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Unconditional and optimal H^2-error estimates of two linear and conservative finite difference schemes for the Klein-Gordon-Schrödinger equation in high dimensions

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Abstract The focus of this paper is on the optimal error bounds of two finite difference schemes for solving the d-dimensional ($d = 2, 3$) nonlinear Klein-Gordon-Schrödinger (KGS) equations. The proposed finite difference schemes not only conserve the mass and energy in the discrete level but also are efficient in practical computation because only two linear systems need to be solved at each time step. Besides the standard energy method, an induction argument as well as a 'lifting' technique are introduced to establish rigorously the optimal H^2-error estimates without any restrictions on the grid ratios, while the previous works either are not rigorous enough or often require certain restriction on the grid ratios. The convergence rates of the proposed schemes are proved to be at $O(h^2 + \tau^2)$ with mesh-size h and time step τ in the discrete H^2-norm. The analysis method can be directly extended to other linear finite difference schemes for solving the KGS equations in high dimensions. Numerical results are reported to confirm the theoretical analysis for the proposed finite difference schemes.

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1 Introduction

This paper aims to analyze two finite difference time domain schemes for solving the dimensionless Klein-Gordon-Schrödinger (KGS) equations

$$i\partial_t\psi(\mathbf{x},t)+\frac{1}{2}\Delta\psi(\mathbf{x},t)+\phi(\mathbf{x},t)\psi(\mathbf{x},t)=0,\quad \mathbf{x}\subset\mathbb{R}^d,\quad t>0, \tag{1.1}$$

$$\partial_{tt}\phi(\mathbf{x},t)-\Delta\phi(\mathbf{x},t)+\mu^2\phi(\mathbf{x},t)=|\psi(\mathbf{x},t)|^2,\quad \mathbf{x}\subset\mathbb{R}^d,\quad t>0, \tag{1.2}$$

$$(\psi,\phi,\partial_t\phi)(\mathbf{x},0)=(\psi_0,\phi_0,\phi_1)(\mathbf{x}),\quad \mathbf{x}\in\mathbb{R}^d, \tag{1.3}$$

which is the classical model representing the dynamics of conserved complex nucleon fields ψ interacting with neutral real scalar meson fields ϕ. See [6, 9, 20] for its derivation and non-dimensionalization. Here, t is time, $\mathbf{x}=(x,y)$ in two dimensions (2D), i.e. $d=2$, and respectively $\mathbf{x}=(x,y,z)$ in three dimensions (3D), i.e. $d=3$, are the Cartesian coordinates, μ describes the ratio of mass between a meson and a nucleon, ψ_0 is a given complex-valued function and ϕ_0 and ϕ_1 are two given real-valued functions. It is clear to see that the KGS equations (1.1)–(1.3) conserve the total *mass*,

$$M(t):=\int_{\mathbb{R}^d}|\psi(\mathbf{x},t)|^2d\mathbf{x}\equiv M(0):=\int_{\mathbb{R}^d}|\psi_0(\mathbf{x})|^2d\mathbf{x},\quad t>0, \tag{1.4}$$

and the total *energy*

$$E(t):=\int_{\mathbb{R}^d}\left[|\nabla\psi|^2+\frac{1}{2}(|\partial_t\phi|^2+|\nabla\phi|^2+\mu^2|\phi|^2)-\phi|\psi|^2\right]d\mathbf{x} \tag{1.5}$$

$$\equiv E(0):=\int_{\mathbb{R}^d}\left[|\nabla\psi_0|^2+\frac{1}{2}(|\partial_t\phi_0|^2+|\nabla\phi_0|^2+\mu^2|\phi_0|^2)-\phi_0|\psi_0|^2\right]d\mathbf{x},\quad t>0.$$

In the literature, extensive mathematical studies have been carried out for the above KGS equations. Along the analytical front, the singular limit, solitary waves and dynamical properties have been investigated and we refer to [1, 4, 6–15, 21, 23] and the references therein. Along the numerical front, various numerical methods including the time-splitting pseudospectral method [5], the conservative spectral method [29], symplectic and multi-symplectic methods [17–19], conservative finite difference methods [25, 26, 30], and orthogonal spline collocation method [24] have been proposed in the literatures. Of course, each method has its advantages and disadvantages. For a comparison between different numerical methods for the KGS equations, we refer to [16].

Among the existing numerical methods for the KGS equations (1.1)–(1.3), most of the methods and error estimates are accomplished in only one space dimension (1D). For instance, a conservative spectral method [29] and a conservative orthogonal spline collocation method [24] were analysed in 1D where the convergences of the schemes were established in the discrete $L^2 \times H^1$-norm. Similarly, the proposed conservative finite difference time domain scheme in [30] was also showed in 1D to converge at second order rate in both space and time in the discrete $L^2 \times H^1$-norm. Later in [25], the authors managed to establish the error estimate in the discrete $H^1 \times H^1$-norm and they considered another conservative finite difference scheme. In [26], the author proposed a conservative compact finite difference scheme and combined a new technique and the standard energy method to obtain the optimal error estimate in the discrete $H^1 \times H^1$-norm.

However, for the KGS equations in high dimensions, few numerical methods have been considered and analysed in the literature. Here, we are particularly interested in the finite difference time domain schemes which are very popular for solving the Schrödinger-type equations [2, 3, 27, 28] due to the discrete conservation laws and the convenience of implementations. In [31], Zhang and Han proposed and analysed a nonlinear and fully implicit finite difference scheme for 3D dissipative KGS equation. However, the scheme is nonlinear and therefore needs multiple iterations in the practical computation. Thus, the first interest of this paper is to propose two finite difference schemes for the d-dimensional ($d = 2, 3$) KGS equations, which not only conserve the total mass and energy in the discrete level but also are linear and therefore do not require any iterations in the practical computation.

On the other hand, the interest of this paper is to establish the optimal error estimates of the proposed schemes in the discrete H^2-norm. It is known that, the proof of the conservative finite difference schemes for the 1D KGS equations relies strongly on the conservative properties of the schemes and the discrete version of the Sobolev inequality in 1D

$$||f||_{L^\infty} \le C_\Omega ||f||_{H^1}, \quad f \in H^1(\Omega) \text{ with } \Omega \subset \mathbb{R}, \tag{1.6}$$

where Ω is a bounded domain in $\mathbb{R}$ and the constant C_Ω depends only on the size of the Ω. However, the extension of the discrete version of the above Sobolev inequality is no longer valid in 2D or 3D. Thus the technique used in [24–27, 29, 30] for obtaining error bounds of the conservative schemes for the KGS equations only works for conservative difference schemes in one dimension and they can not be extended to high dimensions. In fact, for the 2D and 3D cases, we need the discrete version of the following Sobolev embedding inequality

$$||f||_{L^\infty} \le C_\Omega ||f||_{H^2}, \quad f \in H^2(\Omega) \text{ with } \Omega \subset \mathbb{R}^d, \quad d = 2, 3. \tag{1.7}$$

Thus, in order to obtain the *a priori* estimates of the numerical solutions in the discrete L^∞-norm, we have to establish the *a priori* estimates in the discrete H^2-norm. In [28], Wang and Zhao obtained the L^∞-error estimates of some finite difference schemes for the 2D and 3D nonlinear Schrödinger equations, but the error estimates there depend on the grid ratio, though the dependence is weak from the practical point of view. In [31], Zhang and Han proved the stability and optimal error bound of their finite difference scheme in the discrete $H^2 \times H^2$-norm over a finite time interval, and obtained the existence of a maximal attractor for a discrete dynamical system associate with the finite difference scheme. However, their analysis method can not be generalized to other finite difference schemes for solving the KGS equations in 2D or 3D (e.g. the estimate of $|I_4|$ in [31] can not be used in analyzing other schemes). Hence, for the schemes proposed in this work, we are aiming to prove rigorously, without imposing any restrictions on the grid ratios, the optimal error bounds in the discrete H^2-norm. Differing from the analysis method used in [31], we here introduce an induction argument as well as a 'lifting' technique (i.e., by taking the discrete L^2-norm of both sides of the 'error' equations, the estimate of the higher order difference quotient of the error functions can be obtained from the estimate of the lower order difference quotient of the error functions and local truncation error functions) in analysing the convergence and stability of the proposed schemes.

The rest of this paper is organized as follows. In Section 2, we present two linear and conservative finite difference schemes for the KGS equations and state our main error estimate results. In Section 3, we first build the optimal $H^1 \times H^1$-error estimate without any constraints on the grid ratios and obtain the *a priori* estimate of the numerical solution in the maximum norm, then establish the optimal $H^2 \times H^2$-error bounds of the proposed schemes, and then generalize the numerical methods as well as the corresponding theoretical results to nonhomogeneous KGS equations. In Section 4, several numerical results are reported to support our theoretical analysis. Finally, some conclusions are drawn in Section 5.

2 Finite difference scheme and main result

In this section, we shall introduce two finite difference schemes for the KGS equations in three dimensions and then state our main results.

