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A NEW LINEAR AND CONSERVATIVE FINITE DIFFERENCE SCHEME FOR THE GROSS–PITAEVSKII EQUATION WITH ANGULAR MOMENTUM ROTATION

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Abstract

A new linear and conservative finite difference scheme which preserves discrete mass and energy is developed for the two-dimensional Gross–Pitaevskii equation with angular momentum rotation. In addition to the energy estimate method and mathematical induction, we use the lifting technique as well as some well-known inequalities to establish the optimal H^1-error estimate for the proposed scheme with no restrictions on the grid ratio. Unlike the existing numerical solutions which are of second-order accuracy at the most, the convergence rate of the numerical solution is proved to be of order $O(h^4 + \tau^2)$ with time step τ and mesh size h. Numerical experiments have been carried out to show the efficiency and accuracy of our new method.

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1. Introduction

Through proper nondimensionalization and dimension reduction, the dynamics of a rotating Bose–Einstein condensate (BEC) can be well described by the following Gross–Pitaevskii (GP) equation with angular momentum rotation (AMR) in dimensionless form [3, 20]:

$$i\partial_t\psi = [-\tfrac{1}{2}\Delta + V(\mathbf{x}) - \Omega L_z + \beta|\psi|^2]\psi, \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0.$$

Here $i = \sqrt{-1}$, $d = 2, 3$, $\mathbf{x} = (x, y) \in \mathbb{R}^2$ or $(x, y, z) \in \mathbb{R}^3$, t is the time variable and $\psi(\mathbf{x}, t)$ is the unknown complex-valued wave function. Note that $V(\mathbf{x})$ is a real-valued

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function related to the external trap potential and, in most experiments, it is chosen as a harmonic potential, that is, as a quadratic polynomial. The dimensionless constant Ω corresponds to the angular speed of the laser beam in experiments and β characterizes the interaction (positive for repulsive interaction and negative for attractive interaction) between particles in the rotating BEC. Moreover, Δ is the Laplacian operator and L_z is the z-component of the angular momentum defined as

$$L_z = -i(x\partial_y - y\partial_x) = -i\partial_\theta,$$

where (r, θ) and (r, θ, z) are the two-dimensional (2D) polar coordinates and three-dimensional (3D) cylindrical coordinates, respectively. In fact, since the first experimental implementation of a quantized vortex in a gaseous BEC [18, 19], which is relevant to superfluidity, theoretical and experimental advances in rotating BECs [6, 9] have spurred great excitement in atomic physics and the computational and applied mathematics community.

In this paper, we focus numerically on the 2D case

$$i\partial_t\psi = [-\tfrac{1}{2}\Delta + V(x, y) - \Omega L_z + \beta|\psi|^2]\psi, \quad (x, y) \in \mathbb{R} \times \mathbb{R}, \quad 0 < t \leqslant T, \tag{1.1}$$

subject to the (l_1, l_2)-periodic boundary conditions

$$\psi(x, y, t) = \psi(x + l_1, y, t), \quad \psi(x, y, t) = \psi(x, y + l_2, t), \quad (x, y) \in \mathbb{R} \times \mathbb{R}, \quad 0 < t \leqslant T, \tag{1.2}$$

and the initial condition

$$\psi(x, y, 0) = \psi_0(x, y), \quad (x, y) \in \mathbb{R} \times \mathbb{R}, \tag{1.3}$$

where $\psi_0(x, y)$ is a given (l_1, l_2)-periodic smooth complex-valued function. In addition, it can be verified that the initial boundary value problem (1.1)–(1.3) possesses the following mass and energy conservation laws:

$$M(\psi(\cdot, t)) = \int_{\mathcal{D}} |\psi(\cdot, t)|^2 \, dx \, dy \equiv M(\psi_0), \quad t \geqslant 0,$$

and

$$E(\psi(\cdot, t)) = \int_{\mathcal{D}} \Big[\frac{1}{2}|\nabla\psi|^2 + V(x, y)|\psi|^2 - \Omega\bar{\psi}L_z\psi + \frac{\beta}{2}|\psi|^4\Big] \, dx \, dy \equiv E(\psi_0), \quad t \geqslant 0,$$

where $\mathcal{D} = [0, l_1] \times [0, l_2]$ and $\bar{\psi}$ refers to the complex conjugate of ψ.

The GP equation with AMR has been vigorously studied in theoretical analysis and numerical simulations. For the derivation, well-posedness and dynamical properties, we refer to the papers [13, 17], the book [20] and the references therein. Numerically, various algorithms have been developed, including the finite difference method [3, 25], the finite element method [14], the time-splitting pseudo-spectral method [23] and so on. For the 1D GP equation including the nonlinear Schrödinger (NLS) equation, the unconditional and optimal error estimates for conservative finite difference methods have been established by Chang et al. [7] and Guo [12]. Note that their proofs heavily rely on the discrete conservative property and the discrete 1D version of the Sobolev inequality

$$\|f\|_{L^\infty} \leqslant C_{\mathcal{D}}\|f\|_{H^1} \quad \text{for all } f \in H^1(\mathcal{D}) \text{ with } \mathcal{D} \subset \mathbb{R}.$$

Such an inequality in 2D or 3D is no longer valid, which causes serious difficulty in obtaining an a priori uniform estimate of the numerical solution. Thus, few error estimates of the finite difference method are available in the literature for the 2D GP equation with AMR. For the second-order finite difference method of the GP equation with AMR, the first result about the error estimate was given by Bao and Cai [3] with the aid of the cut-off technique [21]. Nevertheless, a weak condition on the time-step size is involved in the corresponding error analysis. For $\Omega \neq 0$, the convergence rate in the discrete H^1-norm is merely of order $O(h^{3/2} + \tau^{3/2})$, which is not optimal according to the numerical results. Further introducing a lifting technique, Wang et al. [25] established an optimal H^1-error estimate for another Crank–Nicolson finite difference scheme; the convergence rate, with no restrictions on the grid ratio, is of order $O(h^2 + \tau^2)$.

Recently, there has been growing interest in high-order methods for solving partial differential equations. It was shown that the high-order difference methods play an important role in the simulation of high frequency wave phenomena. For example, it is convenient to incorporate compact finite difference methods to achieve a high-order scheme. There have been a few fourth-order compact schemes for the NLS equation, which is a special case of the GP equation, as well as their convergence analysis. Liao and Sun [16] established the maximum norm error estimate for linear Schrödinger equations in 2D/3D. However, their analysis technique cannot be directly used in nonlinear problems. Wang et al. [24] developed a new technique to analyse a compact difference scheme for the 2D NLS equation and it was proved to be convergent, with no constrains on the time-step size, at the order of $O(h^4 + \tau^2)$ in the discrete L^2-norm. Nevertheless, due to the introduction of the angular momentum rotation term, this method [24] still cannot be directly extended for the analysis of the GP equation (1.1)–(1.3).

To the best of our knowledge, the compact finite difference method has not been applied to the GP equation with AMR and the existing finite difference schemes are of second-order accuracy at most. Therefore, it is desirable to construct a high-order scheme for the GP equation with AMR. In this paper, we first develop a fourth-order conservative difference scheme for solving the initial boundary value problem (1.1)–(1.3) and then prove that the proposed scheme is convergent at the order $O(h^4 + \tau^2)$ in the discrete H^1-norm, which is optimal according to the local truncation error. The application of the lifting technique [25] removes the restriction on the mesh ratio, which is needed to estimate the maximum norm boundedness of the numerical solution of Bao and Cai [3]. Another aspect of this paper is that we have obtained a higher order of spatial convergence using the fourth-order finite difference scheme. Unlike the known analysis techniques [16, 24], the key strategy in the proof is the

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utilization of the circular matrix operation and the equivalences of several discrete semi-norms for error estimates.

The remainder of the paper is organized as follows. In Section 2 some notation is given and the fourth-order difference scheme is proposed. In Section 3 we introduce some auxiliary lemmas for our error analysis. We discuss the existence of the numerical solution and the discrete conservation laws in Section 4. In Section 5 the convergence and stability of the proposed scheme are analysed. Numerical examples are presented to show the efficiency and accuracy of our method in Section 6 and concluding remarks are given in Section 7.

2. Notation and the fourth-order finite difference scheme

Numerically, we study the initial boundary value problem (1.1)–(1.3) in a finite domain $\mathcal{D} \times [0, T]$. We start with introducing some notation. For $N \in \mathbb{N}$, let the time step $\tau = T/N, t_n = n\tau, 0 \leqslant n \leqslant N$ and denote $\mathcal{T}_\tau = \{t_n = n\tau \mid n = 1, 2, \ldots, N-1\}$, $\mathcal{T}'_\tau = \{t_n = n\tau \mid n = 0, 1, 2, \ldots, N-1\}$ and $\mathcal{T}''_\tau = \{t_n = n\tau \mid n = 0, 1, 2, \ldots, N\}$. Given a temporal discrete function $\{u^n \mid t_n \in \mathcal{T}''_\tau\}$, we denote $\delta_t u^n = (u^{n+1} - u^{n-1})/2\tau, u^{\bar{n}} = (u^{n+1} + u^{n-1})/2, t_n \in \mathcal{T}_\tau$ and $\delta_t^+ u^n = (u^{n+1} - u^n)/\tau, t_n \in \mathcal{T}'_\tau$.

Besides, let $J, K \in \mathbb{N}, h_1 = l_1/J, h_2 = l_2/K, h = \max\{h_1, h_2\}, x_j = jh_1, 0 \leqslant j \leqslant J-1$, $y_k = kh_2, 0 \leqslant k \leqslant K-1$ and the grid $\mathcal{T}_h = \{(x_j, y_k) \mid 0 \leqslant j \leqslant J-1, 0 \leqslant k \leqslant K-1\}$. To approximate the periodic boundary conditions, we assume that $x_{-1} = -h_1$, $x_J = Jh_1$, $y_{-1} = -h_2$, $y_K = Kh_2$ and the extended discrete grid $\mathcal{T}_h^E = \{(x_j, y_k) \mid j = -1, 0, \ldots, J;\ k = -1, 0, 1, \ldots, K\}$. Given a grid function $u = \{u_{jk} \mid (x_j, y_k) \in \mathcal{T}_h^E\}$, we denote

$$\delta_x^+ u_{jk} = \frac{u_{j+1,k} - u_{jk}}{h_1}, \quad \delta_x u_{jk} = \frac{u_{j+1,k} - u_{j-1,k}}{2h_1}, \quad \delta_x^2 u_{jk} = \frac{u_{j-1,k} - 2u_{jk} + u_{j+1,k}}{h_1^2},$$
$$\mathcal{A}_{h_1} u_{jk} = \frac{u_{j-1,k} + 10u_{jk} + u_{j+1,k}}{12}, \quad \mathcal{B}_{h_1} u_{jk} = \frac{u_{j-1,k} + 4u_{jk} + u_{j+1,k}}{6},$$

where $(x_j, y_k) \in \mathcal{T}_h$. Difference operators $\delta_y^+ u_{jk}, \delta_y u_{jk}, \delta_y^2 u_{jk}, \mathcal{A}_{h_2} u_{jk}, \mathcal{B}_{h_2} u_{jk}$ are similarly defined.

