75}$$

Then by using Lemma 3.1 and Theorem 3.1 we obtain

$$|||e_l^n|||_2 \lesssim h^2 + \tau^2, \quad ||e_l^n||_\infty \lesssim h^2 + \tau^2, \quad l = 1, 2, \quad n = 1, 2, \dots, N. \tag{3.76}$$

This completes the proof. ■

Theorem 3.3. *Under Assumptions (A) and (B), there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, the solution of the CNFD scheme (2.5)–(2.8) is unique.*

Thanks to the results given in Theorem 3.2, one can use the standard energy method to prove Theorem 3.3. We here omit the proof for brevity.

Remark 3.1. Based on the results given in Theorem 3.2, one can use the standard energy method to prove that the CNFD scheme is stable in the discrete maximum norm with respect to the initial values. For the sake of brevity, we here omit the detailed proof of the stable result.

Remark 3.2. In fact, the analysis method used in establishing the unconditional and optimal error estimate of the CNFD scheme can be generalized to analyze many other finite difference schemes without any restriction on the grid ratio.

4 | NUMERICAL EXPERIMENT

In this section, we numerically underline the theoretical convergence results and the conservation properties of the CNFD scheme in the previous sections. In addition, several dynamics of the CGPEs are also simulated. The proposed CNFD scheme is a nonlinear scheme, we here adopted an iterative algorithm [23, 37] such as Jacobi iteration [23, 37] to solve the nonlinear scheme.

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Example 4.1. For comparison, we consider the following nonhomogenous CGPEs

$$i\partial_t\psi_1 = \left[-\frac{1}{2}\Delta + V_1 + ik_0\partial_x + \frac{\alpha}{2} + \sum_{l=1}^{2}\beta_{1l}|\psi_l|^2\right]\psi_1 + \frac{\lambda}{2}\psi_2 + f, \quad (x,y)\in\Omega,\ t>0, \tag{4.1}$$

$$i\partial_t\psi_2 = \left[-\frac{1}{2}\Delta + V_2 - ik_0\partial_x - \frac{\alpha}{2} + \sum_{l=1}^{2}\beta_{2l}|\psi_l|^2\right]\psi_2 + \frac{\lambda}{2}\psi_1 + g, \quad (x,y)\in\Omega,\ t>0, \tag{4.2}$$

with homogeneous Dirichlet boundary condition

$$\psi_1(x,y,t)=0, \quad \psi_2(x,y,t)=0, \quad (x,y)\in\partial\Omega, \quad t>0, \tag{4.3}$$

and initial condition

$$\psi_1(x,y,0)=\varphi_1(x,y)=\sin(\pi x)\sin(\pi y), \tag{4.4}$$

$$\psi_2(x,y,0)=\varphi_2(x,y)=\sin(\pi x)\sin(\pi y), \quad (x,y)\in\overline{\Omega}. \tag{4.5}$$

where $\Omega=(0,1)\times(0,1)$, $V_1(x,y)=V_2(x,y)=\frac{1}{2}(x^2+y^2), \beta_{11}=\beta_{22}=1, \beta_{12}=\beta_{21}=2, k_0=1, \alpha=1, \lambda=-1$ and

$$\begin{aligned} f(x,y,t) &= \left[\frac{1}{2}-\pi^2-3\sin^2(\pi x)\sin^2(\pi y)-\frac{1}{2}(x^2+y^2)\right]\sin(\pi x)\sin(\pi y)e^{-it} \\ &\quad - i\pi\cos(\pi x)\sin(\pi y)e^{-it}+\frac{1}{2}\sin(\pi x)\sin(\pi y)e^{-2it}, \\ g(x,y,t) &= \left[\frac{1}{2}-\pi^2-3\sin^2(\pi x)\sin^2(\pi y)-\frac{1}{2}(x^2+y^2)\right]\sin(\pi x)\sin(\pi y)e^{-it} \\ &\quad + i\pi\cos(\pi x)\sin(\pi y)e^{-2it}+\frac{1}{2}\sin(\pi x)\sin(\pi y)e^{-it}. \end{aligned}$$