2.1 Numerical methods

For simplicity, here we only present the schemes in three dimensions, i.e. $d = 3$ and $\Omega = (x_L, x_R) \times (y_L, y_R) \times (z_L, z_R)$ in (1.1)–(1.3). Reductions to 2D are straightforward, and the error estimate results remain valid with little modification. That is, we consider the initial-boundary value problem of the 3D KGS equation as follows

$$i\partial_t \psi + \frac{1}{2}\Delta\psi + \phi\psi = 0, \quad (x, y, z) \in \Omega, \quad t > 0, \tag{2.1}$$

$$\partial_{tt}\phi - \Delta\phi + \mu^2\phi = |\psi|^2, \quad (x, y, z) \in \Omega, \quad t > 0, \tag{2.2}$$

$$\psi(x, y, z, t) = 0, \quad \phi(x, y, z, t) = 0, \quad (x, y, z) \in \partial\Omega, \quad t > 0, \tag{2.3}$$

$$(\psi, \phi, \partial_t\phi)(x, y, z, 0) = (\psi_0, \phi_0, \phi_1)(x, y, z), \quad (x, y, z) \in \overline{\Omega}. \tag{2.4}$$

For a positive integer N, choose time step $\tau = T/N$ and denote time steps $t_n = n\tau$ for $n = 0, 1, 2, \cdots, N$, where $0 < T < T_{\max}$ with $T_{\max}$ the maximal existing time of the solution; choose mesh sizes $h_1 = (x_R - x_L)/J$, $h_2 = (y_R - y_L)/K$ and $h_3 = (z_R - z_L)/L$ with three positive integers J, K and L, and denote $h = \max\{h_1, h_2, h_3\}$ and mesh grids as $(x_j, y_k, z_l) = (x_L + jh_1, y_L + kh_2, z_L + lh_3)$ for $j = 0, 1, \cdots, J$, $k = 0, 1, \cdots, K$ and $l = 0, 1, \cdots, L$. Denote the index sets as

$$\mathcal{T}_h^0 = \{(j, k, l)|\ j = 0, 1, 2, \cdots, J,\ k = 0, 1, 2, \cdots, K,\ l = 0, 1, 2, \cdots, L\},$$
$$\mathcal{T}_h = \{(j, k, l)|\ j = 1, 2, \cdots, J-1,\ k = 1, 2, \cdots, K-1,\ l = 1, 2, \cdots, L-1\},$$

and denote three grid sets as

$$\overline{\Omega}_h := \{(x_j, y_k, z_l) | \, (j,k,l) \in \mathcal{T}_h^0\}, \quad \Omega_h := \overline{\Omega}_h \cap \Omega, \quad \partial\Omega_h := \overline{\Omega}_h \cap \partial\Omega.$$

Let $(\psi_{jkl}^n, \phi_{jkl}^n)$ be the numerical approximation to $\big(\psi(x_j, y_k, z_l, t_n), \phi(x_j, y_k, z_l, t_n)\big)$ for $(j,k,l) \in \mathcal{T}_h^0, n = 0, 1, \cdots, N$, and denote $(\psi^n, \phi^n) \in \mathbb{C}^{(J+1)\times(K+1)\times(L+1)} \times \mathbb{R}^{(J+1)\times(K+1)\times(L+1)}$ be the numerical vector solution at time level $t = t_n$. For a grid function $u^n = (u_{jkl}^n)_{(j,k,l)\in\mathcal{T}_h^0} \in \mathbb{C}^{(J+1)\times(K+1)\times(L+1)}$ with $n = 0, 1, 2, \cdots, N$, we introduce the following finite difference quotient operators:

$$\delta_x^+ u_{jkl}^n = \frac{1}{h_1}\left(u_{j+1kl}^n - u_{jkl}^n\right), \; j = 0, 1, 2, \cdots, J-1,$$
$$\delta_x^2 u_{jkl}^n = \frac{1}{h_1^2}\left(u_{j-1kl}^n - 2u_{jkl}^n + u_{j+1kl}^n\right), \; j = 1, 2, \cdots, J-1,$$
$$\delta_t^+ u_{jkl}^n = \frac{1}{\tau}\left(u_{jkl}^{n+1} - u_{jk}^n\right), \; n = 0, 1, 2, \cdots, N-1,$$
$$\delta_t u_{jkl}^n = \frac{1}{2\tau}\left(u_{jkl}^{n+1} - u_{jkl}^{n-1}\right), \; n = 1, 2, \cdots, N-1,$$
$$\delta_t^2 u_{jkl}^n = \frac{1}{\tau^2}\left(u_{jkl}^{n+1} - 2u_{jkl}^n + u_{jkl}^{n-1}\right), \; n = 1, 2, \cdots, N-1.$$

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

$$\nabla_h u_{jkl}^n = \left(\delta_x^+ u_{jkl}^n, \; \delta_y^+ u_{jkl}^n, \; \delta_z^+ u_{jkl}^n\right)^\top, \quad \Delta_h u_{jkl}^n = \delta_x^2 u_{jkl}^n + \delta_y^2 u_{jkl}^n + \delta_z^2 u_{jkl}^n.$$

We define the space of grid functions

$$X_h := \{u = (u_{jkl})_{(j,k,l)\in\mathcal{T}_h^0} | u_{jkl} = 0 \text{ when } (j,k,l) \notin \mathcal{T}_h\} \subseteq \mathbb{C}^{(J+1)\times(K+1)\times(L+1)},$$

with discrete inner products and norms over X_h as

$$\langle u, v\rangle := h_1h_2h_3 \sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\sum_{l=1}^{L-1} u_{jkl}\overline{v}_{jkl}, \quad \langle u, v\rangle_0 := h_1h_2h_3 \sum_{j=0}^{J-1}\sum_{k=0}^{K-1}\sum_{l=0}^{L-1} u_{jkl}\overline{v}_{jkl},$$

$$||u|| := \langle u, u\rangle^{\frac{1}{2}}, \quad ||u||_\infty := \max_{(j,k,l)\in\mathcal{T}_h} |u_{jkl}|, \quad ||u||_p := \sqrt[p]{h_1h_2h_3 \sum_{j=1}^{J-1}\sum_{k=1}^{K-1}\sum_{l=1}^{L-1} |u_{jkl}|^p},$$

$$|u|_1 := \langle \nabla_h u, \nabla_h u\rangle_0^{\frac{1}{2}} := (\langle \delta_x^+ u, \delta_x^+ u\rangle_0 + \langle \delta_y^+ u, \delta_y^+ u\rangle_0 + \langle \delta_z^+ u, \delta_z^+ u\rangle_0)^{\frac{1}{2}},$$
$$|u|_2 := \langle \Delta_h u, \Delta_h u\rangle^{\frac{1}{2}}, \quad |||u|||_1 := (||u||^2 + |u|_1^2)^{\frac{1}{2}}, \quad |||u|||_2 := (|||u|||_1^2 + |u|_2^2)^{\frac{1}{2}},$$

where $\o v$ represents the conjugate of the grid function $v \in X_h$, $p \in [2, \infty)$, $|u|_k$ and $|||u|||_k$ $(k = 1, 2)$ are respectively Sobolev's semi-norms and norms for the discrete function $u \in X_h$. Let $H^k(\Omega_h)$ denotes the space of complex-vaued or real-valued discrete functions with the Sobolev's norm $||| \cdot |||_k$, $(k = 1, 2)$. Let $H_0^1(\Omega_h)$ be the subspace of the space $H^1(\Omega_h)$ satisfying the homogeneous Dirichlet boundary condition.

Throughout the paper, we denote C as a generic positive constant which may have different values at different circumstances but are independent of the discrete parameters, i.e. the time step τ and mesh size h, and we adopt the notation $w \lesssim v$ to denote $|w| \le Cv$.

We shall consider two finite difference schemes for computing the problem (2.1)–(2.4). The first one is an extension of the scheme given in [30] to the high dimensional case, i.e.,

$$i\delta_t^+\psi_{jkl}^n + \frac{1}{4}\Delta_h(\psi_{jkl}^n + \psi_{jkl}^{n+1}) + \frac{1}{4}(\phi_{jkl}^n + \phi_{jkl}^{n+1})(\psi_{jkl}^n + \psi_{jkl}^{n+1}) = 0, \tag{2.5}$$
$$(j,k,l) \in \mathcal{T}_h, \quad n = 0, 1, \cdots, N-1,$$
$$\delta_t^2\phi_{jkl}^n - \frac{1}{2}\Delta_h(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) + \frac{\mu^2}{2}(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) = |\psi_{jkl}^n|^2, \tag{2.6}$$
$$(j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,$$
$$\psi_{jkl}^0 = \psi_0(x_j, y_k, z_l), \quad \phi_{jkl}^0 = \phi_0(x_j, y_k, z_l), \tag{2.7}$$
$$\delta_t^+\phi_{jkl}^0 = \phi_1(x_j, y_k, z_l) + \frac{\tau}{2}\phi_2(x_j, y_k, z_l), \quad (j,k,l) \in \mathcal{T}_h^0,$$
$$\psi^n \in X_h, \quad \phi^n \in X_h, \quad n = 1, 2, \cdots, N, \tag{2.8}$$