A matrix in the form

$$A = \begin{pmatrix} a_0 & a_1 & \ldots & a_{n-1} \\ a_{n-1} & a_0 & \ldots & a_{n-2} \\ \vdots & \vdots & \ddots & \vdots \\ a_1 & a_2 & \ldots & a_0 \end{pmatrix}$$

is called a *circulant matrix* [11]. Since the matrix A is determined by the entries in the first row, the matrix may be denoted as

$$A = C(a_0, a_1, \ldots, a_{n-1}).$$

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To approximate the Laplacian operator and the rotation operator, we introduce the following matrices: in x-direction,

$$D_2^x = \frac{1}{h_1^2}C(-2,1,0_{J-3},1), \quad D_1^x = \frac{1}{2h_1}C(0,1,0_{J-3},-1), \quad D_+^x = \frac{1}{h_1}C(-1,1,0_{J-2}),$$
$$D_-^x = \frac{1}{h_1}C(1,0_{J-2},-1), \quad A_2^x = \frac{1}{12}C(10,1,0_{J-3},1), \quad A_1^x = \frac{1}{6}C(4,1,0_{J-3},1),$$
$$B_2^x = (A_2^x)^{-1}, \quad B_1^x = (A_1^x)^{-1}, \quad X = \mathrm{diag}(x_0, x_1, \ldots, x_{J-1});$$

and in y-direction,

$$D_2^y = \frac{1}{h_2^2}C(-2,1,0_{K-3},1), \quad D_1^y = \frac{1}{2h_2}C(0,-1,0_{K-3},1), \quad D_+^y = \frac{1}{h_2}C(-1,0_{K-2},1),$$
$$D_-^y = \frac{1}{h_2}C(1,-1,0_{K-2}), \quad A_2^y = \frac{1}{12}C(10,1,0_{K-3},1), \quad A_1^y = \frac{1}{6}C(4,1,0_{K-3},1),$$
$$B_2^y = (A_2^y)^{-1}, \quad B_1^y = (A_1^y)^{-1}, \quad Y = \mathrm{diag}(y_0, y_1, \ldots, y_{K-1}),$$

where 0_m is a row vector with m zero elements. Note that $D_2^w, A_2^w, A_1^w, B_2^w, B_1^w$ are symmetric circulant matrices, D_1^w is an antisymmetric circulant matrix, D_+^w, D_-^w are circulant matrices and $w = x$ or y.

Let $V_h = \{u = (u_{jk}) \mid (x_j, y_k) \in \mathcal{T}_h\}$ be a space of grid functions. For $u \in V_h$, we introduce the discrete version of the Laplacian operator, the gradient operator and the rotation operator in the matrix form as

$$\nabla_h^2 u_{jk} = (D_2^x u + u D_2^y)_{jk}, \quad \Delta_h u_{jk} = (B_2^x D_2^x u + u D_2^y B_2^y)_{jk},$$
$$\nabla_h u_{jk} = ((D_+^x u)_{jk}, (u D_+^y)_{jk})^\top, \quad L_z^h u_{jk} = -i(X u D_1^y B_1^y - B_1^x D_1^x u Y)_{jk},$$

where $(x_j, y_k) \in \mathcal{T}_h$. For any two grid functions $w, v \in V_h$, we define discrete inner products and discrete (semi-)norms, respectively, as

$$(w, v) = h_1 h_2 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} w_{jk}\bar{v}_{jk}, \quad \|w\| = \sqrt{(w,w)}, \quad |w|_h = \sqrt{-(\Delta_h w, w)},$$

$$\|w\|_{1,h} = \sqrt{\|w\|^2 + \|\nabla_h w\|^2}, \quad \|w\|_p = \sqrt[p]{h_1 h_2 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} |w_{jk}|^p}, \quad 1 \leqslant p < \infty,$$

$$\|w\|_\infty = \max_{(x_j,y_k)\in\mathcal{T}_h} |w_{jk}|, \quad \varepsilon(w) = \frac{1}{2}|w|_h^2 + h_1 h_2 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1}(V_{jk}|w_{jk}|^2 - \Omega \bar{w}_{jk} L_z^h w_{jk}).$$

In fact, it can be verified that

$$\begin{aligned}
\|\nabla_h w\| &= \sqrt{(\nabla_h w, \nabla_h w)} = \sqrt{(D_+^x w, D_+^x w) + (w D_+^y, w D_+^y)} \\
&= \sqrt{-(D_+^x D_-^x w, w) - (w D_+^y D_-^y, w)} = \sqrt{-(D_2^x w + w D_2^y, w)} \\
&= \sqrt{-(\nabla_h^2 w, w)}.
\end{aligned}$$

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Throughout the paper, let C be a generic positive constant independent of h and τ; the notation $p \lesssim q$ means that there exists a constant C such that $|p| \leqslant Cq$. To introduce some lemmas for error estimates, we first make the following assumptions.

Assumption 2.1. For the external trapping potential $V(x, y)$ and the rotation speed Ω, we assume that there exists a constant $\mu > 0$ such that

$$V(x, y) \in C(\mathcal{D}), \quad V(x, y) \geqslant \tfrac{1}{2}\mu^2(x^2 + y^2) \quad \text{for all } (x, y) \in \mathcal{D}, |\Omega| < \tfrac{1}{3}\mu.$$

Assumption 2.2. For the regularity of the exact solution ψ, we assume that

$$\psi \in C^3([0, T]; \quad L^\infty(\mathcal{D})) \cap C^2([0, T]; \quad W^{2,\infty}(\mathcal{D})) \cap C^0([0, T]; \quad W^{6,\infty}(\mathcal{D}) \cap H^1_p(\mathcal{D})).$$

2.1. Fourth-order compact approximation of spatial derivatives

Lemma 2.3 [16]. *Let* $g(x) \in C^6([x_{j-1}, x_{j+1}])$ *and* $\zeta(\lambda) = 5(1-\lambda)^3 - 3(1-\lambda)^5$; *then*

$$\frac{g''(x_{j-1}) + 10g''(x_j) + g''(x_{j+1})}{12} = \frac{g(x_{j+1}) - 2g(x_j) + g(x_{j-1})}{h_1^2} + \frac{h_1^4}{360}\int_0^1 [g^{(6)}(x_j - \lambda h_1) + g^{(6)}(x_j + \lambda h_1)]\zeta(\lambda)\, d\lambda.$$

Lemma 2.4. *Let* $g(x) \in C^5([x_{j-1}, x_{j+1}])$ *and* $\bar{\zeta}(\lambda) = 4(1-\lambda)^3 - 3(1-\lambda)^4$; *then*

$$\frac{g'(x_{j-1}) + 4g'(x_j) + g'(x_{j+1})}{6} = \frac{g(x_{j+1}) - g(x_{j-1})}{2h_1} + \frac{h_1^4}{144}\int_0^1 [g^{(5)}(x_j - \lambda h_1) + g^{(5)}(x_j + \lambda h_1)]\bar{\zeta}(\lambda)\, d\lambda.$$

Proof. Taylor's formula with the integral remainder yields the result and we omit the details here for brevity. □

For the discretization of the second- and first-order derivatives ψ_{xx} and ψ_x of the (l_1, l_2)-periodic function $\psi(x, y, t)$, we derive from Lemmas 2.3 and 2.4 that

$$\mathcal{A}_{h_1}\psi_{xx}(x_j, y_k, t_n) = \delta_x^2\psi(x_j, y_k, t_n) + (\eta_2^x)^n_{jk}, \quad (x_j, y_k) \in \mathcal{T}_h,$$
$$\mathcal{B}_{h_1}\psi_x(x_j, y_k, t_n) = \delta_x\psi(x_j, y_k, t_n) + (\eta_1^x)^n_{jk}, \quad (x_j, y_k) \in \mathcal{T}_h,$$

that is,

$$\psi_{xx}(x_j, y_k, t_n) = \mathcal{A}_{h_1}^{-1}\delta_x^2\psi(x_j, y_k, t_n) + \mathcal{A}_{h_1}^{-1}(\eta_2^x)^n_{jk}, \quad (x_j, y_k) \in \mathcal{T}_h,$$
$$\psi_x(x_j, y_k, t_n) = \mathcal{B}_{h_1}^{-1}\delta_x\psi(x_j, y_k, t_n) + \mathcal{B}_{h_1}^{-1}(\eta_1^x)^n_{jk}, \quad (x_j, y_k) \in \mathcal{T}_h,$$

where

$$(\eta_2^x)^n_{jk} = \frac{h_1^4}{360}\int_0^1 [\psi_x^{(6)}(x_j - \lambda h_1, y_k, t_n) + \psi_x^{(6)}(x_j + \lambda h_1, y_k, t_n)]\zeta(\lambda)\, d\lambda,$$
$$(\eta_1^x)^n_{jk} = \frac{h_1^4}{144}\int_0^1 [\psi_x^{(5)}(x_j - \lambda h_1, y_k, t_n) + \psi_x^{(5)}(x_j + \lambda h_1, y_k, t_n)]\bar{\zeta}(\lambda)\, d\lambda.$$

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The corresponding matrix form of the above equations is

$$A_2^x\psi_{xx}^n = D_2^x\psi^n + (\eta_2^x)^n \Rightarrow \psi_{xx}^n = B_2^xD_2^x\psi^n + B_2^x(\eta_2^x)^n, \tag{2.1}$$
$$A_1^x\psi_{x}^n = D_1^x\psi^n + (\eta_1^x)^n \Rightarrow \psi_{x}^n = B_1^xD_1^x\psi^n + B_1^x(\eta_1^x)^n, \tag{2.2}$$

where $\psi_{xx}^n = (\psi_{xx}^n(x_j, y_k)), \psi_x^n = (\psi_x^n(x_j, y_k)), \psi^n = (\psi^n(x_j, y_k)), (\eta_2^x)^n, (\eta_1^x)^n \in V_h$.

Similarly,

$$\psi_{yy}^nA_2^y = \psi^nD_2^y + (\eta_2^y)^n \Rightarrow \psi_{yy}^n = \psi^nD_2^yB_2^y + (\eta_2^y)^nB_2^y, \tag{2.3}$$
$$\psi_{y}^nA_1^y = \psi^nD_1^y + (\eta_1^y)^n \Rightarrow \psi_{y}^n = \psi^nD_1^yB_1^y + (\eta_1^y)^nB_1^y, \tag{2.4}$$

where

$$\psi_{yy}^n = (\psi_{yy}^n(x_j, y_k)), \quad \psi_y^n = (\psi_y^n(x_j, y_k)), \quad (\eta_2^y)^n, \quad (\eta_1^y)^n \in V_h,$$
$$(\eta_2^y)_{jk}^n = \frac{h_2^4}{360}\int_0^1 [\psi_y^{(6)}(x_j, y_k - \lambda h_2, t_n) + \psi_y^{(6)}(x_j, y_k + \lambda h_2, t_n)]\zeta(\lambda)\,d\lambda,$$
$$(\eta_1^y)_{jk}^n = \frac{h_2^4}{144}\int_0^1 [\psi_y^{(5)}(x_j, y_k - \lambda h_2, t_n) + \psi_y^{(5)}(x_j, y_k + \lambda h_2, t_n)]\bar{\zeta}(\lambda)\,d\lambda.$$

Using (2.1) and (2.3), we represent the action of the Laplacian operator as

$$\begin{aligned}\Delta\psi^n &= \psi_{xx}^n + \psi_{yy}^n \\ &= B_2^xD_2^x\psi^n + \psi^nD_2^yB_2^y + B_2^x(\eta_2^x)^n + (\eta_2^y)^nB_2^y \\ &= \Delta_h\psi^n + B_2^x(\eta_2^x)^n + (\eta_2^y)^nB_2^y.\end{aligned} \tag{2.5}$$

Then, for the rotation operator, we derive from the identities (2.2) and (2.4) that

$$\begin{aligned}L_z\psi^n &= -i(X\psi_y^n - \psi_x^nY) \\ &= -i[X(\psi^nD_1^yB_1^y + (\eta_1^y)^nB_1^y) - (B_1^xD_1^x\psi^n + B_1^x(\eta_1^x)^n)Y] \\ &= -i(X\psi^nD_1^yB_1^y - B_1^xD_1^x\psi^nY) - iX(\eta_1^y)^nB_1^y + iB_1^x(\eta_1^x)^nY \\ &= L_z^h\psi^n - iX(\eta_1^y)^nB_1^y + iB_1^x(\eta_1^x)^nY.\end{aligned} \tag{2.6}$$

2.2. Fourth-order linear finite difference method

Now we can incorporate the fourth-order compact approximations (2.5) and (2.6) into the initial boundary value problem (1.1)–(1.3) in space and use a three-level linear difference method in time to arrive at a full-discrete system:

$$i\delta_t\psi_{jk}^n = (-\tfrac{1}{2}\Delta_h + V_{jk} - \Omega L_z^h)\psi_{jk}^{\bar{n}} + \beta|\psi_{jk}^n|^2\psi_{jk}^{\bar{n}}, \quad (x_j, y_k) \in \mathcal{T}_h, \quad t_n \in \mathcal{T}_\tau, \tag{2.7}$$
$$\psi^n \in V_h, \quad t_n \in \mathcal{T}_\tau'', \tag{2.8}$$
$$\psi_{jk}^0 = \psi_0(x_j, y_k), \quad (x_j, y_k) \in \mathcal{T}_h, \tag{2.9}$$

where $V_{jk} = V(x_j, y_k)$. As a three-level scheme, the above scheme cannot start by itself. We can compute the numerical solution at the first step by any explicit second-