The problem (4.1)–(4.5) has an exact solution in the following form,

$$\psi_1(x,y,t)=\sin(\pi x)\sin(\pi y)e^{-it}, \quad \psi_2(x,y,t)=\sin(\pi x)\sin(\pi y)e^{-2it}.$$

In virtue of the good stability, we measure the temporal errors and the spatial errors of the CNFD scheme separately. To test the spatial error analysis, we choose different h, and use $\tau=0.0001$ which is small enough to ignore the temporal error. In the same way, to test the temporal error analysis, we choose different τ (here we take $\tau=0.12, 0.1, 0.08, 0.06$, respectively, which are much bigger than the value of h), and fix $h=h_1=h_2=0.005$ which is small enough to ignore the spatial error. The errors are presented at time $t=1.2$. Data in Tables 1 and 2 verify our main theoretical results given in Theorem 3.2 and Remark 3.1.

Let $e_1(h,\tau)$ and $e_2(h,\tau)$ denote the errors $||e_1^N||_\infty$ and $||e_2^N||_\infty$, respectively, with time step τ and mesh-size $h=h_1=h_2$. For simplicity, we denote

TABLE 1 Spatial errors of the CNFD scheme in computing Example 1 with $\tau=0.0001$ at $t=1.2$.

CNFD	$h=0.2$	$h=0.1$	$h=0.05$	$h=0.025$
$\|\|e_1^N\|\|_\infty$	2.8311e−02	6.8706e−03	1.6844e−03	4.1088e−04
	rate1	2.04	2.03	2.04
$\|\|e_2^N\|\|_\infty$	3.2910e−02	1.0078e−02	2.3247e−03	5.8717e−04
	rate2	1.71	2.11	1.99

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TABLE 2 Temporal errors of the CNFD scheme in computing Example 1 with $h = 0.005$ at $t = 1.2$.

CNFD	$\tau = 0.12$	$\tau = 0.1$	$\tau = 0.08$	$\tau = 0.06$
$\|\|e_1^N\|\|_\infty$	4.1838e−03	2.8466e−03	1.8575e−03	1.0259e−03
	rate3	2.11	1.91	2.06
$\|\|e_2^N\|\|_\infty$	1.3793e−02	9.1109e−03	5.7059e−03	2.9527e−03
	rate4	2.27	2.10	2.29