where $\phi_2(x_j, y_k, z_l) = \Delta_h^c\phi_0(x_j, y_k, z_l) - \mu^2\phi_0(x_j, y_k, z_l) + |\psi_0(x, y, z)|^2$ with $\Delta_h^c = (1 + \frac{h_1^2}{12}\delta_x^2)^{-1}\delta_x^2 + (1 + \frac{h_2^2}{12}\delta_y^2)^{-1}\delta_y^2 + (1 + \frac{h_3^2}{12}\delta_z^2)^{-1}\delta_z^2$ a 3D compact discrete Laplace operator. As will be proved in Section 3, the above finite difference scheme conserves the total mass and energy of the system in the discrete sense. The order of the execution of the scheme (2.5)–(2.8) is aligned as follows: ψ^0, ϕ^0 are directly given in (2.7), and ϕ^1 is obtained by computing the third equality of (2.7), then ψ^1 is obtained by computing (2.5), and then ϕ^2 is gotten by computing (2.6),$\cdots$. If ψ^n, ϕ^n for $n = 2, 3, \cdots, N-1$ are obtained, then ϕ^{n+1} is obtained by computing (2.6), and then ψ^{n+1} is obtained by computing (2.5), until $n+1 = N$. In the following, we refer to the scheme (2.5)–(2.8) as the coupled implicit finite difference (CIFD) method. Though the CIFD scheme is linear in the computation, it is still coupled at each time level. Therefore, the two linear systems cannot be solved simultaneously by parallel computing. This motivates us also to consider the following linear, decoupled and implicit finite difference (DIFD) scheme which is an extension of the second scheme studied in [25] to high dimensions,

$$i\delta_t\psi_{jkl}^n + \frac{1}{4}\Delta_h(\psi_{jkl}^{n-1} + \psi_{jkl}^{n+1}) + \frac{1}{2}\phi_{jkl}^n(\psi_{jkl}^{n-1} + \psi_{jkl}^{n+1}) = 0, \tag{2.9}$$
$$(j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,$$
$$\delta_t^2\phi_{jkl}^n - \frac{1}{2}\Delta_h(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) + \frac{\mu^2}{2}(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) = |\psi_{jkl}^n|^2, \tag{2.10}$$
$$(j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,$$
$$\psi_{jkl}^0 = \psi_0(x_j, y_k, z_l), \ \phi_{jkl}^0 = \phi_0(x_j, y_k, z_l), \tag{2.11}$$
$$\delta_t^+\phi_{jkl}^0 = \phi_1(x_j, y_k, z_l) + \frac{\tau}{2}\phi_2(x_j, y_k, z_l), \quad (j,k,l) \in \mathcal{T}_h^0,$$
$$\psi^n \in X_h, \quad \phi^n \in X_h, \quad n = 1, 2, \cdots, N. \tag{2.12}$$

As will be proved in Section 3, the above finite difference scheme also conserves the total mass and energy of the system in the discrete level. Obviously, (2.9) is a three-level scheme which can not start by itself. Thus, the first step has to be computed by a two-level scheme such as the scheme (2.5). In practical computation, ψ^0, ϕ^0 are directly given in (2.7), and ψ^1, ϕ^1 are obtained by computing the third equality of (2.7) and the scheme (2.5), respectively, then ψ^2 and ϕ^2 are obtained by computing (2.9) and (2.10) simultaneously and independently, $\cdots$. If ψ^n, ϕ^n for $n = 2, 3, \cdots, N-1$ are obtained, ψ^{n+1} and ϕ^{n+1} are obtained by computing (2.9) and (2.10) simultaneously and independently, until $n + 1 = N$.

2.2 Main error estimate results

To state our main results, we make the following assumptions on the exact solution ψ and ϕ of the problem (2.5)–(2.8) in order to achieve the optimal error estimate results:

$$\begin{aligned} &\psi \in C^4(0,T;W^{0,\infty}(\Omega))\cap C^3(0,T;W^{2,\infty}(\Omega))\cap C^1(0,T;W^{4,\infty}(\Omega)\cap H_0^1(\Omega)),\\ &\phi \in C^5(0,T;W^{0,\infty}(\Omega))\cap C^3(0,T;W^{2,\infty}(\Omega))\cap C^1(0,T;W^{4,\infty}(\Omega)\cap H_0^1(\Omega)). \end{aligned} \tag{A}$$

Denote

$$u_{jkl}^n = \psi(x_j, y_k, z_l, t_n), \quad v_{jkl}^n = \phi(x_j, y_k, z_l, t_n), \quad (j,k,l) \in \mathcal{T}_h^0, \quad n = 0, 1, \cdots, N,$$

and define the error functions $e^n, \theta^n \in X_h$ as

$$e_{jkl}^n = u_{jkl}^n - \psi_{jkl}^n, \quad \theta_{jkl}^n = v_{jkl}^n - \phi_{jkl}^n, \quad (j,k,l) \in \mathcal{T}_h^0, \quad n = 0, 1, \cdots, N. \tag{2.13}$$

Then for the finite difference schemes proposed in this section, we have the following error estimates and stability result.

Theorem 2.1 *Under assumption (A), there exist two constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, we have the following optimal error estimates for the proposed CIFD scheme (2.5)–(2.8) as:*

$$|||e^n|||_2 + |||\theta^n|||_2 \lesssim h^2 + \tau^2, \quad ||e^n||_\infty + ||\theta^n||_\infty \lesssim h^2 + \tau^2, \quad n = 0, 1, \cdots, N. \tag{2.14}$$

Theorem 2.2 *Under assumption (A), there exist two constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, we have the following optimal error estimates for the proposed DIFD scheme (2.9)–(2.12) as:*

$$|||e^n|||_2 + |||\theta^n|||_2 \lesssim h^2 + \tau^2, \quad ||e^n||_\infty + ||\theta^n||_\infty \lesssim h^2 + \tau^2, \quad n = 0, 1, \cdots, N. \tag{2.15}$$

Theorem 2.3 *Under assumption (A), there exist two constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, the proposed finite difference schemes (2.5)–(2.8) and (2.9)–(2.12) are stable (finite time boundedness) on $H^2(\Omega_h) \times H^2(\Omega_h)$ over a finite time interval $[0, T]$ with respect to the initial conditions.*

3 Discrete conservation laws

Corresponding to the conservation laws (1.4) and (1.5) preserved by the continuous problem (2.1)–(2.4), the scheme CIFD (2.5)–(2.8) conserves the total mass and energy in the discrete level.

Lemma 3.1 *The scheme CIFD (2.5)–(2.8) satisfies the following discrete conservation laws*

$$
\begin{aligned}
M^n &:= ||\psi^n||^2 \equiv M^0, \quad n = 0, 1, \cdots, N, && (3.1)\\
E^n &:= |\psi^{n+1}|_1^2 + \frac{1}{2}||\delta_t^+\phi^n||^2 + \frac{1}{4}\left(|\phi^n|_1^2 + |\phi^{n+1}|_1^2\right) && (3.2)\\
&\quad + \frac{\mu^2}{4}\left(||\phi^n||^2 + ||\phi^{n+1}||^2\right) - \frac{1}{2}\langle\phi^n + \phi^{n+1}, |\psi^{n+1}|^2\rangle\\
&\equiv E^0, \quad n = 0, 1, \cdots, N-1.
\end{aligned}
$$

Here M^n and E^n are the called total mass and energy in the discrete level.

Proof Multiplying both sides of (2.5) by $\tau h_1 h_2 h_3(\o\psi^n_{jkl} + \o\psi^{n+1}_{jkl})$ and summing up for $(j, k, l) \in \mathcal{T}_h$, then taking the imaginary part, we obtain

$$
||\psi^{n+1}||^2 - ||\psi^n||^2 = 0, \quad n = 0, 1, \cdots, N. \tag{3.3}
$$

This immediately gives (3.1).

Multiplying both sides of (2.5) by $2h_1h_2h_3(\o\psi^{n+1}_{jk} - \o\psi^n_{jk})$ and summing up for $(j, k, l) \in \mathcal{T}_h$, then taking the real part, we obtain

$$
\begin{aligned}
&|\psi^{n+1}|_1^2 - \frac{1}{2}\langle\phi^n + \phi^{n+1}, |\psi^{n+1}|^2\rangle && (3.4)\\
&= |\psi^n|_1^2 - \frac{1}{2}\langle\phi^{n-1} + \phi^n, |\psi^n|^2\rangle - \frac{1}{2}\langle\phi^{n+1} - \phi^{n-1}, |\psi^n|^2\rangle.
\end{aligned}
$$

Multiplying both sides of (2.6) by $\frac{1}{2}\tau h_1h_2h_3(\delta_t^+\o\phi^n_{jk} - \delta_t^+\o\phi^{n-1}_{jk})$ and summing up for $(j, k, l) \in \mathcal{T}_h$ give

$$
\begin{aligned}
&\frac{1}{2}||\delta_t^+\phi^n||_1^2 + \frac{1}{4}\left(|\phi^n|_1^2 + |\phi^{n+1}|_1^2\right) + \frac{\mu^2}{4}\left(||\phi^n||^2 + ||\phi^{n+1}||^2\right) && (3.5)\\
&= ||\delta_t^+\phi^{n-1}||_1^2 + \frac{1}{4}\left(|\phi^{n-1}|_1^2 + |\phi^n|_1^2\right) + \frac{\mu^2}{4}\left(||\phi^{n-1}||^2 + ||\phi^n||^2\right)\\
&\quad + \frac{1}{2}\langle\phi^{n+1} - \phi^{n-1}, |\psi^n|^2\rangle.
\end{aligned}
$$

Adding (3.5) to (3.4) immediately gives (3.2). □

Similarly, one can prove that the scheme (2.9)–(2.12) is also a conservative type scheme which preserves the total mass and energy in the discrete level, i.e.