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or higher-order time integrator, for example the following second-order modified Euler method:

$$i\delta_t^+\psi_{jk}^0 = \Big(-\frac{1}{2}\Delta_h + V_{jk} - \Omega L_z^h\Big)\psi_{jk}^{1/2} + \beta|\psi_{jk}^{1/2}|^2\psi_{jk}^{1/2}, \quad (x_j, y_k) \in \mathcal{T}_h, \tag{2.10}$$

$$\psi_{jk}^{1/2} = \psi_{jk}^0 - i\frac{\tau}{2}\Big[\Big(-\frac{1}{2}\Delta_h + V_{jk} - \Omega L_z^h\Big)\psi_{jk}^0 + \beta|\psi_{jk}^0|^2\psi_{jk}^0\Big]. \tag{2.11}$$

In practical computation, the order of the execution of the scheme (2.7)–(2.11) is aligned as follows. If ψ^0 is directly given in (2.9), then ψ^1 is obtained from (2.10) and (2.11). If ψ^{n-1}, ψ^n for $n = 1, 2, \ldots, N-1$ are obtained, then ψ^{n+1} can be derived by solving a linear system defined in scheme (2.7) as

$$\Big(I - i\frac{\tau}{2}\Delta_h + i\tau V - i\tau\Omega L_z^h\Big)\psi^{n+1} + i\tau\beta|\psi^n|^2\cdot\psi^{n+1} = \Big(I + i\frac{\tau}{2}\Delta_h - i\tau V + i\tau\Omega L_z^h\Big)\psi^{n-1} - i\tau\beta|\psi^n|^2\cdot\psi^{n-1}$$

and the computational cost is apparently cheaper than the conservative Crank–Nicolson finite difference method [3, 25], which is globally nonlinear and implicit at each discrete time step, and a set of nonlinear algebraic equations has to be solved.

3. Some useful lemmas

To establish an optimal H^1-error estimate for the approximate solution of the proposed scheme, we need the following lemmas.

Lemma 3.1. *For matrices D_2^w, D_1^w, D_+^w and D_-^w,*

$$D_+^{w\top} = -D_-^w, \quad D_2^w = D_-^w D_+^w = D_+^w D_-^w, \quad D_1^w = \tfrac{1}{2}(D_+^w + D_-^w), \quad w = x \text{ or } y.$$

Proof. It can be directly verified by using the definition of the matrices D_2^w, D_1^w, D_+^w and D_-^w. □

Lemma 3.2 [11]. *For a real circulant matrix $A = C(a_0, a_1, \ldots, a_{n-1})$, all eigenvalues of A are given by*

$$f(\varepsilon_k), \quad k = 0, 1, \ldots, n-1,$$

where $f(x) = a_0 + a_1x + a_2x^2 + \cdots + a_{n-1}x^{n-1}$ and $\varepsilon_k = e^{i(2k\pi/n)}$.

Lemma 3.3. *For circulant matrices $A_2^x, A_2^y, A_1^x, A_1^y$,*

$$A_2^x = F_J^H\Lambda_1F_J, \quad A_2^y = F_K^H\Lambda_2F_K, \quad A_1^x = F_J^H\Lambda_3F_J, \quad A_1^y = F_K^H\Lambda_4F_K, \tag{3.1}$$

respectively, where F_J is the discrete Fourier transform matrix with elements $(F_J)_{j,k} = (1/\sqrt{J})e^{-i(2\pi jk/J)}$, F_J^H is the conjugate transpose matrix of F_J and F_K, F_K^H are defined

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similarly. Furthermore,

$$\Lambda_1 = \operatorname{diag}(\lambda_{A_2^x,0}, \lambda_{A_2^x,1}, \ldots, \lambda_{A_2^x,J-1}), \quad \lambda_{A_2^x,j} = \frac{5}{6} + \frac{1}{6}\cos\frac{2j\pi}{J}, \quad 0 \leqslant j \leqslant J-1,$$
$$\Lambda_2 = \operatorname{diag}(\lambda_{A_2^y,0}, \lambda_{A_2^y,1}, \ldots, \lambda_{A_2^y,K-1}), \quad \lambda_{A_2^y,k} = \frac{5}{6} + \frac{1}{6}\cos\frac{2k\pi}{K}, \quad 0 \leqslant k \leqslant K-1,$$
$$\Lambda_3 = \operatorname{diag}(\lambda_{A_1^x,0}, \lambda_{A_1^x,1}, \ldots, \lambda_{A_1^x,J-1}), \quad \lambda_{A_1^x,j} = \frac{2}{3} + \frac{1}{3}\cos\frac{2j\pi}{J}, \quad 0 \leqslant j \leqslant J-1,$$
$$\Lambda_4 = \operatorname{diag}(\lambda_{A_1^y,0}, \lambda_{A_1^y,1}, \ldots, \lambda_{A_1^y,K-1}), \quad \lambda_{A_1^y,k} = \frac{2}{3} + \frac{1}{3}\cos\frac{2k\pi}{K}, \quad 0 \leqslant k \leqslant K-1.$$

Proof. It follows from Lemma 3.2 that

$$\lambda_{A_2^x,j} = \frac{1}{12}\{10 + e^{i(2j\pi/J)} + e^{i(2j\pi/J)(J-1)}\} = \frac{1}{6}\Big(5 + \cos\frac{2j\pi}{J}\Big).$$

Then $\lambda_{A_2^y,k}$, $\lambda_{A_1^x,j}$ and $\lambda_{A_1^y,k}$ can be similarly obtained. Since $A_2^x, A_2^y, A_1^x, A_1^y$ are circulant matrices [11], we have (3.1). Further, it may be verified that

$$1 \leqslant \lambda_{B_2^x}, \quad \lambda_{B_2^y} \leqslant \tfrac{3}{2}, \quad 1 \leqslant \lambda_{B_1^x}, \quad \lambda_{B_1^y} \leqslant 3, \tag{3.2}$$

which completes the proof. □

Lemma 3.4. *For circulant matrices $A, B \in \mathbb{R}^{J\times J}$ and $C, D \in \mathbb{R}^{K\times K}$,*

$$AB = BA, \quad CD = DC.$$

Proof. Noticing that A, B are circulant matrices [11] of order J,

$$AB = F_J^H\Lambda_A F_J F_J^H \Lambda_B F_J = F_J^H \Lambda_A\Lambda_B F_J = F_J^H\Lambda_B\Lambda_A F_J = BA,$$

using the fact that $F_J F_J^H = I$. Similarly, we have $CD = DC$. □

Lemma 3.5 [10]. *For any $A \in \mathbb{C}^{J\times J}$, $B \in \mathbb{C}^{K\times K}$ and $u, v \in V_h$, there exist identities*

$$(Au, v) = (u, A^H v), \quad (uB, v) = (u, vB^H).$$

Lemma 3.6. *For $u, v \in V_h$,*

$$(\Delta_h u, v) = (u, \Delta_h v), \quad (L_z^h u, v) = (u, L_z^h v).$$

Proof. It follows from Lemmas 3.4 and 3.5 that

$$\begin{aligned}
(\Delta_h u, v) &= (B_2^x D_2^x u, v) + (u D_2^y B_2^y, v)\\
&= (u, D_2^x B_2^x v) + (u, v B_2^y D_2^y)\\
&= (u, B_2^x D_2^x v + v D_2^y B_2^y)\\
&= (u, \Delta_h v),\\
(L_z^h u, v) &= -i(X u D_1^y B_1^y - B_1^x D_1^x u Y, v)\\
&= i(u, X v B_1^y D_1^y) - i(u, D_1^x B_1^x v Y)\\
&= i(u, X v D_1^y B_1^y - B_1^x D_1^x v Y)\\
&= (u, L_z^h v),
\end{aligned}$$

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which yield

$$(L_z^h u, u) = (u, L_z^h u) \in \mathbb{R} \tag{3.3}$$

and this completes the proof. □

Unlike the analysis techniques [16, 24], we here utilize the circulant matrix operation to prove the following equivalences of discrete semi-norms:

$$|u|_h \sim \|\nabla_h u\|, \quad \|\Delta_h u\| \sim \|\nabla_h^2 u\|.$$

LEMMA 3.7. *For any grid function $u \in V_h$, the following inequalities hold:*

$$\|\nabla_h u\| \leqslant |u|_h \leqslant \frac{\sqrt{6}}{2}\|\nabla_h u\|. \tag{3.4}$$

PROOF. Using the definitions of $\|\nabla_h\cdot\|$ and $|\cdot|_h$, we obtain from Lemmas 3.1, 3.4 and 3.5 that

$$\begin{aligned}\|\nabla_h u\|^2 &= -(D_2^x u, u) - (uD_2^y, u)\\ &= (D_+^x u, D_+^x u) + (uD_+^y, uD_+^y)\end{aligned}$$

and

$$\begin{aligned}|u|_h^2 &= -(B_2^x D_2^x u, u) - (uD_2^y B_2^y, u)\\ &= (B_2^x D_+^x u, D_+^x u) + (uD_+^y B_2^y, uD_+^y)\\ &= (\Lambda_{B_2^x} F_J D_+^x u, F_J D_+^x u) + (uD_+^y F_K^H \Lambda_{B_2^y}, uD_+^y F_K^H).\end{aligned}$$

Comparing the above equations, and using inequalities (3.2) and the equations

$$F_J^H F_J = I, \quad F_K^H F_K = I, \tag{3.5}$$

we immediately obtain inequalities (3.4). □

LEMMA 3.8. *For any grid function $u \in V_h$, the following inequalities hold:*

$$\|\nabla_h^2 u\| \leqslant \|\Delta_h u\| \leqslant \tfrac{3}{2}\|\nabla_h^2 u\|. \tag{3.6}$$

PROOF. The definitions of $\|\nabla_h^2\cdot\|$ and $\|\Delta_h\cdot\|$, along with Lemmas 3.1, 3.4 and 3.5, yield

$$\begin{aligned}\|\nabla_h^2 u\|^2 &= (D_2^x u + uD_2^y, D_2^x u + uD_2^y)\\ &= (D_2^x u, D_2^x u) + (D_2^x u, uD_2^y) + (uD_2^y, D_2^x u) + (uD_2^y, uD_2^y)\\ &= (D_2^x u, D_2^x u) + 2(D_+^x uD_+^y, D_+^x uD_+^y) + (uD_2^y, uD_2^y)\\ &:= \mathrm{I} + 2\mathrm{II} + \mathrm{III},\\ \|\Delta_h u\|^2 &= (B_2^x D_2^x u + uD_2^y B_2^y, B_2^x D_2^x u + uD_2^y B_2^y)\\ &= (B_2^x D_2^x u, B_2^x D_2^x u) + (B_2^x D_2^x u, uD_2^y B_2^y) + (uD_2^y B_2^y, B_2^x D_2^x u)\\ &\quad + (uD_2^y B_2^y, uD_2^y B_2^y)\\ &= (\Lambda_{B_2^x}^2 F_J D_2^x u, F_J D_2^x u) + 2(\Lambda_{B_2^x} F_J D_+^x uD_+^y F_K^H, F_J D_+^x uD_+^y F_K^H \Lambda_{B_2^y})\\ &\quad + (uD_2^y F_K^H \Lambda_{B_2^y}^2, uD_2^y F_K^H)\\ &:= \widehat{\mathrm{I}} + 2\widehat{\mathrm{II}} + \widehat{\mathrm{III}}.\end{aligned}$$

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From (3.2) and (3.5),

$$\mathrm{II} \leqslant \widehat{\mathrm{II}} \leqslant \tfrac{9}{4}\mathrm{II} \quad \text{and similarly} \quad \mathrm{I} \leqslant \widehat{\mathrm{I}} \leqslant \tfrac{9}{4}\mathrm{I}, \quad \mathrm{III} \leqslant \widehat{\mathrm{III}} \leqslant \tfrac{9}{4}\mathrm{III}.$$

Combining these inequalities immediately yields inequalities (3.6). □

Lemma 3.9. *Under Assumption 2.1,*

$$\frac{1}{2}\Big(1 - \frac{9\Omega^2}{\mu^2}\Big)\|\nabla_h u\|^2 \leqslant \varepsilon(u) \lesssim \|\nabla_h u\|^2 + \|u\|^2. \tag{3.7}$$