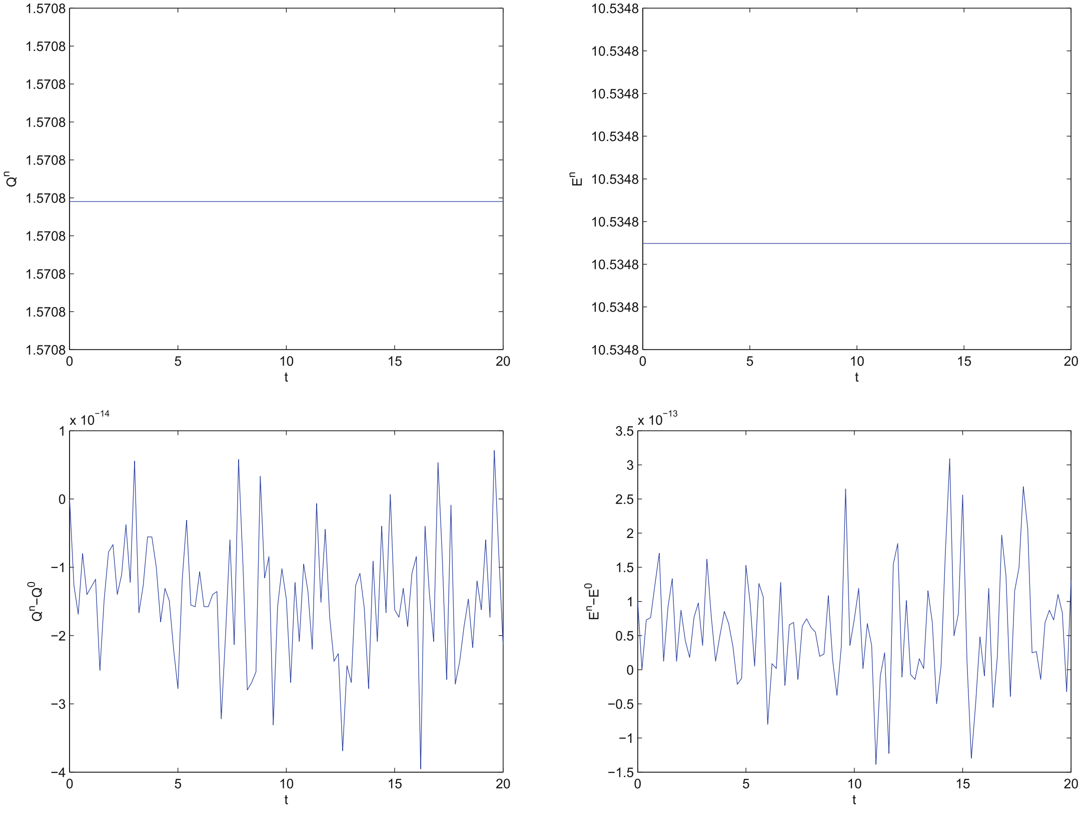

FIGURE 1 Total mass (left column) and energy (right column) and their differences from initial values computed by the CNFD scheme with $\gamma = 0.5, \beta = 1, h = 0.5, \tau = 0.4, T = 40$.

$$\text{rate1} = \frac{\log\big(e_1(h,\tau)/e_1(\tilde{h},\tau)\big)}{\log(h/\tilde{h})}, \quad \text{rate2} = \frac{\log\big(e_2(h,\tau)/e_2(\tilde{h},\tau)\big)}{\log(h/\tilde{h})}, \tag{4.6}$$

$$\text{rate3} = \frac{\log(e_1(h,\tau)/e_1(h,\tilde{\tau}))}{\log(\tau/\tilde{\tau})}, \quad \text{rate4} = \frac{\log(e_2(h,\tau)/e_2(h,\tilde{\tau}))}{\log(\tau/\tilde{\tau})}. \tag{4.7}$$

Example 4.2. *In the initial-boundary value problem (2.1)–(2.4), we take* $\Omega = (-20, 20)\times(-20, 20)$, $V_1(\mathbf{x}) = V_2(\mathbf{x}) = \frac{1}{2}(x^2 + y^2)$, $\beta_{11} = \beta_{22} = 1$, $\beta_{12} = \beta_{21} = 2$, $k_0 = 1, \alpha = 1, \lambda = 0.1$ *in (2.1)-(2.2) and* $\varphi_1 = \varphi_2 = \exp(-4((x-2)^2 + y^2)) + \exp(-4((x+2)^2 + y^2))$ *in (2.4).*

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To test the conservation properties possessed by the CNFD scheme, we draw the total mass and energy of Example 2 computed by the CNFD scheme in Figure 1. One can observe from the figure that the CNFD scheme preserves well the total mass and energy in the discrete sense, as verifies the result given in Lemma 2.2. To figure out the collision of two waves described by the CGPEs, we set the solution at the initial time to be two Gaussian waves and simulate the evolution of the solutions of the CGPEs, see Figures 2 and 3.