Lemma 3.2 *The finite difference scheme DIFD (2.9)–(2.12) where ψ^1 is computed by the finite difference scheme (2.9)–(2.12) satisfies the following discrete conservation laws*

$$M^n := ||\psi^n||^2 \equiv M^0, \quad n = 0, 1 \cdots, N, \tag{3.6}$$

$$\begin{aligned} E^n &:= \frac{1}{2}\left(|\psi^n|_1^2 + |\psi^{n+1}|_1^2\right) + \frac{1}{2}||\delta_t^+\phi^n||^2 + \frac{1}{4}\left(|\phi^n|_1^2 + |\phi^{n+1}|_1^2\right) \\ &\quad + \frac{\mu^2}{4}\left(||\phi^n||^2 + ||\phi^{n+1}||^2\right) - \frac{1}{2}\left(\langle\phi^n, |\psi^{n+1}|^2\rangle + \langle\phi^{n+1}, |\psi^n|^2\rangle\right) \\ &\equiv E^0, \quad n = 0, 1, \cdots, N-1. \end{aligned} \tag{3.7}$$

4 Error estimates

In this section, we rigorously prove the error estimate results stated in Theorems 2.1, 2.2 and 2.3. Here, we mainly discuss the error estimate of the CIFD (2.5)–(2.8), and the error estimate of the DIFD (2.9)–(2.12) can be done in the similar way. To do so, besides the standard energy method, we firstly introduce an induction argument as well as a 'lifting' technique to obtain the error estimate in H^1 norm and the *a priori* estimate of the numerical solution in maximum norm, then establish the optimal H^2 error estimates without imposing any restrictions on the grid ratios.

In our analysis, we need the following interpolation formula and discrete Sobolev inequality.

Lemma 4.1 *For any function $u \in H_0^1(\Omega_h)$, we have*

$$||u||_p \le C|u|_1^\alpha \cdot ||u||^{1-\alpha}, \quad \alpha = \frac{d}{2} - \frac{d}{p}, \tag{4.1}$$

$$p \in \begin{cases} [2, 6] & \textit{for } d = 3, \\ [2, \infty) & \textit{for } d = 1, 2. \end{cases}$$

In general, for any function $u \in H^1(\Omega_h)$, we have

$$||u||_p \le C(|u|_1 + ||u||)^\alpha \cdot ||u||^{1-\alpha}, \quad \alpha = \tfrac{d}{2} - \tfrac{d}{p}, \tag{4.2}$$

$$p \in \begin{cases} [2, 6] & \textit{for } d = 3, \\ [2, \infty) & \textit{for } d = 1, 2. \end{cases}$$

Proof For the proof of (4.1), we refer to [33] for the case $d = 1$, [27, 32] for $d = 2$, and [31] for $d = 3$. □

Lemma 4.2 *For any grid function $w \in H^2(\Omega_h) \cap H_0^1(\Omega_h)$, we have*

$$||w||_\infty \lesssim |w|_2, \quad d = 2, 3. \tag{4.3}$$

Proof Though there is a little difference between our definition of $|\cdot|_2$ and that in [31, 34], one can prove that they are equivalent. Therefore, by using the similar proof used in [31, 34], one can prove that (4.3) still holds. □

4.1 Proof of error estimates

We define the local truncation error $\eta^n \in X_h$ and $\xi^n \in X_h$ of the conservative scheme (2.5)–(2.8) for $n = 0, 1, 2, \ldots, N-1$ as

$$\eta^n_{jkl} := i\delta_t^+ u^n_{jkl} + \frac{1}{2}\Delta_h(u^n_{jkl} + u^{n+1}_{jkl}) + \frac{1}{4}(v^n_{jkl} + v^{n+1}_{jkl})(u^n_{jkl} + u^{n+1}_{jkl}), \quad (j,k,l) \in \mathcal{T}_h, \quad n = 0, 1, \cdots, N-1, \tag{4.4}$$

$$\xi^n_{jkl} := \delta_t^2 v^n_{jkl} - \frac{1}{2}\Delta_h(v^{n-1}_{jkl} + v^{n+1}_{jkl}) + \frac{\mu^2}{2}(v^{n-1}_{jkl} + v^{n+1}_{jkl}) - |u^n_{jkl}|^2, \quad (j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1, \tag{4.5}$$

$$\xi^0_{jkl} := \delta_t^+ v^0_{jkl} - \phi_1(x_j, y_k, z_l), \; u^0_{jkl} = \psi_0(x_j, y_k, z_l), \; v^0_{jkl} = \phi_0(x_j, y_k, z_l), \quad (j,k,l) \in \mathcal{T}_h^0, \tag{4.6}$$

$$u^n \in X_h, \quad v^n \in X_h, \quad n = 1, 2, \cdots, N. \tag{4.7}$$

Then, under the assumption (A), we obtain by using Taylor's expansion that

Lemma 4.3 (Local truncation errors) *Under assumption* (*A*)*, we have*

$$|\eta^n_{jkl}| \lesssim \tau^2 + h^2, \quad |\xi^0_{jkl}| \lesssim \tau^2 + h^4, \quad (j,k,l) \in \mathcal{T}_h, \quad 0 \le n < N, \tag{4.8}$$

$$|\Delta_h \xi^0_{jkl}| \lesssim \tau^2 + h^4, \quad |\xi^n_{jkl}| \lesssim \tau^2 + h^2, \quad (j,k,l) \in \mathcal{T}_h, \quad 0 < n < N, \tag{4.9}$$

$$|\delta_t^+ \eta^n_{jkl}| \lesssim \tau^2 + h^2, \quad |\delta_t^+ \xi^n_{jkl}| \lesssim \tau^2 + h^2, \quad (j,k,l) \in \mathcal{T}_h, \quad 0 \le n < N-1. \tag{4.10}$$

For the finite difference scheme (2.5)–(2.8), we have the following theorem,

Theorem 4.1 *Under assumption (A), there exist two constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, we have the following error estimates for the proposed finite difference scheme CIFD* (2.5)–(2.8) *as:*

$$|||e^n|||_1 + |||\theta^n|||_1 + ||\delta_t^+ \theta^{n-1}|| \lesssim h^2 + \tau^2, \quad n = 1, 2, \cdots, N, \tag{4.11}$$

$$|e^n|_2 + |\theta^n|_2 \lesssim 1, \quad ||e^n||_\infty + ||\theta^n||_\infty \lesssim 1, \quad n = 1, 2, \cdots, N. \tag{4.12}$$

Proof Subtracting (2.5)–(2.8) from (4.4)–(4.7) gives the 'error' equations as follows

$$i\delta_t^+ e^n_{jkl} + \frac{1}{2}\Delta_h(e^n_{jkl} + e^{n+1}_{jkl}) + p^{n+1}_{jkl} = \eta^n_{jkl}, \quad (j,k,l) \in \mathcal{T}_h, \quad 0 \le n < N, \tag{4.13}$$

$$\delta_t^2 \theta^n_{jkl} - \frac{1}{2}\Delta_h(\theta^{n-1}_{jkl} + \theta^{n+1}_{jkl}) + \frac{\mu^2}{2}(\theta^{n-1}_{jkl} + \theta^{n+1}_{jkl}) - q^n_{jkl} = \xi^n_{jkl}, \quad (j,k,l) \in \mathcal{T}_h, \quad 0 < n < N, \tag{4.14}$$

$$\theta^1_{jkl} = \tau \xi^0_{jkl}, \quad e^0_{jkl} = 0, \quad \theta^0_{jkl} = 0, \quad (j,k,l) \in \mathcal{T}_h^0, \tag{4.15}$$

$$e^n \in X_h, \quad \theta^n \in X_h, \quad 0 < n \le N. \tag{4.16}$$

where

$$p_{jkl}^{n+1} := \frac{1}{4}(v_{jkl}^n + v_{jkl}^{n+1})(u_{jkl}^n + u_{jkl}^{n+1}) - \frac{1}{4}(\phi_{jkl}^n + \phi_{jkl}^{n+1})(\psi_{jkl}^n + \psi_{jkl}^{n+1}) \tag{4.17}$$

$$= \frac{1}{4}(\theta_{jkl}^n + \theta_{jkl}^{n+1})(u_{jkl}^n + u_{jkl}^{n+1}) + \frac{1}{4}(\phi_{jkl}^n + \phi_{jkl}^{n+1})(e_{jkl}^n + e_{jkl}^{n+1}),$$

$$q_{jkl}^n := |u_{jkl}^n|^2 - |\psi_{jkl}^n|^2 = u_{jkl}^n \o e_{jkl}^n - e_{jkl}^n \o \psi_{jkl}^n. \tag{4.18}$$

Next, we use an induction argument as well as a 'lifting' technique to prove the error estimate (4.11) in two steps.