Proof. From Lemmas 3.1 and 3.5,

$$\begin{aligned}
\|uD_1^y\|^2 + \|D_1^x u\|^2 &= \tfrac{1}{4}[\|u(D_+^y + D_-^y)\|^2 + \|(D_+^x + D_-^x)u\|^2] \\
&\leqslant \tfrac{1}{2}(\|uD_+^y\|^2 + \|uD_-^y\|^2 + \|D_+^x u\|^2 + \|D_-^- u\|^2) \\
&= \|uD_+^y\|^2 + \|D_+^x u\|^2 \\
&= -(uD_2^y + D_2^x u, u) \\
&= \|\nabla_h u\|^2.
\end{aligned} \tag{3.8}$$

Under Assumption 2.1, from (3.2), (3.3), (3.5) and (3.8),

$$\begin{aligned}
-\Omega(L_z^h u, u) &= \Omega i(XuD_1^y B_1^y - B_1^x D_1^x uY, u) \\
&= \Omega i(uD_1^y B_1^y, Xu) - \Omega i(B_1^x D_1^x u, uY) \\
&\geqslant -|\Omega| \cdot \|uD_1^y B_1^y\| \cdot \|Xu\| - |\Omega| \cdot \|B_1^x D_1^x u\| \cdot \|uY\| \\
&\geqslant -\frac{\Omega^2}{2\mu^2}\|uD_1^y B_1^y\|^2 - \frac{\mu^2}{2}\|Xu\|^2 - \frac{\Omega^2}{2\mu^2}\|B_1^x D_1^x u\|^2 - \frac{\mu^2}{2}\|uY\|^2 \\
&= -\frac{\Omega^2}{2\mu^2}[(uD_1^y (B_1^y)^2, uD_1^y) + ((B_1^x)^2 D_1^x u, D_1^x u)] - \frac{\mu^2}{2}(\|Xu\|^2 + \|uY\|^2) \\
&\geqslant -\frac{9\Omega^2}{2\mu^2}(\|uD_1^y\|^2 + \|D_1^x u\|^2) - h_1 h_2 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} \frac{\mu^2}{2}(x_j^2 + y_k^2)|u_{jk}|^2 \\
&\geqslant -\frac{9\Omega^2}{2\mu^2}\|\nabla_h u\|^2 - h_1 h_2 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} V_{jk}|u_{jk}|^2
\end{aligned} \tag{3.9}$$

and

$$\begin{aligned}
\|L_z^h u\|^2 &= \|XuD_1^y B_1^y - B_1^x D_1^x uY\|^2 \\
&\leqslant 2(\|XuD_1^y B_1^y\|^2 + \|B_1^x D_1^x uY\|^2) \\
&= 2[(X^2 uD_1^y (B_1^y)^2, uD_1^y) + ((B_1^x)^2 D_1^x uY^2, D_1^x u)] \\
&\lesssim \|uD_1^y\|^2 + \|D_1^x u\|^2 \\
&\leqslant \|\nabla_h u\|^2.
\end{aligned} \tag{3.10}$$

Along with the definition of $\varepsilon(u)$, we derive (3.7) from (3.4), (3.9) and (3.10). □

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LEMMA 3.10. *For the approximation $\psi^n \in V_h$, there exist the following identities:*

$$\mathrm{Im}(-\tfrac{1}{2}\Delta_h\psi^{\bar{n}} + V\cdot\psi^{\bar{n}} - \Omega L_z^h\psi^{\bar{n}}, \psi^{\bar{n}}) = 0, \tag{3.11}$$

$$\mathrm{Re}\Big(-\frac{1}{2}\Delta_h\psi^{\bar{n}} + V\cdot\psi^{\bar{n}} - \Omega L_z^h\psi^{\bar{n}}, \delta_t\psi^n\Big) = \frac{1}{4\tau}[\varepsilon(\psi^{n+1}) - \varepsilon(\psi^{n-1})], \tag{3.12}$$

where "$\mathrm{Im}(s)$*" and "*$\mathrm{Re}(s)$*" mean the imaginary part and the real part of a complex number s, respectively.*

PROOF. The definition of $\varepsilon(\psi^n)$ together with Lemma 3.9 gives

$$\mathrm{Im}(-\tfrac{1}{2}\Delta_h\psi^{\bar{n}} + V\cdot\psi^{\bar{n}} - \Omega L_z^h\psi^{\bar{n}}, \psi^{\bar{n}}) = \mathrm{Im}\varepsilon(\psi^{\bar{n}}) = 0,$$

which is (3.11). From Lemma 3.6,

$$\mathrm{Re}[-(\Delta_h\psi^{n+1}, \psi^{n-1}) + (\Delta_h\psi^{n-1}, \psi^{n+1})] = 0,$$
$$\mathrm{Re}[-(L_z^h\psi^{n+1}, \psi^{n-1}) + (L_z^h\psi^{n-1}, \psi^{n+1})] = 0.$$

Using the above identities,

$$\begin{aligned}
\mathrm{Re}\Big(-\frac{1}{2}\Delta_h\psi^{\bar{n}}, \delta_t\psi^n\Big) &= -\frac{1}{8\tau}\mathrm{Re}(\Delta_h\psi^{n+1} + \Delta_h\psi^{n-1}, \psi^{n+1} - \psi^{n-1})\\
&= \frac{1}{8\tau}(|\psi^{n+1}|_h^2 - |\psi^{n-1}|_h^2),\\
\mathrm{Re}(V\cdot\psi^{\bar{n}}, \delta_t\psi^n) &= \frac{1}{4\tau}\mathrm{Re}\Big[h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}V_{jk}(\psi_{jk}^{n+1} + \psi_{jk}^{n-1})(\bar{\psi}_{jk}^{n+1} - \bar{\psi}_{jk}^{n-1})\Big]\\
&= \frac{1}{4\tau}h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}V_{jk}(|\psi_{jk}^{n+1}|^2 - |\psi_{jk}^{n-1}|^2),\\
-\Omega\mathrm{Re}(L_z^h\psi^{\bar{n}}, \delta_t\psi^n) &= -\frac{\Omega}{4\tau}\mathrm{Re}(L_z^h\psi^{n+1} + L_z^h\psi^{n-1}, \psi^{n+1} - \psi^{n-1})\\
&= -\frac{\Omega}{4\tau}[(L_z^h\psi^{n+1}, \psi^{n+1}) - (L_z^h\psi^{n-1}, \psi^{n-1})].
\end{aligned}$$

Adding the above equations yields (3.12). □

LEMMA 3.11 [27]. *For any grid function $u \in V_h$,*

$$\|u\|_\infty \leqslant C\|u\|^{1-d/4}(\|\nabla_h^2 u\| + \|u\|)^{d/4}$$

for $d = 2, 3$.

4. Existence of solution and conservation laws

In this section, we show that the proposed scheme is solvable and it possesses the discrete mass and energy conservation laws.

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Lemma 4.1 (Browder fixed point theorem [5]). *Let $(H, \langle\cdot,\cdot\rangle)$ be a finite-dimensional inner product space, $\|\cdot\|$ the associated norm and $g : H \to H$ a continuous function. If*

$$\text{there exists } \alpha > 0 \quad \text{for all } z \in H \quad \|z\| = \alpha, \text{ such that } \mathrm{Re}\langle g(z), z\rangle \geqslant 0,$$

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

Theorem 4.2. *The linearized equation system in scheme (2.7)–(2.11) is solvable.*

Proof. Note that the assertion for (2.10) is true. For a fixed n, (2.7) can be written as

$$\psi^{\bar{n}} = \psi^{n-1} - i\tau(-\tfrac{1}{2}\Delta_h\psi^{\bar{n}} + V\cdot\psi^{\bar{n}} - \Omega L_z^h\psi^{\bar{n}} + \beta|\psi^n|^2\cdot\psi^{\bar{n}}),$$
$$\psi^{n-1} \in V_h, \quad \psi^{\bar{n}} \in V_h,$$

where $|\psi^n|^2 \cdot \psi^{\bar{n}} = (|\psi^n_{jk}|^2\psi^{\bar{n}}_{jk})$. We define a mapping $\mathcal{F} : V_h \to V_h$ as follows:

$$\mathcal{F}w = w - \psi^{n-1} + i\tau(-\tfrac{1}{2}\Delta_h w + V\cdot w - \Omega L_z^h w + \beta|\psi^n|^2\cdot w), \tag{4.1}$$

which is continuous. Computing the inner product of (4.1) with w and taking the real part, we obtain from Cauchy–Schwarz inequalities and Lemma 3.9 that

$$\begin{aligned}\mathrm{Re}(\mathcal{F}w, w) &= \|w\|^2 - \mathrm{Re}(\psi^{n-1}, w) - \tau\mathrm{Im}\Big(\varepsilon(u) + \beta h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}|\psi^n_{jk}|^2|w_{jk}|^2\Big)\\ &= \|w\|^2 - \mathrm{Re}(\psi^{n-1}, w)\\ &\geqslant \|w\|^2 - \|\psi^{n-1}\|\cdot\|w\|\\ &\geqslant \tfrac{1}{2}(\|w\|^2 - \|\psi^{n-1}\|^2).\end{aligned}$$

Hence, taking $\alpha = \sqrt{\|\psi^{n-1}\|^2 + 2}$ for $\|w\| = \alpha$, we have $\mathrm{Re}(\mathcal{F}w, w) \geqslant 1$. Thus, the existence of $\psi^{\bar{n}}$ follows from Lemma 4.1 and, consequently, the existence of ψ^{n+1} is obtained. □

Theorem 4.3. *The proposed scheme (2.7)–(2.11) is conservative in the sense that for $t_n \in \mathcal{T}_\tau$,*

$$M^n = \tfrac{1}{2}(\|\psi^{n+1}\|^2 + \|\psi^n\|^2) \equiv M^0, \tag{4.2}$$

$$E^n = \frac{1}{2}[\varepsilon(\psi^{n+1}) + \varepsilon(\psi^n)] + \frac{\beta}{2}h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}|\psi^{n+1}_{jk}|^2|\psi^n_{jk}|^2 \equiv E^0. \tag{4.3}$$

Proof. Computing the discrete inner product of (2.7) with $\psi^{\bar{n}}$ and then taking the imaginary part, we derive from the identity (3.11),

$$\frac{1}{4\tau}(\|\psi^{n+1}\|^2 - \|\psi^{n-1}\|^2) = 0,$$

which yields (4.2).

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Similarly, computing the discrete inner product of (2.7) with $2\tau\delta_t\psi^n$ and then taking the real part, we obtain from the identity (3.12),

$$\frac{1}{2}[\varepsilon(\psi^{n+1}) - \varepsilon(\psi^{n-1})] + \frac{\beta}{2}h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}|\psi_{jk}^n|^2(|\psi_{jk}^{n+1}|^2 - |\psi_{jk}^{n-1}|^2) = 0, \quad t_n \in \mathcal{T}_\tau,$$

that is,

$$\frac{1}{2}\varepsilon(\psi^{n+1}) + \frac{\beta}{2}h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}|\psi_{jk}^{n+1}|^2|\psi_{jk}^n|^2 = \frac{1}{2}\varepsilon(\psi^{n-1}) + \frac{\beta}{2}h_1h_2\sum_{j=0}^{J-1}\sum_{k=0}^{K-1}|\psi_{jk}^n|^2|\psi_{jk}^{n-1}|^2,$$

which gives (4.3). □

5. Error estimate of the scheme

In this section, we establish an optimal H^1-error estimate for the proposed scheme, without any constraints on the grid ratio. We define the local truncation error $\eta^n \in V_h$ by

$$\eta_{jk}^n = i\delta_t\phi_{jk}^n + (\tfrac{1}{2}\Delta_h - V_{jk} + \Omega L_z^h)\phi_{jk}^{\bar{n}} - \beta|\phi_{jk}^n|^2\phi_{jk}^{\bar{n}}, \quad (x_j, y_k) \in \mathcal{T}_h, \quad t_n \in \mathcal{T}_\tau, \tag{5.1}$$

$$\eta_{jk}^0 = i\delta_t^+\phi_{jk}^0 + (\tfrac{1}{2}\Delta_h - V_{jk} + \Omega L_z^h)\phi_{jk}^{1/2} - \beta|\phi_{jk}^{1/2}|^2\phi_{jk}^{1/2}, \quad (x_j, y_k) \in \mathcal{T}_h, \tag{5.2}$$

$$\phi_{jk}^{1/2} = \phi_{jk}^0 - i\frac{\tau}{2}\Big[\Big(-\frac{1}{2}\Delta_h + V_{jk} - \Omega L_z^h\Big)\phi_{jk}^0 + \beta|\phi_{jk}^0|^2\phi_{jk}^0\Big], \quad (x_j, y_k) \in \mathcal{T}_h, \tag{5.3}$$

where

$$\phi_{jk}^n = \psi(x_j, y_k, t_n), \quad \phi_{jk}^{\bar{n}} = \frac{1}{2}(\phi_{jk}^{n+1} + \phi_{jk}^{n-1}), \quad \delta_t\phi_{jk}^n = \frac{1}{2\tau}(\phi_{jk}^{n+1} - \phi_{jk}^{n-1}).$$

LEMMA 5.1 (Local truncation error). *If Assumptions 2.1 and 2.2 hold, then the local truncation error of the proposed scheme satisfies the following inequalities:*

$$\|\eta^n\| \leqslant C(h^4 + \tau^2), \quad t_n \in \mathcal{T}_\tau, \tag{5.4}$$

$$\|\eta^0\| \leqslant C(h^4 + \tau^2), \quad \|\nabla_h\eta^0\| \leqslant C(h^4 + \tau^2), \quad \|\eta^0\|_\infty \leqslant C. \tag{5.5}$$

The proof of this result is presented in Appendix A.