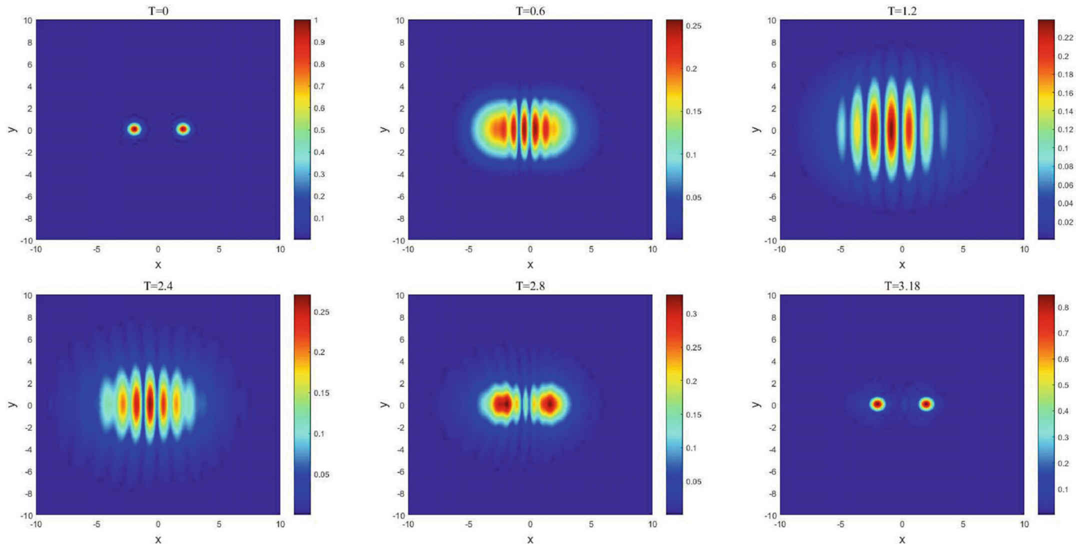

FIGURE 2 Collision of two waves for ψ_1 computed by the CNFD scheme with $\gamma = 0.5, \beta = 1, h = 0.1, \tau = 0.02$ at different times.

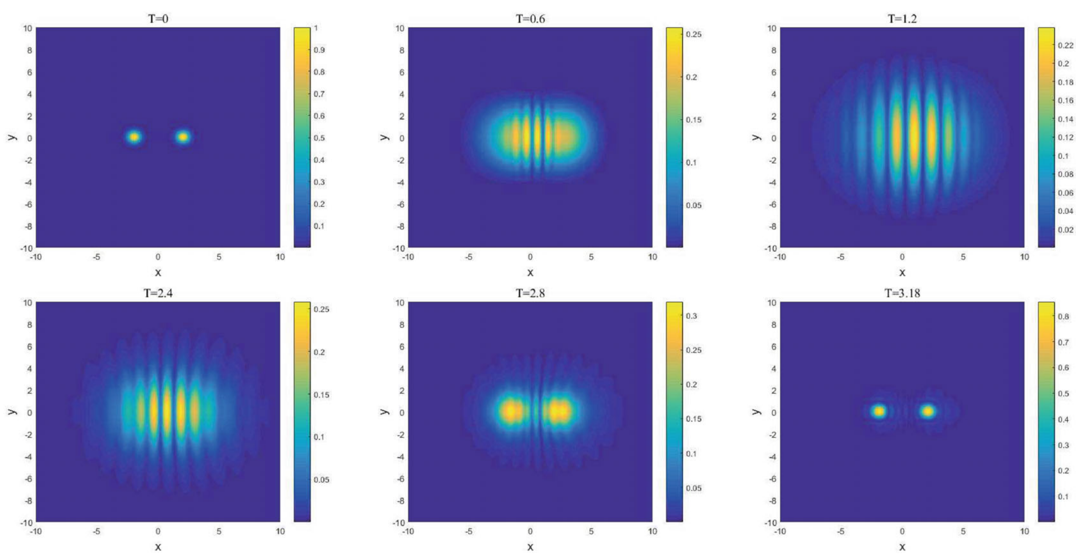

FIGURE 3 Collision of two waves for ψ_2 computed by the CNFD scheme with $\gamma = 0.5, \beta = 1, h = 0.1, \tau = 0.02$ at different times.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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REFERENCES