Step 1. Error estimates at the first time step

It follows from (4.15) and Lemma 4.3 that

$$||\theta^1||_\infty = ||\tau\xi^0||_\infty \lesssim \tau(\tau^2 + h^4), \quad |\theta^1|_2 = |\tau\xi^0|_2 \lesssim \tau(\tau^2 + h^4), \tag{4.19}$$

$$||\delta_t^+\theta^0|| = ||\xi^0|| \lesssim \tau^2 + h^4, \quad ||\phi^1||_\infty \le ||v^1||_\infty + ||\theta^1||_\infty \lesssim 1, \tag{4.20}$$

This gives

$$||p^1|| \lesssim ||\theta^1|| + ||e^1||. \tag{4.21}$$

Multiplying both sides of (4.13) with $n = 0$ by $h_1 h_2 h_3 \o e_{jkl}^1$ and summing up for $(j, k, l) \in \mathcal{T}_h$, then taking the imaginary part, we obtain

$$||e^1||^2 + \tau \mathrm{Im}\langle p^1, e^1\rangle = \tau \mathrm{Im}\langle \eta^0, e^1\rangle. \tag{4.22}$$

By using Cauchy-Schwartz inequality, (4.19), (4.21) and Lemma 4.3, we obtain from (4.22) that

$$||e^1||^2 \lesssim \tau(||\theta^1||^2 + ||e^1||^2 + ||\eta^0|^2) \lesssim \tau[\tau^2(\tau^2 + h^2)^2 + ||e^1||^2 + (\tau^2 + h^2)^2], \tag{4.23}$$

Then, for a sufficiently small τ, it follows from (4.23) that

$$||e^1|| \lesssim \tau^2 + h^2, \tag{4.24}$$

On the one hand, by using a 'lifting' technique (i.e., by taking the L^2 norm of both sides of the 'error' equation, then the estimate of the higher order difference quotient of the error function can be obtained from the estimate of the lower order difference quotients of the error functions and local truncation error functions), we obtain from (4.13) that

$$|e^1|_2 = 2||i\delta_t^+ e^0 + p^1 - \eta^0|| \lesssim \frac{1}{\tau}||e^1|| + ||p^1|| + ||\eta^0|| \lesssim \tau^{-1}(h^2 + \tau^2), \tag{4.25}$$

this implies that, if h is small enough such that $\tau^{-1}h^2 \lesssim 1$, there is

$$|e^1|_2 \lesssim 1. \tag{4.26}$$

On the other hand, by using the inverse Sobolev inequality, we obtain that

$$|e^1|_2 \lesssim h^{-2}||e^1|| \lesssim h^{-2}(h^2 + \tau^2), \tag{4.27}$$

this implies that, if τ is small enough such that $h^{-1}\tau \lesssim 1$, there still is

$$|e^1|_2 \lesssim 1. \tag{4.28}$$

Hence, for sufficiently small h and τ, it is always true to have

$$|e^1|_2 \lesssim 1, \tag{4.29}$$

and this together with (4.19) and Lemma 4.2 gives

$$||e^1||_\infty + ||\theta^1||_\infty \lesssim |e^1|_2 + |\theta^1|_2 \lesssim 1. \tag{4.30}$$

Then from (4.17) we get

$$|p^1|_1 \lesssim ||\theta^1|| + ||e^1|| + |\theta^1|_1 + |e^1|_1. \tag{4.31}$$

Multiplying both sides of (4.13) with $n = 0$ by $2h_1h_2h_3 \o e^1_{jkl}$ and summing up for $(j,k,l) \in \mathcal{T}_h$, then taking the real part, we obtain

$$|e^1|_1^2 = 2\tau \mathrm{Re}\langle p^1, \delta_t^+ e^0\rangle - 2\mathrm{Re}\langle \eta^0, e^1\rangle, \quad n = 0, 1, \cdots, N-1. \tag{4.32}$$

For the last two terms of (4.32), by using Cauchy's inequality, (4.19), (4.24), (4.31) and Lemma 4.3, we have the following estimates,

$$\begin{aligned} |2\tau \mathrm{Re}\langle p^1, \delta_t^+ e^0\rangle| &= \tau |2\mathrm{Re}\langle p^1, \frac{i}{2}\Delta_h e^1 + ip^1 - i\eta^0\rangle| & (4.33)\\ &\le \tau|\langle \nabla_h p^1, \nabla_h e_0^1\rangle| + 2\tau|\langle p^1, \eta^0\rangle| \\ &\le C\tau(||\eta^0||^2 + ||\theta^1||^2 + |\theta^1|_1^2 + ||e^1||^2 + |e^1|_1^2), \\ &\le C\tau[(\tau^2 + h^2)^2 + |e^1|_1^2], \\ |2\mathrm{Re}\langle \eta^0, e^1\rangle| &\le ||\eta^0||^2 + ||e^1||^2 \le C(\tau^2 + h^2)^2. & (4.34) \end{aligned}$$

Substituting (4.33)-(4.34) into (4.32) gives

$$|e^1|_1^2 \le C\tau|e^1|_1^2 + C(\tau^2 + h^2)^2. \tag{4.35}$$

Then, for a sufficiently small τ, one can obtain from (4.35) that

$$|e^1|_1 \lesssim \tau^2 + h^2. \tag{4.36}$$

This together with (4.24) gives

$$|||e^1|||_1 \lesssim \tau^2 + h^2. \tag{4.37}$$

In addition, it is follows from (4.19) that

$$|||\theta^1|||_1 \lesssim |\theta^1|_2 \lesssim \tau^2 + h^2. \tag{4.38}$$

Step 2. Error estimates at the n-th ($n > 1$) time step

Assuming that (4.11) holds for $n = m$ $(1 \le m \le N-1)$, i.e.,

$$|||e^m|||_1 + |||\theta^m|||_1 + ||\delta_t^+\theta^{m-1}|| \lesssim h^2 + \tau^2, \quad ||e^m||_\infty + ||\theta^m||_\infty \lesssim 1. \tag{4.39}$$

Then we aim to prove that (4.11) still holds for $n = m + 1$. The assumption (4.39) together with (4.18) gives

$$||q^m|| \lesssim ||e^m|| \lesssim \tau^2 + h^2. \tag{4.40}$$

Multiplying both sides of (4.14) with $n = m$ by $h_1 h_2 h_3(\theta_{jkl}^{m+1} - \theta_{jkl}^{m-1})$ and summing up for $(j,k,l) \in \mathcal{T}_h^0$ give

$$\begin{aligned} &||\delta_t^+\theta^m||^2 + \frac{1}{2}|\theta^{m+1}|_1^2 + \frac{\mu^2}{2}||\theta^{m+1}||^2 \\ =\ &||\delta_t^+\theta^{m-1}||^2 + \frac{1}{2}|\theta^{m-1}|_1^2 + \frac{\mu^2}{2}||\theta^{m-1}||^2 + 2\tau\langle q^m, \delta_t\theta^m\rangle + 2\tau\langle \xi^m, \delta_t\theta^m\rangle. \end{aligned} \tag{4.41}$$

By using Cauchy's inequality and (4.39)–(4.40), we obtain

$$||\delta_t^+\theta^{m-1}||^2 + \frac{1}{2}|\theta^{m-1}|_1^2 + \frac{\mu^2}{2}||\theta^{m-1}||^2 \lesssim (h^2+\tau^2)^2, \tag{4.42}$$

$$\begin{aligned} \left|2\tau\langle q^m, \delta_t\theta^m\rangle\right| &\lesssim \tau(||\delta_t^+\theta^m||^2 + ||\delta_t^+\theta^{m-1}||^2 + ||e^m||^2) \\ &\lesssim \tau||\delta_t^+\theta^m||^2 + \tau(h^2+\tau^2)^2, \end{aligned} \tag{4.43}$$

$$\begin{aligned} \left|2\tau\langle \xi^m, \delta_t\theta^k\rangle\right| &\lesssim \tau(||\delta_t^+\theta^m||^2 + ||\delta_t^+\theta^{m-1}||^2 + ||\xi^m||^2) \\ &\lesssim \tau||\delta_t^+\theta^m||^2 + \tau(h^2+\tau^2)^2. \end{aligned} \tag{4.44}$$

Substituting (4.42)–(4.44) into (4.41) that

$$||\delta_t^+\theta^m||^2 + \frac{1}{2}|\theta^{m+1}|_1^2 + \frac{\mu^2}{2}||\theta^{m+1}||^2 \lesssim \tau||\delta_t^+\theta^m||^2 + (h^2+\tau^2)^2. \tag{4.45}$$