Let us now define an error function $e^n \in V_h$ by

$$e_{jk}^n = \phi_{jk}^n - \psi_{jk}^n, \quad (x_j, y_k) \in \mathcal{T}_h, \quad t_n \in \mathcal{T}_\tau''.$$

Then, for the convergence analysis for the proposed scheme, we have the following theorem.

THEOREM 5.2. *If Assumptions 2.1 and 2.2 hold, then there are $h_0 > 0$ and $\tau_0 > 0$ such that for all $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, the error of the proposed scheme (2.7)–(2.11) satisfies the inequalities*

$$\|e^n\| \leqslant C(h^4 + \tau^2), \quad t_n \in \mathcal{T}_\tau'', \tag{5.6}$$

$$\|e^n\|_\infty \leqslant C, \quad \|\psi^n\|_\infty \leqslant C, \quad t_n \in \mathcal{T}_\tau'', \tag{5.7}$$

$$\|\nabla_h e^2\| \leqslant C(h^4 + \tau^2). \tag{5.8}$$

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PROOF. Subtracting (2.7) and (2.10) from (5.1) and (5.2), respectively,

$$i\delta_t e^n_{jk} = (-\tfrac{1}{2}\Delta_h + V_{jk} - \Omega L^h_z)e^{\bar{n}}_{jk} + \xi^n_{jk} + \eta^n_{jk}, \quad t_n \in \mathcal{T}_\tau, \tag{5.9}$$

$$i\delta^+_t e^0_{jk} = \eta^0_{jk}, \tag{5.10}$$

where

$$\begin{aligned}\xi^n_{jk} &= \beta|\phi^n_{jk}|^2\phi^{\bar{n}}_{jk} - \beta|\psi^n_{jk}|^2\psi^{\bar{n}}_{jk}\\ &= \beta(|\phi^n_{jk}|^2 - |\psi^n_{jk}|^2)\phi^{\bar{n}}_{jk} + \beta|\psi^n_{jk}|^2 e^{\bar{n}}_{jk}\\ &= \beta(e^n_{jk}\bar{\phi}^n_{jk} + \psi^n_{jk}\bar{e}^n_{jk})\phi^{\bar{n}}_{jk} + \beta|\psi^n_{jk}|^2 e^{\bar{n}}_{jk}.\end{aligned} \tag{5.11}$$

Here we use mathematical induction. From (1.3) and (2.9), we find that (5.6) and (5.7) are apparently true when $n = 0$. Then it follows from (5.5) and (5.10) that

$$\|e^1\| = \|-i\tau\eta^0\| \leqslant C\tau(h^4 + \tau^2), \tag{5.12}$$

$$\|\nabla_h e^1\| = \tau\|\nabla_h\eta^0\| \leqslant C\tau(h^4 + \tau^2), \tag{5.13}$$

$$\|e^1\|_\infty = \|-i\tau\eta^0\|_\infty \leqslant C, \tag{5.14}$$

$$\|\psi^1\|_\infty \leqslant \|\phi^1\|_\infty + \|e^1\|_\infty \leqslant C,$$

which implies the validity of inequalities (5.6) and (5.7) when $n = 1$. Now we assume that (5.6)–(5.7) are true for all $0 \leqslant n \leqslant m-1$ $(2 \leqslant m \leqslant N)$; then, from (5.11),

$$\|\xi^n\| \leqslant C(\|e^{n+1}\| + \|e^n\| + \|e^{n-1}\|), \quad 1 \leqslant n \leqslant m-1. \tag{5.15}$$

First, we need to prove that (5.6) is still true when $n = m$. Computing the inner product of (5.9) with $e^{\bar{n}}$ and taking the imaginary part, from (3.11), (5.4) and (5.15),

$$\begin{aligned}\|e^{n+1}\|^2 - \|e^{n-1}\|^2 &= 2\tau\,\mathrm{Im}(\xi^n + \eta^n, e^{n+1} + e^{n-1})\\ &\leqslant 2\tau(\|\xi^n\|^2 + \|\eta^n\|^2 + \|e^{n+1}\|^2 + \|e^{n-1}\|^2)\\ &\leqslant C\tau(\|e^{n+1}\|^2 + \|e^n\|^2 + \|e^{n-1}\|^2) + C\tau(h^4 + \tau^2)^2,\end{aligned}$$

that is,

$$\|e^{n+1}\|^2 - \|e^{n-1}\|^2 \leqslant C\tau(\|e^{n+1}\|^2 + \|e^n\|^2 + \|e^{n-1}\|^2) + C\tau(h^4 + \tau^2)^2.$$

Summing all these inequalities with n changing from 1 to $m-1$,

$$\|e^m\|^2 + \|e^{m-1}\|^2 - \|e^1\|^2 - \|e^0\|^2 \leqslant C\tau\sum_{l=1}^{m}\|e^l\|^2 + CT(h^4 + \tau^2)^2.$$

Using (5.12), we rewrite the last inequality as

$$\|e^m\|^2 \leqslant C\tau\sum_{l=1}^{m}\|e^l\|^2 + C(h^4 + \tau^2)^2.$$

This, together with the Gronwall inequality [15], yields (5.6) for $n = m$. Then

$$\|e^n\| \leqslant C(h^4 + \tau^2), \quad 0 \leqslant n \leqslant m. \tag{5.16}$$

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Next, we need to show that (5.7) is also true when $n = m$. From inequality (3.10),

$$\begin{aligned}
\|L_z^h e^n\|^2 &\leqslant C\|\nabla_h e^n\|^2 \\
&= -C(\nabla_h^2 e^n, e^n) \\
&\leqslant C\|\nabla_h^2 e^n\| \cdot \|e^n\| \\
&\leqslant \frac{1}{4\varepsilon^2}\|\nabla_h^2 e^n\|^2 + \varepsilon^2 C^2\|e^n\|^2 \\
&\leqslant \left(\frac{1}{2\varepsilon}\|\nabla_h^2 e^n\| + \varepsilon C\|e^n\|\right)^2,
\end{aligned}$$

that is,

$$\|L_z^h e^n\| \leqslant \frac{1}{2\varepsilon}\|\nabla_h^2 e^n\| + \varepsilon C\|e^n\| \quad \text{for all } \varepsilon > 0. \tag{5.17}$$

We now utilize the lifting technique [25] to prove the boundedness of $\|e^m\|_\infty$. It follows from (5.9) and Assumption 2.1 that for $n = 1, 2, \ldots, m-1$,

$$\|\Delta_h(e^{n+1} + e^{n-1})\| \leqslant C(\|\delta_t e^n\| + \|e^{n+1} + e^{n-1}\| + \|L_z^h(e^{n+1} + e^{n-1})\| + \|\xi^n\| + \|\eta^n\|). \tag{5.18}$$

Considering each term in the right-hand side of (5.18) and using (5.4) and (5.15)–(5.17),

$$\begin{aligned}
\|\delta_t e^n\| &\leqslant C\tau^{-1}(\|e^{n+1}\| + \|e^{n-1}\|) \leqslant C\tau^{-1}(h^4 + \tau^2), \\
\|e^{n+1} + e^{n-1}\| &\leqslant \|e^{n+1}\| + \|e^{n-1}\| \leqslant C(h^4 + \tau^2), \\
\|L_z^h(e^{n+1} + e^{n-1})\| &\leqslant \frac{1}{2\varepsilon}\|\nabla_h^2(e^{n+1} + e^{n-1})\| + \varepsilon C\|e^{n+1} + e^{n-1}\| \\
&\leqslant \frac{1}{2\varepsilon}\|\nabla_h^2(e^{n+1} + e^{n-1})\| + \varepsilon C(h^4 + \tau^2), \\
\|\xi^n\| + \|\eta^n\| &\leqslant C(h^4 + \tau^2).
\end{aligned}$$

Substituting these estimates into (5.18) and taking $\varepsilon = C$, one can obtain from (3.6),

$$\|\nabla_h^2(e^{n+1} + e^{n-1})\| \leqslant C\tau^{-1}(h^4 + \tau^2), \quad n = 1, 2, \ldots, m-1. \tag{5.19}$$

Therefore, starting with Lemma 3.11 and using inequalities (5.16) and (5.19),

$$\begin{aligned}
\|e^{n+1} + e^{n-1}\|_\infty &\leqslant C\|e^{n+1} + e^{n-1}\|^{1/2}(\|\nabla_h^2(e^{n+1} + e^{n-1})\| + \|e^{n+1} + e^{n-1}\|)^{1/2} \\
&\leqslant C\tau^{-1/2}(h^4 + \tau^2), \quad n = 1, 2, \ldots, m-1.
\end{aligned}$$

The last inequality also implies that

$$\begin{aligned}
\|e^{n+1}\|_\infty - \|e^{n-1}\|_\infty &\leqslant \|e^{n+1} + e^{n-1}\|_\infty \\
&\leqslant C\tau^{-1/2}(h^4 + \tau^2), \quad n = 1, 2, \ldots, m-1,
\end{aligned}$$

and, summing all such estimates with n changing from 1 to $m-1$,

$$\begin{aligned}\|e^m\|_\infty + \|e^{m-1}\|_\infty - \|e^1\|_\infty - \|e^0\|_\infty &\leqslant C(m-1)\tau^{-1/2}(h^4+\tau^2)\\ &\leqslant CT\tau^{-3/2}(h^4+\tau^2).\end{aligned}$$

This, together with inequality (5.14), gives

$$\|e^m\|_\infty \leqslant C[1+\tau^{-3/2}(h^4+\tau^2)].$$

On the other hand, by using the inverse inequality [22],

$$\|e^m\|_\infty \leqslant Ch^{-1}\|e^m\| \leqslant Ch^{-1}(h^4+\tau^2).$$

Therefore, with no constraints on the time-step size, it is always true to have

$$\|e^m\|_\infty \leqslant C, \quad \|\psi^m\|_\infty \leqslant \|\phi^m\|_\infty + \|e^m\|_\infty \leqslant C.$$

This implies that (5.7) is true for $n=m$; thus, the validity of (5.6) and (5.7) for $t_n \in \mathcal{T}_\tau''$ is proved by induction.

Finally, we present the proof of (5.8). Noticing that $e_{jk}^0 = 0$, we rewrite (5.9) for $n=1$ as

$$\frac{i}{2\tau}e_{jk}^2 = \frac{1}{2}\Big(-\frac{1}{2}\Delta_h + V_{jk} - \Omega L_z^h\Big)e_{jk}^2 + \xi_{jk}^1 + \eta_{jk}^1. \tag{5.20}$$

Computing the inner product of (5.20) with $2e^2$ and taking the real part,

$$\varepsilon(e^2) = -2\mathrm{Re}(\xi^1, e^2) - 2\mathrm{Re}(\eta^1, e^2).$$

This, along with inequalities (3.7), (5.4), (5.6) and (5.15), yields

$$\|\nabla_h e^2\|^2 \leqslant C(\|\xi^1\|^2 + \|\eta^1\|^2 + \|e^2\|^2) \leqslant C(h^4+\tau^2)^2,$$

which completes the proof. □

Further, in the following, we make higher temporal regularity assumption on the solution of the problem (1.1)–(1.3).