[1] N. B. Abdallah, F. Méhats, C. Schmeiser, and R. M. Weishäupl, *The nonlinear Schrödinger equation with a strongly anisotropic harmonic potential*, SIAM J. Math. Anal. 37 (2005), 189–199.
[2] G. Akrivis, V. Dougalis, and O. Karakashian, *On fully discrete Galerkin methods of secondorder temporal accuracy for the nonlinear Schrödinger equation*, Numer. Math. 59 (1991), 31–53.
[3] X. Antoine, W. Bao, and C. Besse, *Computational methods for the dynamics of the nonlinear Schrödinger/Gross-Pitaevskii equations*, Comput. Phys. Commun. 184 (2013), 2621–2633.
[4] X. Antoine, C. Besse, and V. Rispoli, *High-order IMEX-spectral schemes for computing the dynamics of systems of nonlinear Schrödinger/Gross-Pitaevskii equations*, J. Comput. Phys. 327 (2016), 252–269.
[5] W. Bao and Y. Cai, *Mathematical theory and numerical methods for Bose-Einstein condensation*, Kinet. Relat. Model 6 (2013), 1–135.
[6] W. Bao and Y. Cai, *Optimal error estimates of finite difference methods for the Gross-Pitaevskii equation with angular momentum rotation*, Math. Comput. 82 (2013), 99–128.
[7] W. Bao and Y. Cai, *Ground states and dynamics of spin-orbit-coupled Bose-Einstein condensates*, SIAM J. Appl. Math. 75 (2015), 492–517.
[8] W. Bao, Q. Du, and Y. Zhang, *Dynamics of rotating Bose-Einstein condensates and its efficient and accurate numerical computation*, SIAM J. Appl. Math. 66 (2006), 758–786.
[9] W. Bao, H. Li, and J. Shen, *A generalized-Laguerre-Fourier-Hermite pseudospectral method for computing the dynamics of rotating Bose-Einstein condensates*, SIAM J. Sci. Comput. 31 (2009), 3685–3711.
[10] W. Bao and H. Wang, *An efficient and spectrally accurate numerical method for computing dynamics of rotating Bose-Einstein condensates*, J. Comput. Phys. 217 (2006), 612–626.
[11] W. Bao, H. Wang, and P. A. Markowich, *Ground, symmetric and central vortex states in rotating Bose-Einstein condensates*, Commun. Math. Sci. 3 (2005), 57–88.
[12] F. E. Browder, "Existence and uniqueness theorems for solutions of nonlinear boundary value problems," *Application of nonlinear partial differential equations in mathematical physics*, Proceedings of symposia in applied mathematics, Vol 17, R. Finn (ed.), AMS, Providence, RI, 1965, pp. 24–49.
[13] J. Cai and J. Shen, *Two classes of linearly implicit local energy-preserving approach for general multi-symplectic Hamiltonian PDEs*, J. Comput. Phys. 401 (2020), 108975.
[14] Q. Chang, B. Guo, and H. Jiang, *Finite difference method for generalized Zakharov equations*, Math. Comput. 64 (1995), 537–553.
[15] Q. Chang, E. Jia, and W. Sun, *Difference schemes for solving the generalized nonlinear Schrödinger equation*, J. Comput. Phys. 148 (1999), 397–415.
[16] S. Chippada and C. N. Dawson, *Finite element approximations to the system of shallow water equations, part II: Discrete time a priori error estimates*, SIAM J. Numer. Anal. 36 (1999), 226–250.
[17] C. N. Dawson, *A characteristic-Galerkin approximation to a system of shallow water equations*, Numer. Math. 86 (2000), 239–256.
[18] X. Feng, B. Li, and S. Ma, *High-order mass- and energy-conserving SAV-Gauss collocation finite element methods for the nonlinear Schrödinger equation*, SIAM J. Numer. Anal. 59 (2021), 1566–1591. https://www.researchgate.net/publication/342094165.
[19] C. Hao, L. Hsiao, and H. Li, *Global well posedness for the Gross-Pitaevskii equation with an angular momentum rotational term in three dimensions*, J. Math. Phys. 48 (2007), 102105.
[20] C. Hao, L. Hsiao, and H. Li, *Global well posedness for the Gross-Pitaevskii equation with an angular momentum rotational term*, Math. Methods Appl. Sci. 31 (2008), 655–664.
[21] C. Hamner, Y. Zhang, M. A. Khamehchi, M. J. Davis, and P. Engels, *Spin-orbit coupled Bose-Einstein condensates in a one-dimensional optical lattice*, Phys. Rev. Lett. 114 (2015), 070401.