This means that, for a sufficiently small τ, there is

$$||\delta_t^+\theta^m||^2 + |\theta^{m+1}|_1^2 + ||\theta^{m+1}||^2 \lesssim (h^2+\tau^2)^2. \tag{4.46}$$

On the one hand, by using the 'lifting' technique (4.39) and (4.46) together with Minkowski's inequality, one can obtain from (4.14) with $n = m$ that

$$\begin{aligned} &|\theta^{m+1}|_2 - |\theta^{m-1}|_2 \lesssim |\theta^{m+1} + \theta^{m-1}|_2 \\ &\lesssim \frac{1}{\tau}(||\delta_t^+\theta^m|| + ||\delta_t^+\theta^{m-1}||) + ||\theta^{m+1}|| + ||\theta^{m-1}|| + ||q^m|| + ||\xi^m|| \\ &\lesssim \tau^{-1}(h^2+\tau^2). \end{aligned} \tag{4.47}$$

Summing up the above inequality for m gives

$$|\theta^{m+1}|_2 \lesssim |\theta^1|_2 + \tau^{-2}(h^2+\tau^2) \lesssim \tau^{-2}(h^2+\tau^2). \tag{4.48}$$

This means that, if h is small enough such that $\tau^{-1}h \lesssim 1$, there is

$$|\theta^{m+1}|_2 \lesssim 1. \tag{4.49}$$

On the other hand, by using the inverse Sobolev inequality, one can obtain that

$$|\theta^{m+1}|_2 \lesssim h^{-2}||\theta^{m+1}|| \lesssim h^{-2}(h^2+\tau^2). \tag{4.50}$$

This means that, if τ is small enough such that $\tau h^{-1} \lesssim 1$, there is

$$|\theta^{m+1}|_2 \lesssim 1. \tag{4.51}$$

Hence, for sufficiently small h, τ, we always have

$$|\theta^{m+1}|_2 \lesssim 1. \tag{4.52}$$

This together with Lemma 4.2 gives

$$||\theta^{m+1}||_\infty \lesssim 1, \quad ||\phi^{m+1}||_\infty \leq ||v^{m+1}||_\infty + ||\theta^{m+1}||_\infty \lesssim 1. \tag{4.53}$$

This together with (4.39) gives

$$||p^{m+1}|| \lesssim ||e^m|| + ||\theta^m|| + ||e^{m+1}|| + ||\theta^{m+1}||, \tag{4.54}$$

Multiplying both sides of (4.13) with $n = m$ by $h_1h_2h_3(øe^m_{jkl} + øe^{m+1}_{jkl})$ and summing up for $(j, k, l) \in \mathcal{T}_h$, then taking the imaginary part, we obtain

$$||e^{m+1}||^2 - ||e^m||^2 + \tau \mathrm{Im}\langle p^{m+1}, e^m + e^{m+1}\rangle = \tau \mathrm{Im}\langle \eta^m, e^m + e^{m+1}\rangle. \tag{4.55}$$

By using Cauchy's inequality, (4.39), (4.46), (4.54) and Lemma 4.3, we obtain from (4.55) that

$$\begin{aligned} ||e^{m+1}||^2 - ||e^m||^2 &\lesssim \tau(||p^{m+1}||^2 + ||e^{m+1}||^2 + ||e^m||^2 + ||\eta^m||^2) \\ &\lesssim \tau[||e^{m+1}||^2 + ||e^m||^2 + (h^2 + \tau^2)^2]. \end{aligned} \tag{4.56}$$

Applying Gronwall's inequality to (4.56) gives that, if τ is small enough, there is

$$||e^{m+1}|| \lesssim h^2 + \tau^2. \tag{4.57}$$

By using the similar analysis as (4.25)-(4.30), one can obtain that, if h, τ are small enough, there always is

$$|e^{m+1}|_2 \lesssim 1, \quad ||e^{m+1}||_\infty \lesssim 1. \tag{4.58}$$

This together with (4.53) and (4.17) gives

$$|p^{m+1}|_1 \lesssim |||e^m|||_1 + |||\theta^m|||_1 + |||e^{m+1}|||_1 + |||\theta^{m+1}|||_1. \tag{4.59}$$

Multiplying both sides of (4.13) with $n = m$ by $2h_1h_2h_3(øe^m_{jkl} - øe^{m+1}_{jkl})$ and summing up for $(j, k, l) \in \mathcal{T}_h$, then taking the real part, we obtain

$$|e^{m+1}|_1^2 - |e^m|_1^2 = 2\tau \mathrm{Re}\langle p^{m+1}, \delta_t^+ e^m\rangle - 2\mathrm{Re}\langle \eta^m, e^{m+1} - e^m\rangle. \tag{4.60}$$

Summing up the above equation over m from 0 to s then replacing s by m give

$$|e^{m+1}|_1^2 = 2\tau \sum_{l=0}^{m} \mathrm{Re}\langle p^{l+1}, \delta_t^+ e^l\rangle - 2\sum_{l=0}^{m} \mathrm{Re}\langle \eta^l, e^{l+1} - e^l\rangle. \tag{4.61}$$

For the last two term of (4.61), by using Cauchy's inequality, (4.39), (4.46), (4.57), (4.59) and Lemma 4.3, we have the following estimates,

$$\begin{aligned} |2\tau \mathrm{Re}\langle p^{m+1}, \delta_t^+ e^m\rangle| &= \tau|2\mathrm{Re}\langle p^{m+1}, \frac{i}{2}\Delta_h(e^m + e^{k+1}) + ip^{m+1} - i\eta^m\rangle| \\ &= \tau|2\mathrm{Re}\langle p^{m+1}, \frac{i}{2}\Delta_h(e^m + e^{m+1}) - i\eta^m\rangle| \\ &\leq \tau|\langle \nabla_h p^{m+1}, \nabla_h(e^m + e^{m+1})\rangle| + 2\tau|\langle p^{m+1}, \eta^m\rangle| \\ &\leq C\tau(||\eta^m||^2 + ||p^{m+1}||^2 + |p^{m+1}|_1^2 + |e^m|_1^2 + |e^{m+1}|_1^2), \\ &\leq C\tau[(\tau^2 + h^2)^2 + |e^{m+1}|_1^2], \end{aligned} \tag{4.62}$$

$$|2\sum_{l=0}^{m}\mathrm{Re}\langle\eta^l, e^{l+1}-e^l\rangle| = |-2\tau\sum_{l=1}^{m}\mathrm{Re}\langle\delta_t^+\eta^{l-1}, e^l\rangle + 2\mathrm{Re}\langle\eta^m, e^{m+1}\rangle| \quad (4.63)$$

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

$$\leq C(\tau^2+h^2)^2.$$

Substituting (4.62)–(4.63) into (4.61) gives

$$|e^{m+1}|_1^2 \leq C\tau\sum_{l=1}^{m+1}|e^l|_1^2 + C(\tau^2+h^2)^2. \quad (4.64)$$

By using Gronwall's inequality, we obtain that, for sufficiently small τ, there is

$$|e^{m+1}|_1 \leq C_T(\tau^2+h^2), \quad (4.65)$$

where C_T depends on T but is independent of m, h and τ. This completes the induction argument and consequently completes the proof. □

Now, we are ready to prove the main error estimate results (i.e. Theorem 2.1).

Proof of Theorem 2.1 Multiplying both sides of (4.13) by $2h_1h_2h_3(\Delta_h\o e_{jkl}^{n+1} - \Delta_h\o e_{jkl}^n)$ and summing up for $(j,k,l)\in\mathcal{T}_h$, then taking the real part, we obtain

$$\begin{aligned}&|e^{n+1}|_2^2 - |e^n|_2^2 \quad (4.66)\\ =\ & -2\tau\mathrm{Re}\langle p^{n+1}, \Delta_h\delta_t^+e^n\rangle + 2\mathrm{Re}\langle\eta^n, \Delta_h e^{n+1}-\Delta_h e^n\rangle, \quad n=0,1,\cdots,N.\end{aligned}$$

For the third term of (4.66), we have the following estimate,

$$\begin{aligned}&|2\tau\mathrm{Re}\langle\Delta_h p^{n+1}, \delta_t^+e^n\rangle| \quad (4.67)\\ =\ & \tau|2\mathrm{Re}\langle\Delta_h p^{n+1}, i\frac{1}{2}\Delta_h(e^n+e^{n+1}) + ip^{n+1} - i\eta^n\rangle|\\ \leq\ & \tau|\langle\Delta_h p^{n+1}, \Delta_h(e^n+e^{n+1})\rangle| + 2\tau|\langle\Delta_h p^{n+1}, \eta^n\rangle|.\end{aligned}$$