Assumption 5.3. For the exact solution ψ, we assume that

$$\psi \in C^4([0,T];L^\infty(\mathcal{D})) \cap C^3([0,T];W^{2,\infty}(\mathcal{D})) \cap C^1([0,T];W^{6,\infty}(\mathcal{D}) \cap H_p^1(\mathcal{D})).$$

Then we have the following result.

Theorem 5.4. *If Assumptions 2.1 and 5.3 hold, then there are $h_0 > 0$ and $\tau_0 > 0$ such that for all $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, the error of the proposed scheme satisfies the inequality*

$$\|e^n\|_{1,h} \leqslant C(h^4+\tau^2), \quad t_n \in \mathcal{T}_\tau''.$$

PROOF. With Assumptions 2.1 and 5.3, by utilizing (A.8) in Appendix A, we have the following result on the local truncation error:

$$\|\delta_t \eta^n\| \leqslant C(h^4 + \tau^2), \quad n = 2, \dots, N-2. \tag{5.21}$$

Then the boundedness of the approximate solution can now be utilized to establish semi-norm estimates of the nonlinear term ξ^n in (5.9). Invoking (5.7) and (5.11), we first estimate

$$\|\delta_x^+ \xi^n\| \leqslant C(\|\delta_x^+ e^{n+1}\| + \|\delta_x^+ e^n\| + \|\delta_x^+ e^{n-1}\| + \|e^{n+1}\| + \|e^n\| + \|e^{n-1}\|),$$
$$\|\delta_y^+ \xi^n\| \leqslant C(\|\delta_y^+ e^{n+1}\| + \|\delta_y^+ e^n\| + \|\delta_y^+ e^{n-1}\| + \|e^{n+1}\| + \|e^n\| + \|e^{n-1}\|)$$

and these inequalities lead to the estimate

$$\|\nabla_h \xi^n\| \leqslant C(\|\nabla_h e^{n+1}\| + \|\nabla_h e^n\| + \|\nabla_h e^{n-1}\| + \|e^{n+1}\| + \|e^n\| + \|e^{n-1}\|), \quad t_n \in \mathcal{T}_\tau. \tag{5.22}$$

Computing the inner product of both sides of (5.9) with $4\tau\delta_t e^n$ and taking the real part, we obtain from identity (3.12) that

$$\varepsilon(e^{n+1}) - \varepsilon(e^{n-1}) = -4\tau \mathrm{Re}(\xi^n, \delta_t e^n) - 4\tau \mathrm{Re}(\eta^n, \delta_t e^n), \quad n = 2, \dots, N-1.$$

These equations can be summed with n ranging from 2 to m. Now, using the identity

$$2\tau \sum_{l=2}^{m} (\eta^l, \delta_t e^l) = -2\tau \sum_{l=2}^{m-1} (\delta_t \eta^l, e^l) + (\eta^m, e^{m+1}) + (\eta^{m-1}, e^m) - (\eta^1, e^2) - (\eta^2, e^1)$$

and then replacing m by n,

$$\begin{aligned}\varepsilon(e^{n+1}) + \varepsilon(e^n) - \varepsilon(e^2) - \varepsilon(e^1) &= -4\tau \sum_{l=2}^{n} \mathrm{Re}(\xi^l, \delta_t e^l) + 4\tau \sum_{l=2}^{n-1} \mathrm{Re}(\delta_t \eta^l, e^l) \\ &\quad - 2\mathrm{Re}[(\eta^n, e^{n+1}) + (\eta^{n-1}, e^n) - (\eta^1, e^2) - (\eta^2, e^1)].\end{aligned} \tag{5.23}$$

Before estimating the right-hand terms, we first derive from Lemma 3.1, (3.2) and (3.5),

$$\begin{aligned}|(\xi^l, \Delta_h e^l)| &= |(\xi^l, B_2^x D_2^x e^l + e^l D_2^y B_2^y)| \\ &\leqslant |(\xi^l, B_2^x D_2^x e^l)| + |(\xi^l, e^l D_2^y B_2^y)| \\ &= |(D_+^x \xi^l, B_2^x D_+^x e^l)| + |(\xi^l D_+^y, e^l D_+^y B_2^y)| \\ &\leqslant \tfrac{1}{2}\|D_+^x \xi^l\|^2 + \tfrac{1}{2}\|B_2^x D_+^x e^l\|^2 + \tfrac{1}{2}\|\xi^l D_+^y\|^2 + \tfrac{1}{2}\|e^l D_+^y B_2^y\|^2 \\ &= -\tfrac{1}{2}(D_2^x \xi^l + \xi^l D_2^y, \xi^l) + \tfrac{1}{2}((B_2^x)^2 D_+^x e^l, D_+^x e^l) + \tfrac{1}{2}(e^l D_+^y (B_2^y)^2, e^l D_+^y) \\ &\leqslant \tfrac{1}{2}\|\nabla_h \xi^l\|^2 + \tfrac{9}{8}[(D_+^x e^l, D_+^x e^l) + (e^l D_+^y, e^l D_+^y)] = \tfrac{1}{2}\|\nabla_h \xi^l\|^2 + \tfrac{9}{8}\|\nabla_h e^l\|^2.\end{aligned} \tag{5.24}$$

Let us now estimate each term in the right-hand side of (5.23). For this, we use the triangle and Cauchy inequalities, along with inequalities (3.10), (5.4), (5.6), (5.15),

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(5.21), (5.22) and (5.24), to arrive at the estimates

$$\begin{aligned}
|\mathrm{Re}(\xi^l, \delta_t e^l)| &= \Big|\mathrm{Re}\Big(\xi^l, i\Big(\frac{1}{2}\Delta_h - V + \Omega L_z^h\Big)e^{\bar{l}} - i\xi^l - i\eta^l\Big)\Big| \\
&\leqslant \frac{1}{2}|\mathrm{Im}(\xi^l, \Delta_h e^{\bar{l}})| + |\mathrm{Im}(\xi^l, V\cdot e^{\bar{l}})| + |\mathrm{Im}(\xi^l, \Omega L_z^h e^{\bar{l}})| + |\mathrm{Im}(\xi^l, \eta^l)| \\
&\leqslant \frac{1}{4}\|\nabla_h \xi^l\|^2 + \frac{9}{16}\|\nabla_h e^{\bar{l}}\|^2 + \frac{1}{2}\|\xi^l\|^2 + \frac{1}{2}\|V\|_\infty^2 \|e^{\bar{l}}\|^2 \\
&\quad + \frac{|\Omega|}{2}\|\xi^l\|^2 + \frac{|\Omega|}{2}\|L_z^h e^{\bar{l}}\|^2 + \frac{1}{2}\|\xi^l\|^2 + \frac{1}{2}\|\eta^l\|^2 \\
&\leqslant C(\|\nabla_h e^{l+1}\|^2 + \|\nabla_h e^l\|^2 + \|\nabla_h e^{l-1}\|^2) + C(h^4 + \tau^2)^2, \quad 2 \leqslant l \leqslant n, \\
|\mathrm{Re}(\delta_t \eta^l, e^l)| &\leqslant \tfrac{1}{2}\|\delta_t \eta^l\|^2 + \tfrac{1}{2}\|e^l\|^2 \leqslant C(h^4 + \tau^2)^2, \quad 2 \leqslant l \leqslant n-1,
\end{aligned}$$

$$\begin{aligned}
&|2\mathrm{Re}[(\eta^n, e^{n+1}) + (\eta^{n-1}, e^n) - (\eta^1, e^2) - (\eta^2, e^1)]| \\
&\qquad \leqslant C(\|\eta^n\|^2 + \|e^{n+1}\|^2 + \|\eta^{n-1}\|^2 + \|e^n\|^2 + \|\eta^1\|^2 + \|e^2\|^2 + \|\eta^2\|^2 + \|e^1\|^2) \\
&\qquad \leqslant C(h^4 + \tau^2)^2.
\end{aligned}$$

Substituting these estimates into (5.23) and using inequalities (3.7), (5.6), (5.8) and (5.13) yield

$$\|\nabla_h e^{n+1}\|^2 \leqslant C\tau \sum_{l=1}^{n+1} \|\nabla_h e^l\|^2 + C(h^4 + \tau^2)^2, \quad n = 2, \ldots, N-1.$$

Finally, using the discrete Gronwall inequality [15], we obtain $\|\nabla_h e^n\| \leqslant C(h^4 + \tau^2)$, $n = 3, \ldots, N$. Incorporating estimates (5.6), (5.8), (5.13) into the last inequality gives

$$\|e^n\|_{1,h} \leqslant C(h^4 + \tau^2), \quad t_n \in \mathcal{T}_\tau'',$$

which completes the proof. □

Similarly, we have the following stability result.

Theorem 5.5. *If Assumptions 2.1 and 5.3 hold, then there are $h_0 > 0$ and $\tau_0 > 0$ such that for all $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, the proposed scheme (2.7)–(2.11) is unconditionally stable with respect to the initial data in the discrete H^1-norm.*

Remark 5.6. In fact, the existence of the discrete conservation laws is essential to guarantee the convergence and unconditional stability of the proposed scheme [1, 8, 26] and it will not yield numerical "blow-up" for the approximate solution [26].

6. Numerical examples

In this section, results of some experiments are presented to verify the theoretical analysis on convergence and conservation of mass and energy.

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TABLE 1. Temporal errors of the numerical solutions with $t = 1, h = 1/32$.

		$\tau_0 = 1/400$	$\tau_0/2$	$\tau_0/4$	$\tau_0/8$
$\Omega = 0$	$\|\|e\|\|_{1,h}$	0.0973	0.0259	0.0064	0.0014
	Rate	1.94	2.01	2.08	*
	$\|\|e\|\|_\infty$	0.0048	0.0012	2.94e-004	6.82e-5
	Rate	2.00	2.02	2.07	*
$\Omega = 0.5$	$\|\|e\|\|_{1,h}$	0.0957	0.0254	0.0063	0.0014
	Rate	1.93	2.01	2.08	*
	$\|\|e\|\|_\infty$	0.0048	0.0016	4.02e-004	9.32e-5
	Rate	1.73	1.99	2.07	*
$\Omega = 0.9$	$\|\|e\|\|_{1,h}$	0.0925	0.0247	0.0061	0.0014
	Rate	1.93	2.01	2.08	*
	$\|\|e\|\|_\infty$	0.0059	0.0015	3.89e-004	9.09e-005
	Rate	1.96	1.97	2.07	*

EXAMPLE 6.1. We set $\mathcal{D} = [-2, 2]^2$, $V(x, y) = (x^2 + y^2)/2$ and $\beta = 1$. The initial condition is taken as $\psi_0 = (2/\sqrt{\pi})(x + iy)e^{-8(x^2+y^2)}$. For comparison, the numerical "exact" solution ψ_e is obtained by the proposed scheme with a very fine mesh and a small time step, for example $h = 1/128$ and $\tau = 0.00001$. Let $e(\tau, h)$ denote the error of the numerical solution with time step τ and mesh size h. The convergence rate is calculated using the following formula:

$$\text{Rate} = \frac{\ln(\text{error}_1/\text{error}_2)}{\ln(\delta_1/\delta_2)},$$

where $\delta_l, \text{error}_l (l = 1, 2)$ are step size and the error with step size δ_l, respectively.

Convergence tests are presented in Tables 1 and 2 with different angular speeds Ω, respectively. The accuracy of second order in time and fourth order in space is clearly observed, which verifies the preceding theoretical analysis. For brevity, we define the Crank–Nicolson finite difference method [3] as "CNFD" and denote the proposed scheme (2.7)–(2.11) as "LCFD". The comparison of the spatial convergence rate between CNFD and LCFD is presented in Table 3 and the numerical results show that our method has higher efficiency and accuracy.

Moreover, we further demonstrate the long-time behaviour by employing a larger time period $T = 10$. As we can see from Figure 1, the errors of discrete mass and energy reach machine accuracy for all the choices of Ω, which uniformly illustrate the conservative properties of the proposed scheme. Notice that the small time step $\tau = 0.001$ is used in the simulation so as to guarantee that every iteration of BiCGSTAB used for solving the linear system can converge to the desired tolerance. Otherwise, the evolution of the errors may exhibit a slightly linear growth but with the ending error at $T = 10$ of magnitude 10^{-12}, which usually is also considered as a rigorous conservation.