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[22] M. Z. Hasan and C. L. Kane, *Colloquium: Topological insulators*, Rev. Mod. Phys. 82 (2010), 3045–3067.
[23] X. Li, Y. Cai, and P. Wang, *Operator-compensation methods with mass and energy conservation for solving the Gross-Pitaevskii equation*, Appl. Numer. Math. 151 (2020), 337–353.
[24] Y. Li, L. Pitaevskii, and S. Stringari, *Quantum tricriticality and phase transitions in spin-orbit coupled Bose-Einstein condensates*, Phys. Rev. Lett. 108 (2012), 225301.
[25] Y. Li, G. I. Martone, L. Pitaevskii, and S. Stringari, *Superstripes and the excitation spectrum of a spin-orbit-coupled Bose-Einstein condensate*, Phys. Rev. Lett. 110 (2013), 235302.
[26] E. H. Lieb, R. Seiringer, and J. Yngvason, *Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional*, Phys. Rev. A 61 (2000), 043602.
[27] Y. J. Lin, K. Jiménez-Garcia, and I. B. Spielman, *Spin-orbit-coupled Bose-Einstein condensates*, Nature 471 (2011), 83–86.
[28] L. P. Pitaevskii and S. Stringary, *Bose-Einstein condensation*, Clarendon Press, Oxford, 2003.
[29] J. Shen and J. Xu, *Unconditionally bound preserving and energy dissipative schemes for a class of Keller-Segel equations*, SIAM J. Numer. Anal. 58 (2020), 1674–1695.
[30] V. Thomée, *Galerkin finite element methods for parabolic problems*, Springer-Verlag, Berlin, 1997.
[31] Y. Tian, M. Qin, and Y. Zhang, *The multisymplectic numerical method for Gross-Pitaevskii equation*, Comput. Phys. Commun. 178 (2008), 449–458.
[32] M. S. Ismail and T. R. Taha, *Numerical simulation of coupled nonlinear Schrödinger equation*, Math. Comput. Simul. 56 (2001), 547–562.
[33] M. S. Ismail and S. Z. Alamri, *Highly accurate finite difference method for coupled nonlinear Schrödinger equation*, Int. J. Comput. Math. 81 (2004), 333–351.
[34] M. S. Ismail and T. R. Taha, *A linearly implicit conservative scheme for the coupled nonlinear Schrödinger equation*, Math. Comput. Simul. 74 (2007), 302–311.
[35] H. Wang, *A time-splitting spectral method for coupled Gross-Pitaevskii equations with applications to rotating Bose-Einstein condensates*, J. Comput. Appl. Math. 205 (2007), 88–104.
[36] H. Wang, X. Ma, J. Lu, and W. Gao, *An efficient time-splitting compact finite difference method for Gross-Pitaevskii equation*, Appl. Math. Comput. 297 (2017), 131–144.
[37] P. Wang and C. Huang, *An energy conservative difference scheme for the nonlinear fractional Schrodinger equations*, J. Comput. Phys. 293 (2015), 238–251.
[38] T. Wang, B. Guo, and Q. Xu, *Fourth-order compact and energy conservative difference schemes for the nonlinear Schrödinger equation in two dimensions*, J. Comput. Phys. 243 (2013), 382–399.
[39] T. Wang and X. Zhao, *Optimal l^∞ error estimates of finite difference methods for the coupled Gross-Pitaevskii equations in high dimensions*, Sci. China Math. 57 (2014), no. 10, 2189–2214.
[40] T. Wang, X. Zhao, and J. Jiang, *Unconditional and optimal H^2-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrödinger equation in high dimensions*, Adv. Comput. Math. 44 (2018), 477–503.
[41] T. Wang, *Optimal point-wise error estimate of a compact difference scheme for the coupled Gross-Pitaevskii equations in one dimension*, J. Sci. Comput. 59 (2014), no. 1, 158–186.
[42] B. Wang and X. Wu, *Functionally-fitted energy-preserving integrators for Poisson systems*, J. Comput. Phys. 364 (2018), 137–152.
[43] D. Xiao, M. Chang, and Q. Niu, *Berry phase effects on electronic properties*, Rev. Mod. Phys. 82 (2010), 1959–2007.
[44] J. Zhang, S. Ji, Z. Chen, L. Zhang, Z. Du, B. Yan, G. Pan, B. Zhao, Y. Deng, H. Zhai, S. Chen, and J. Pan, *Collective dipole oscillations of a spin-orbit coupled Bose-Einstein condensate*, Phys. Rev. Lett. 109 (2012), 115301.
[45] Y. Zhou, *Applications of discrete functional analysis to the finite difference method*, International Academic Publishers, Beijing, 1991.

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