Noticing that

$$||w|| + |w|_1 \lesssim |w|_2 \quad (4.68)$$

for any $w\in H^2(\Omega_h)$, and using Cauchy's inequality, Lemma 4.1 and Theorem 4.1, we obtain that

$$\begin{aligned}&|\langle\Delta_h p^{n+1}, \Delta_h(e^n+e^{n+1})\rangle_0| \leq |p^n|_2(|e^n|_2+|e^{n+1}|_2) \quad (4.69)\\ \leq\ & \big(|e^n|_2+|e^{n+1}|_2+|\theta^n|_2+|\theta^{n+1}|_2+\|e^n\|_2+\|e^{n+1}\|_2+\|\theta^n\|_2+\|\theta^{n+1}\|_2\\ &+||\nabla_h(e^n+e^{n+1})||_4+||\nabla_h(\theta^n+\theta^{n+1})||_4\big)(|e^n|_2+|e^{n+1}|_2)\\ \leq\ & |e^n|_2^2+|e^{n+1}|_2^2+|\theta^n|_2^2+|\theta^{n+1}|_2^2,\\ &|\langle\Delta_h p^{n+1}, \eta^n\rangle| \leq |p^{n+1}|_2^2 + ||\eta^n||^2\\ \lesssim\ & |e^n|_2+|e^{n+1}|_2+|\theta^n|_2+|\theta^{n+1}|_2+(h^2+\tau^2)^2. \quad (4.70)\end{aligned}$$

Substituting (4.69)–(4.70) into (4.67) gives

$$\begin{aligned} &|2\mathrm{Re}\langle p^{n+1}, \Delta_h e^{n+1} - \Delta_h e^n\rangle| \\ &\le \tau(|e^n|_2^2 + |e^{n+1}|_2^2 + |\theta^n|_2^2 + |\theta^{n+1}|_2^2) + (h^2+\tau^2)^2. \end{aligned} \tag{4.71}$$

Substituting (4.71) into (4.66) and summing up for n from 0 to s then replacing s by n, we obtain

$$\begin{aligned} |e^{n+1}|_2^2 \le\ & 2\sum_{l=0}^{n} \mathrm{Re}\langle \eta^l, \Delta_h e^{l+1} - \Delta_h e^l\rangle + C(h^2+\tau^2)^2 \\ & + C\tau\sum_{l=1}^{n+1}(|e^l|_2^2 + |\theta^l|_2^2), \quad n = 0, 1, \cdots, N. \end{aligned} \tag{4.72}$$

For the second term of (4.72), by using the summation of parts formula, one can obtain that

$$\begin{aligned} & 2\sum_{l=0}^{n} \mathrm{Re}\langle \eta^l, \Delta_h e^{l+1} - \Delta_h e^l\rangle \\ &= -2\tau\sum_{l=1}^{n}\mathrm{Re}\langle \delta_t^+\eta^{l-1}, \Delta_h e^l\rangle + 2\mathrm{Re}\langle \eta^n, \Delta_h e^{n+1}\rangle \\ &\le \tau\sum_{l=1}^{n}(||\delta_t^+\eta^{l-1}||^2 + |e^l|_2^2) + \frac{1}{2}|e^{n+1}|_2^2 + 2||\eta^n||^2. \end{aligned} \tag{4.73}$$

Substituting (4.73) into (4.72) and using Lemma 4.3 gives

$$|e^{n+1}|_2^2 \le C\tau\sum_{l=1}^{n+1}(|\theta^l|_2^2 + |e^l|_2^2) + C(h^2+\tau^2)^2, \quad n = 0, 1, \cdots, N. \tag{4.74}$$

Multiplying both sides of (4.14) by $h_1h_2h_3(\Delta_h\theta_{jkl}^{n+1} - \Delta_h\theta_{jkl}^{n-1})$ and summing up for $(j,k,l) \in \mathcal{T}_h$ give

$$\begin{aligned} & |\delta_t^+\theta^n|_1^2 + \frac{1}{2}(|\theta^{n+1}|_2^2 + |\theta^n|_2^2) + \frac{\mu^2}{2}(|\theta^{n+1}|_1^2 + |\theta^n|_1^2) \\ &= |\delta_t^+\theta^{n-1}|_1^2 + \frac{1}{2}(|\theta^n|_2^2 + |\theta^{n-1}|_2^2) + \frac{\mu^2}{2}(|\theta^n|_1^2 + |\theta^{n-1}|_1^2) \\ &\quad + \tau\langle \delta_t^+\nabla_h\theta^n + \delta_t^+\nabla_h\theta^{n-1}, \nabla_h q^n\rangle_0 - 2\tau\langle \xi^n, \delta_t\Delta_h\theta^n\rangle, \quad 1 \le n < N. \end{aligned} \tag{4.75}$$

Summing up (4.75) for n from 1 to m then replacing m by n, we obtain

$$\begin{aligned} & |\delta_t^+\theta^n|_1^2 + \frac{1}{2}(|\theta^{n+1}|_2^2 + |\theta^n|_2^2) + \frac{\mu^2}{2}(|\theta^{n+1}|_1^2 + |\theta^n|_1^2) \\ &= |\delta_t^+\theta^0|_1^2 + \frac{1}{2}|\theta^1|_2^2 + \frac{\mu^2}{2}|\theta^1|_1^2 - 2\tau\sum_{l=1}^{n}\langle \xi^l, \delta_t\Delta_h\theta^l\rangle \\ &\quad + \tau\sum_{l=1}^{n}\langle \delta_t^+\nabla_h\theta^l + \delta_t^+\nabla_h\theta^{l-1}, \nabla_h q^l\rangle_0, \quad 1 \le n < N. \end{aligned} \tag{4.76}$$

For the last two terms of (4.76), we have

$$
\begin{aligned}
& |2\tau \sum_{l=1}^{n} \langle \xi^l, \delta_t \Delta_h \theta^l \rangle| \qquad (4.77)\\
&= |\langle \xi^n, \Delta_h \theta^{n+1} \rangle + \langle \xi^{n-1}, \Delta_h \theta^n \rangle - \langle \xi^2, \Delta_h \theta^1 \rangle - 2\tau \sum_{l=2}^{n-1} \langle \delta_t \xi^l, \Delta_h \theta^l \rangle| \\
&\leq \frac{1}{4}(|\theta^{n+1}|_2^2 + |\theta^n|_2^2 + |\theta^1|_2^2) + ||\xi^n||^2 + ||\xi^{n-1}||^2 + ||\xi^2||^2 \\
&\quad + \tau \sum_{l=2}^{n-1} |\theta^l|_2^2 + \tau \sum_{l=2}^{n-1} ||\delta_t \xi^l||^2 \leq \frac{1}{4}(|\theta^{n+1}|_2^2 + |\theta^n|_2^2) + C(h^2 + \tau^2)^2,
\end{aligned}
$$

$$
\begin{aligned}
& \tau \sum_{l=1}^{n} \langle \delta_t^+ \nabla_h \theta^l + \delta_t^+ \nabla_h \theta^{l-1}, \nabla_h q^l \rangle_0 \leq \tau \sum_{l=0}^{n} |\delta_t^+ \theta^l|_1^2 + \tau \sum_{l=0}^{n} |q^l|_1^2 \qquad (4.78)\\
&\leq \tau \sum_{l=0}^{n} |\delta_t^+ \theta^l|_1^2 + C(h^2 + \tau^2)^2,
\end{aligned}
$$

where Lemma 4.3 and Theorem 4.1 were used.

Substituting (4.77) and (4.78) into (4.76) and using (4.19)–(4.20) gives

$$
\begin{aligned}
& |e^{n+1}|_2^2 + |\delta_t^+ \theta^n|_1^2 + \frac{1}{4}(|\theta^{n+1}|_2^2 + |\theta^n|_2^2) \qquad (4.79)\\
&\leq C\tau \sum_{l=1}^{n+1} (|\delta_t^+ \theta^{l-1}|_1^2 + |\theta^l|_2^2 + |e^l|_2^2) + C(\tau^2 + h^2)^2, \quad 1 \leq n < N.
\end{aligned}
$$

By applying Gronwall's inequality, we obtain from (4.77) that, if τ is small enough, there is

$$
|e^{n+1}|_2^2 + |\delta_t^+ \theta^n|_1^2 + \frac{1}{2}(|\theta^{n+1}|_2^2 + |\theta^n|_2^2) \leq C(\tau^2 + h^2)^2, \quad 1 \leq n < N. \qquad (4.80)
$$

This completes the proof. □

Remark 4.1 By using the similar producer, we can obtain the results in Theorems 2.2 and 2.3.

4.2 Extension to nonhomogeneous KGS equations

In this section, we extend the numerical schemes and corresponding analysis result to the following nonhomogeneous KGS equations in three dimensions.

$$
i\partial_t \psi + \frac{1}{2}\Delta \psi + \phi \psi = f, \quad (x, y, z) \in \Omega, \quad t > 0, \qquad (4.81)
$$

$$
\partial_{tt} \phi - \Delta \phi + \mu^2 \phi = |\psi|^2 + g, \quad (x, y, z) \in \Omega, \quad t > 0, \qquad (4.82)
$$

$$
\psi(x, y, z, t) = 0, \quad \phi(x, y, z, t) = 0, \quad (x, y, z) \in \partial\Omega, \quad t > 0, \qquad (4.83)
$$

$$
(\psi, \phi, \partial_t \phi)(x, y, z, 0) = (\psi_0, \phi_0, \phi_1)(x, y, z), \quad (x, y, z) \in \overline{\Omega}, \qquad (4.84)
$$

where $f = f(x, y, z, t)$ and $g = g(x, y, z, t)$ are given complex-valued function and real-valued function, respectively.