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TABLE 2. Spatial errors of the numerical solutions with $t = 0.05, \tau = 0.00001$.

		$h_0 = 4/32$	$h_0/2$	$h_0/4$	$h_0/8$
$\Omega = 0$	$\|\|e\|\|_{1,h}$	6.9895e-004	4.4488e-005	2.7732e-006	1.6315e-007
	Rate	3.96	4.00	4.12	*
	$\|\|e\|\|_\infty$	1.4387e-004	8.6196e-006	5.3437e-007	3.1465e-008
	Rate	4.08	4.00	4.12	*
$\Omega = 0.5$	$\|\|e\|\|_{1,h}$	6.9054e-004	4.4015e-005	2.7445e-006	1.6147e-007
	Rate	3.96	4.00	4.12	*
	$\|\|e\|\|_\infty$	1.4268e-004	8.5519e-006	5.2969e-007	3.1196e-008
	Rate	4.08	4.01	4.12	*
$\Omega = 0.9$	$\|\|e\|\|_{1,h}$	6.8409e-004	4.3650e-005	2.7224e-006	1.6017e-007
	Rate	3.95	4.00	4.12	*
	$\|\|e\|\|_\infty$	1.4173e-004	8.4978e-006	5.2596e-007	3.0981e-008
	Rate	4.08	4.01	4.12	*

TABLE 3. Comparisons of spatial convergence rate with $t = 0.05, \tau = 0.00001, \Omega = 0.3$.

		$h_0 = 4/32$	$h_0/2$	$h_0/4$	$h_0/8$
CNFD	$\|\|e\|\|_{1,h}$	0.0075	0.0020	4.9496e-004	9.9510e-005
	Rate	1.93	2.02	2.23	*
	$\|\|e\|\|_\infty$	0.0017	4.3523e-004	1.0454e-004	2.0955e-005
	Rate	1.97	2.04	2.23	*
LCFD	$\|\|e\|\|_{1,h}$	6.9386e-004	4.4202e-005	2.7559e-006	1.6213e-007
	Rate	3.96	4.00	4.12	*
	$\|\|e\|\|_\infty$	1.4316e-004	8.5790e-006	5.3156e-007	3.1304e-008
	Rate	4.08	4.01	4.12	*

EXAMPLE 6.2. In this example, we consider the dynamics of vortex lattices in rotating BECs. The initial datum is chosen as the L^2-normalized ground state eigenvector of the Gross–Pitaevskii operator

$$G_0(v) = -\Delta v/2 + V_0 v - \Omega L_z v + \beta|v|^2 v$$

with $V_0(x, y) = (x^2 + y^2)/2$. We compute this ground state using the backward Euler centred finite difference (BEFD) method [4], which is also equipped in the GPELab program [2]. The parameters are chosen as $\Omega = 0.7$, $\beta = 100$ firstly and we solve the problem on $\mathcal{D} = [-6, 6]^2$ with mesh size $h = 12/128$. Figures 2 and 3 display the corresponding initial stationary vortex as well as the contour plots of the density function $|\psi|^2$ for the dynamics of vortex lattices simulated at different times by the proposed scheme. It is clearly observed that during the dynamics the number of

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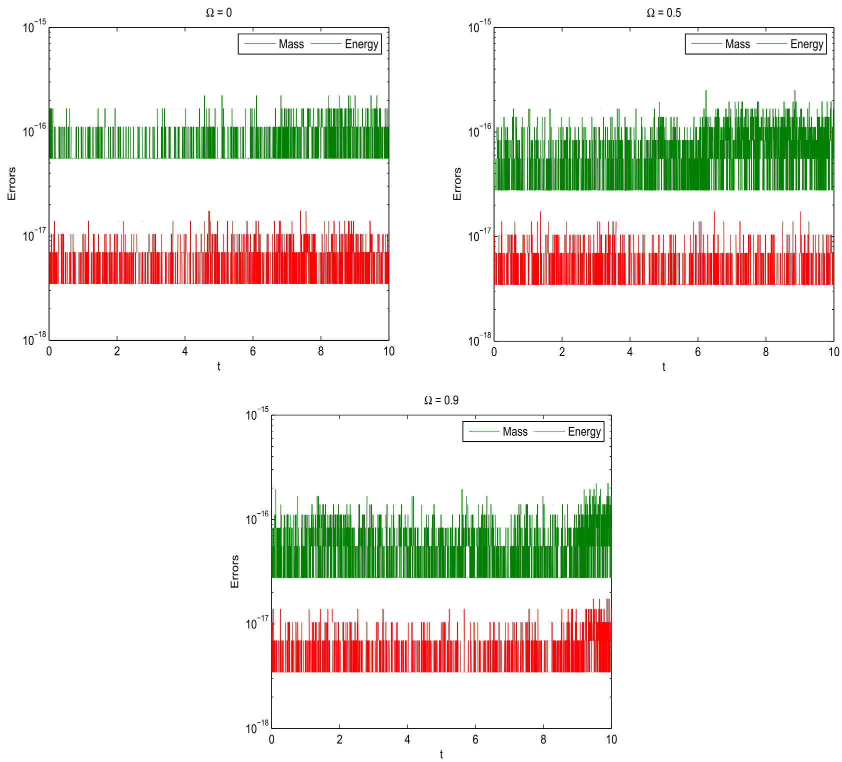

FIGURE 1. Evolutions of discrete mass and energy errors with different angular speeds Ω and $h = 4/128$, $\tau = 0.001$.

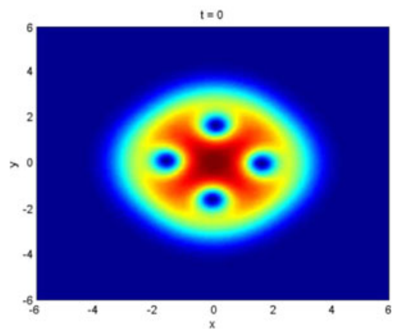

FIGURE 2. Vortex lattices of condensate ground state in a rotating BEC with $\beta = 100$.

vortices is conserved and the discrete mass and energy are also preserved to round-off errors in Figure 4. We also present the comparison of different iterative methods for solving the resulting linear system in Figure 4. For the simple Jacobi iteration, the errors exhibit an apparent linear growth although the error magnitudes are still rather

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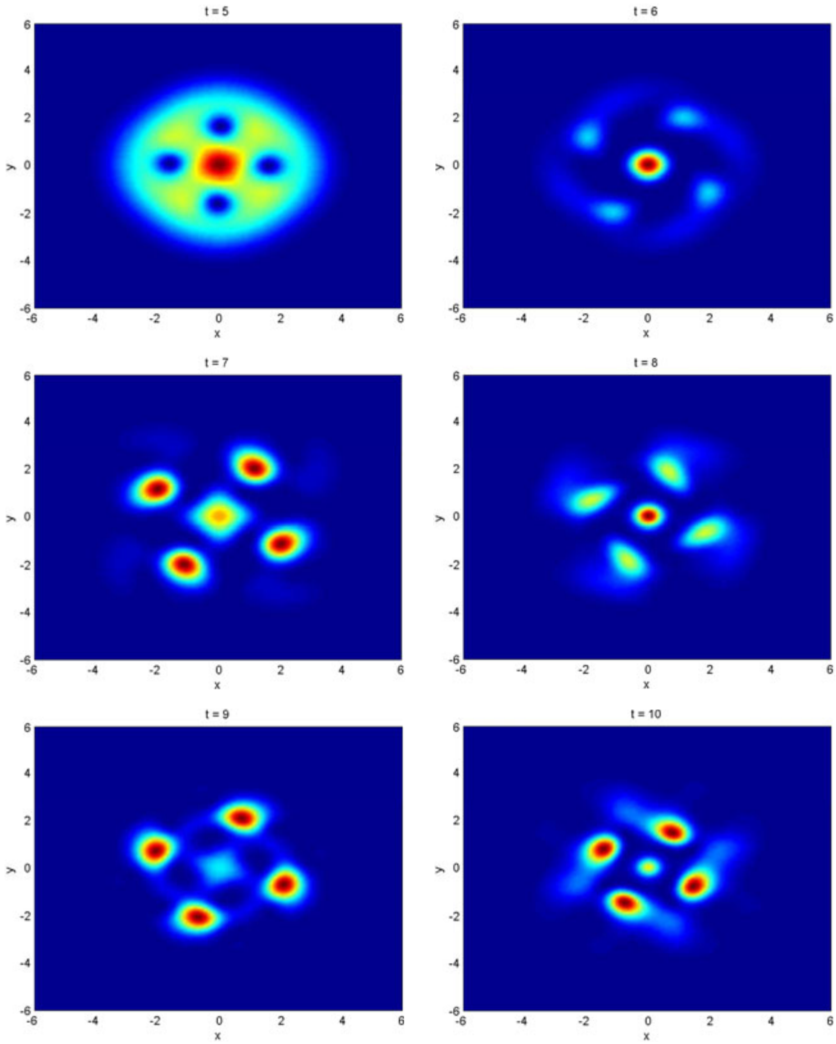

FIGURE 3. Contour plots of the density function $|\psi|^2$ for the dynamics of vortex lattices in a rotating BEC with $\beta = 100$ at different times.

small. For the BiCGSTAB iteration, the errors are just oscillating near the round-off error with no drift observed. Consequently, it relies heavily on the choice of iteration methods to demonstrate the exact conservation of physical quantities numerically. However, to the best of our knowledge, there is no clear result about the criterion to select an effective iteration method, which is worthy of being investigated.

Notice that the choice of the parameter β can directly impact the vortex lattice structures of the condensate ground state. Basically, the increase in β will cause more vortices and the lattice will thereby becomes more dense. As a consequence,

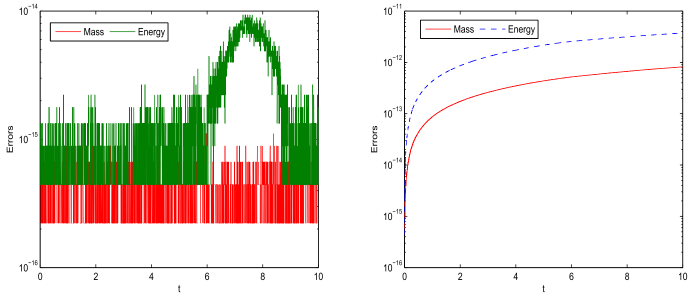

FIGURE 4. Evolution of discrete mass and energy errors by solving the linear system with BiCGSTAB iteration (left) and Jacobi iteration (right).

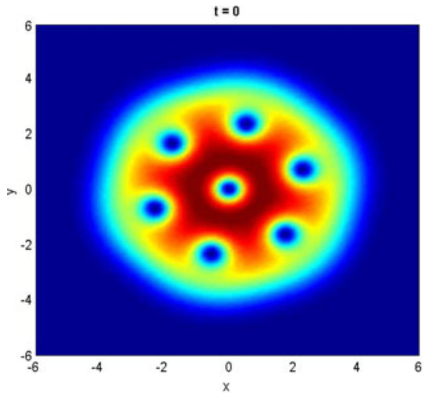

FIGURE 5. Vortex lattices of condensate ground state in a rotating BEC with $\beta = 200$.

high-order numerical methods are preferred for the sake of capturing the feather of each vortex. In the additional example, we set $\beta = 200$ and display the corresponding vortex lattice in Figure 5. Again our methods can resolve these lattice structures very well with the discrete mass and energy being conserved precisely, as Figures 6 and 7 demonstrate. Meanwhile, the influence on numerical errors of conserved quantities of different iteration methods is also revealed in Figure 7 for this example.

7. Conclusions

In this paper, we propose a new linear and conservative finite difference scheme which preserves the discrete mass and energy for the 2D GP equation with AMR. Our key strategy is using the circulant matrix operation and the equivalences of several discrete semi-norms for error analysis. With no constraints on the time-step size, we establish optimal H^1-error estimates for the proposed scheme. Unlike the existing finite difference methods, which are of second-order accuracy at the most, the convergence rate of the approximate solution proved here is of order $O(h^4 + \tau^2)$. Two

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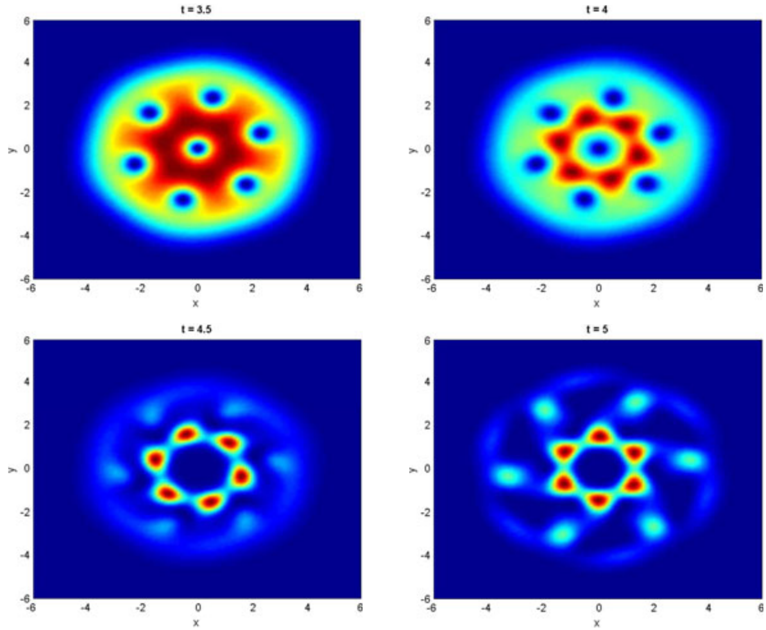

FIGURE 6. Contour plots of the density function $|\psi|^2$ for the dynamics of vortex lattices in a rotating BEC with $\beta = 200$ at different times.

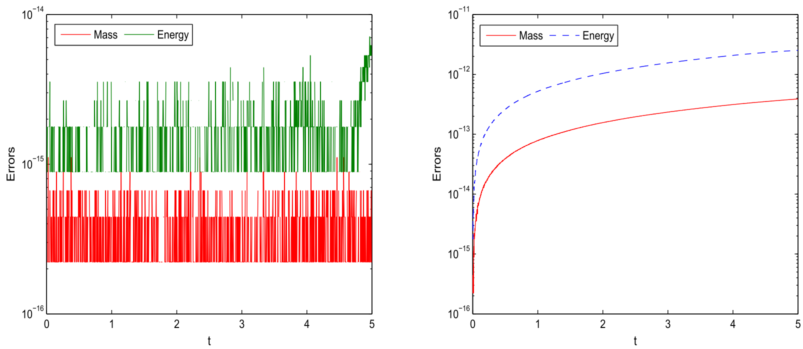

FIGURE 7. Evolution of discrete mass and energy errors by solving the linear system with BiCGSTAB iteration (left) and Jacobi iteration (right).

numerical examples are presented to illustrate the efficiency and accuracy of our new scheme.

Work on optimal error estimates for Fourier pseudo-spectral methods for the 3D GP equation with AMR is under way and future works may focus on the unconditional maximum norm convergence of high-order accurate numerical schemes for the general NLS/GP equations in higher dimensions.

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Appendix A.

LEMMA A.1. *For any grid function* $u \in V_h$,

$$\|B_2^x u\| \leqslant \tfrac{3}{2}\|u\|, \quad \|uB_2^y\| \leqslant \tfrac{3}{2}\|u\|, \quad \|B_1^x u\| \leqslant 3\|u\|, \quad \|uB_1^y\| \leqslant 3\|u\|.$$

PROOF. Using (3.2),

$$\|B_2^x u\|^2 = (B_2^x u, B_2^x u) = ((B_2^x)^2 u, u) = (\Lambda_{B_2^x}^2 F_J u, F_J u) \leqslant \tfrac{9}{4}(F_J u, F_J u) = \tfrac{9}{4}\|u\|^2,$$

that is, $\|B_2^x u\| \leqslant (3/2)\|u\|$. Similarly,

$$\|uB_2^y\| \leqslant \tfrac{3}{2}\|u\|, \quad \|B_1^x u\| \leqslant 3\|u\|, \quad \|uB_1^y\| \leqslant 3\|u\|.$$

This completes the proof. □

PROOF OF LEMMA 5.1. Considering the problem (1.1)–(1.3) at the point (x_j, y_k, t_n),

$$i\partial_t\psi(x_j, y_k, t_n) + (\tfrac{1}{2}\Delta - V_{jk} + \Omega L_z)\psi(x_j, y_k, t_n) - \beta(|\psi|^2\psi)(x_j, y_k, t_n) = 0 \qquad \text{(A.1)}$$

with $(x_j, y_k) \in \mathcal{T}_h$, $t_n \in \mathcal{T}_\tau$. Then, using the Taylor expansion with integral remainder and using (2.5) and (2.6),

$$\partial_t\psi(x_j, y_k, t_n) = \delta_t\phi_{jk}^n - (\eta^t)_{jk}^n, \qquad \text{(A.2)}$$

$$\Delta\psi(x_j, y_k, t_n) = \Delta_h\phi_{jk}^{\bar{n}} + [B_2^x(\eta_2^x)^{\bar{n}}]_{jk} + [(\eta_2^y)^{\bar{n}}B_2^y]_{jk} - (\widetilde{\eta}^{\Delta})_{jk}^n, \qquad \text{(A.3)}$$

$$\psi(x_j, y_k, t_n) = \phi_{jk}^{\bar{n}} - (\widetilde{\eta})_{jk}^n, \qquad \text{(A.4)}$$

$$L_z\psi(x_j, y_k, t_n) = L_z^h\phi_{jk}^{\bar{n}} - ix_j[(\eta_1^y)^{\bar{n}}B_1^y]_{jk} + iy_k[B_1^x(\eta_1^x)^{\bar{n}}]_{jk} + ix_j(\widetilde{\eta}^y)_{jk}^n - iy_k(\widetilde{\eta}^x)_{jk}^n, \qquad \text{(A.5)}$$

$$(|\psi|^2\psi)(x_j, y_k, t_n) = |\phi_{jk}^n|^2\phi_{jk}^{\bar{n}} - |\phi_{jk}^n|^2(\widetilde{\eta})_{jk}^n, \qquad \text{(A.6)}$$

$$(x_j, y_k) \in \mathcal{T}_h, \quad t_n \in \mathcal{T}_\tau, \qquad \text{(A.7)}$$

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where the local truncation errors are

$$(\eta^t)^n_{jk} = \frac{\tau^2}{4}\int_0^1\Big[\frac{\partial^3\psi}{\partial t^3}(x_j,y_k,t_n+\tau s)+\frac{\partial^3\psi}{\partial t^3}(x_j,y_k,t_n-\tau s)\Big](1-s)^2\,ds,$$

$$(\widetilde{\eta}^{\Delta})^n_{jk} = \frac{\tau^2}{2}\int_0^1\Big[\frac{\partial^2}{\partial t^2}\Delta\psi(x_j,y_k,t_n+\tau s)+\frac{\partial^2}{\partial t^2}\Delta\psi(x_j,y_k,t_n-\tau s)\Big](1-s)\,ds,$$

$$(\widetilde{\eta})^n_{jk} = \frac{\tau^2}{2}\int_0^1\Big[\frac{\partial^2\psi}{\partial t^2}(x_j,y_k,t_n+\tau s)+\frac{\partial^2\psi}{\partial t^2}(x_j,y_k,t_n-\tau s)\Big](1-s)\,ds,$$

$$(\widetilde{\eta}^{y})^n_{jk} = \frac{\tau^2}{2}\int_0^1\Big[\frac{\partial^3\psi}{\partial t^2\partial y}(x_j,y_k,t_n+\tau s)+\frac{\partial^3\psi}{\partial t^2\partial y}(x_j,y_k,t_n-\tau s)\Big](1-s)\,ds,$$

$$(\widetilde{\eta}^{x})^n_{jk} = \frac{\tau^2}{2}\int_0^1\Big[\frac{\partial^3\psi}{\partial t^2\partial x}(x_j,y_k,t_n+\tau s)+\frac{\partial^3\psi}{\partial t^2\partial x}(x_j,y_k,t_n-\tau s)\Big](1-s)\,ds$$

and $(\eta_2^x)^n_{jk}, (\eta_2^y)^n_{jk}, (\eta_1^x)^n_{jk}, (\eta_1^y)^n_{jk}$ are defined in (2.1)–(2.4). Substituting (A.2)–(A.6) into (A.1),

$$i\delta_t\phi^n_{jk} + (\tfrac{1}{2}\Delta_h - V_{jk} + \Omega L^h_z)\phi^{\bar{n}}_{jk} - \beta(|\phi^n_{jk}|^2)\phi^{\bar{n}}_{jk} = \eta^n_{jk}, \quad (x_j,y_k)\in\mathcal{T}_h, \quad t_n\in\mathcal{T}_\tau,$$

where

$$\begin{aligned}\eta^n_{jk} = {}& i(\eta^t)^n_{jk} - \tfrac{1}{2}[B^x_2(\eta^x_2)^{\bar{n}}]_{jk} - \tfrac{1}{2}[(\eta^y_2)^{\bar{n}}B^y_2]_{jk} + \tfrac{1}{2}(\widetilde{\eta}^{\Delta})^n_{jk} - V_{jk}(\widetilde{\eta})^n_{jk} + \Omega i x_j[(\eta^y_1)^{\bar{n}}B^y_1]_{jk}\\ & - \Omega i y_k[B^x_1(\eta^x_1)^{\bar{n}}]_{jk} - \Omega i x_j(\widetilde{\eta}^{y})^n_{jk} + \Omega i y_k(\widetilde{\eta}^{x})^n_{jk} - \beta|\phi^n_{jk}|^2(\widetilde{\eta})^n_{jk}.\end{aligned} \tag{A.8}$$

It follows from Assumption 2.2, Lemma A.1 and (A.8) that

$$\begin{aligned}\|\eta^n\| &\leqslant C(\|(\eta^t)^n\| + \|(\eta^x_2)^{\bar{n}}\| + \|(\eta^y_2)^{\bar{n}}\| + \|\widetilde{\eta}^{\Delta}\| + \|V\|_{L^\infty}\|(\widetilde{\eta})^n\|\\ &\quad + \|(\eta^y_1)^{\bar{n}}\| + \|(\eta^x_1)^{\bar{n}}\| + \|(\widetilde{\eta}^{y})^n\| + \|(\widetilde{\eta}^{x})^n\| + \|\psi\|_{L^\infty}\|(\widetilde{\eta})^n\|)\\ &\leqslant Ch^4\Big(\Big\|\frac{\partial^6\psi}{\partial x^6}\Big\|_{L^\infty} + \Big\|\frac{\partial^6\psi}{\partial y^6}\Big\|_{L^\infty} + \Big\|\frac{\partial^5\psi}{\partial x^5}\Big\|_{L^\infty} + \Big\|\frac{\partial^5\psi}{\partial y^5}\Big\|_{L^\infty}\Big)\\ &\quad + C\tau^2\Big(\Big\|\frac{\partial^3\psi}{\partial t^3}\Big\|_{L^\infty} + \Big\|\frac{\partial^4\psi}{\partial t^2\partial x^2}\Big\|_{L^\infty} + \Big\|\frac{\partial^4\psi}{\partial t^2\partial y^2}\Big\|_{L^\infty} + \|V\|_{L^\infty}\Big\|\frac{\partial^2\psi}{\partial t^2}\Big\|_{L^\infty}\\ &\quad + \Big\|\frac{\partial^3\psi}{\partial t^2\partial x}\Big\|_{L^\infty} + \Big\|\frac{\partial^3\psi}{\partial t^2\partial y}\Big\|_{L^\infty} + \|\psi\|_{L^\infty}\Big\|\frac{\partial^2\psi}{\partial t^2}\Big\|_{L^\infty}\Big)\\ &\leqslant C(h^4+\tau^2), \quad t_n\in\mathcal{T}_\tau.\end{aligned}$$

Similarly, from (5.2) and (5.3),

$$\|\eta^0\| \leqslant C(h^4+\tau^2), \quad \|\nabla_h\eta^0\| \leqslant C(h^4+\tau^2), \quad \|\eta^0\|_\infty \leqslant C,$$

which completes the proof. □

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