Extension of the CIFD scheme and the DIFD scheme to the problem (4.81)–(4.84) reads

$$
\begin{aligned}
& i\delta_t^+\psi_{jkl}^n + \frac{1}{4}\Delta_h(\psi_{jkl}^n + \psi_{jkl}^{n+1}) + \frac{1}{4}(\phi_{jkl}^n + \phi_{jkl}^{n+1})(\psi_{jkl}^n + \psi_{jkl}^{n+1}) = f_{jkl}^{n+\frac{1}{2}}, \quad (4.85)\\
& \qquad (j,k,l) \in \mathcal{T}_h, \quad n = 0, 1, \cdots, N-1,\\
& \delta_t^2\phi_{jkl}^n - \frac{1}{2}\Delta_h(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) + \frac{\mu^2}{2}(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) = |\psi_{jkl}^n|^2 + g_{jkl}^n, \quad (4.86)\\
& \qquad (j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,\\
& \psi_{jkl}^0 = \psi_0(x_j, y_k, z_l), \quad \phi_{jkl}^0 = \phi_0(x_j, y_k, z_l), \quad (4.87)\\
& \delta_t^+\phi_{jkl}^0 = \phi_1(x_j, y_k, z_l) + \frac{\tau}{2}\phi_2(x_j, y_k, z_l), \qquad (j,k,l) \in \mathcal{T}_h^0,\\
& \psi^n \in X_h, \quad \phi^n \in X_h, \quad n = 1, 2, \cdots, N, \quad (4.88)
\end{aligned}
$$

and

$$
\begin{aligned}
& i\delta_t\psi_{jkl}^n + \frac{1}{4}\Delta_h(\psi_{jkl}^{n-1} + \psi_{jkl}^{n+1}) + \frac{1}{2}\phi_{jkl}^n(\psi_{jkl}^{n-1} + \psi_{jkl}^{n+1}) = f_{jkl}^n, \quad (4.89)\\
& \qquad (j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,\\
& \delta_t^2\phi_{jkl}^n - \frac{1}{2}\Delta_h(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) + \frac{\mu^2}{2}(\phi_{jkl}^{n-1} + \phi_{jkl}^{n+1}) = |\psi_{jkl}^n|^2 + g_{jkl}^n, \quad (4.90)\\
& \qquad (j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,\\
& \psi_{jkl}^0 = \psi_0(x_j, y_k, z_l), \ \phi_{jkl}^0 = \phi_0(x_j, y_k, z_l), \quad (4.91)\\
& \delta_t^+\phi_{jkl}^0 = \phi_1(x_j, y_k, z_l) + \frac{\tau}{2}\phi_2(x_j, y_k, z_l), \qquad (j,k,l) \in \mathcal{T}_h^0,\\
& \psi^n \in X_h, \quad \phi^n \in X_h, \quad n = 1, 2, \cdots, N. \quad (4.92)
\end{aligned}
$$

where $f_{jkl}^n = f(x_j, y_k, z_l, t_n)$, $f_{jkl}^{n+\frac{1}{2}} = f(x_j, y_k, z_l, t_{n+\frac{1}{2}})$, $g_{jkl}^n = g(x_j, y_k, z_l, t_n)$.

In addition for comparison, Zhang and Han proposed a fully nonlinear scheme in [31] for the KGS (4.81)–(4.84). The schemes reads

$$
\begin{aligned}
& i\delta_t^+\psi_{jkl}^n + \frac{1}{4}\Delta_h(\psi_{jkl}^n + \psi_{jkl}^{n+1}) + \frac{1}{4}(\phi_{jkl}^n + \phi_{jkl}^{n+1})(\psi_{jkl}^n + \psi_{jkl}^{n+1}) = f_{jkl}^{n+\frac{1}{2}}, \quad (4.93)\\
& \qquad (j,k,l) \in \mathcal{T}_h, \quad n = 0, 1, \cdots, N-1,\\
& \delta_t^2\phi_{jkl}^n - \frac{1}{4}\Delta_h(\phi_{jkl}^{n-1} + 2\phi_{jkl}^n + \phi_{jkl}^{n+1}) + \frac{\mu^2}{4}(\phi_{jkl}^{n-1} + 2\phi_{jkl}^n + \phi_{jkl}^{n+1}) \quad (4.94)\\
= \ & \frac{1}{4}(|\psi_{jkl}^{n-1}|^2| + 2|\psi_{jkl}^n|^2| + |\psi_{jkl}^{n+1}|^2) + \frac{1}{2}(g_{jkl}^{n-\frac{1}{2}} + g_{jkl}^{n+\frac{1}{2}}),\\
& \qquad (j,k,l) \in \mathcal{T}_h, \quad n = 1, 2, \cdots, N-1,\\
& \psi_{jkl}^0 = \psi_0(x_j, y_k, z_l), \quad \phi_{jkl}^0 = \phi_0(x_j, y_k, z_l), \quad (4.95)\\
& \delta_t^+\phi_{jkl}^0 = \phi_1(x_j, y_k, z_l) + \frac{\tau}{2}\phi_2(x_j, y_k, z_l), \qquad (j,k,l) \in \mathcal{T}_h^0,\\
& \psi^n \in X_h, \quad \phi^n \in X_h, \quad n = 1, 2, \cdots, N, \quad (4.96)
\end{aligned}
$$

Obviously, this is an implicit and coupled scheme which needs multiple iterations at each time step, so it is more costly. In the following, we address the nonlinear scheme (4.93)–(4.96) as ZHFD.

Remark 4.2 We remark that the original form of ZHFD given in [31] contains an auxiliary variable which is not convenient for implementation. Here the presented ZHFD (4.93)–(4.96) is an equivalent form for $n = 2, 3, \cdots, N-1$, but it differs at the value for $n = 1$.

By using similar method in analysing Theorem 2.1, one can obtain the error estimates of the finite difference schemes for solving the nonhomogeneous KGS equations, i.e.,

Theorem 4.2 *Under assumption (A), there exist two constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, we have the following optimal error estimates for the proposed CIFD scheme* (4.85)–(4.88) *and the proposed DIFD scheme* (4.89)–(4.92) *as:*

$$|||e^n|||_2 + |||\theta^n|||_2 \lesssim h^2 + \tau^2, \quad ||e^n||_\infty + ||\theta^n||_\infty \lesssim h^2 + \tau^2, \quad n = 0, 1, \cdots, N. \tag{4.97}$$

Remark 4.3 Though the proposed schemes and their analysis results are given in the uniform grids, the two schemes can be used to solve the KGS equations in the nonuniform grids, and the corresponding conservation laws, error estimates and stability results can be obtained by using the similar analysis method.

5 Numerical results

In this section, we report the numerical results of the proposed finite difference schemes to confirm our theoretical studies.

Example 5.1 For comparison, we consider the following two-dimensional nonhomogeneous KGS equations,

$$i\partial_t\psi + \frac{1}{2}(\partial_{xx}\psi + \partial_{yy}\psi) + \phi\psi = f(x, y, t), \quad (x, y) \in \Omega, \quad t > 0, \tag{5.1}$$

$$\partial_{tt}\phi - \partial_{xx}\phi - \partial_{yy}\phi + \mu^2\phi - |\psi|^2 = g(x, y, t), \quad (x, y) \in \Omega, \quad t > 0, \tag{5.2}$$

with boundary conditions

$$\psi(x, y, t) = 0, \quad \phi(x, y, t) = 0, \quad (x, y) \in \partial\Omega, \quad t > 0, \tag{5.3}$$

and initial conditions

$$\begin{aligned} &\psi(x, y, 0) = \psi_0(x, y), \quad \phi(x, y, 0) = \phi_0(x, y), \\ &\partial_t\phi(x, y, 0) = \phi_1(x, y), \quad (x, y) \in \overline{\Omega}, \end{aligned} \tag{5.4}$$

where $\Omega = (0, \pi) \times (0, \pi)$ and

$$\begin{aligned} &f(x, y, t) = (1 + \sin(x)\sin(y)\sin(\mu t))\sin(x)\sin(y)\exp(-2it), \\ &g(x, y, t) = 2\sin(x)\sin(y)\sin(\mu t) - \sin^2(x)\sin^2(y), \\ &\psi_0(x, y) = \sin(x)\sin(y), \quad \phi_0(x, y) = 0, \quad \phi_1(x, y) = \mu\sin(x)\sin(y). \end{aligned}$$

Table 1 Temporal error analysis of the CIFD scheme at time $t = 1.2$ with time step τ under mesh size $h = \pi/128$

τ	$\tau = 0.3$	$\tau = 0.24$	$\tau = 0.2$	$\tau = 0.15$	$\tau = 0.12$
$\|e^n\|_\infty$	1.77E-02	5.08E-03	3.60E-03	2.28E-03	1.58E-03
	rate	1.85	1.89	1.58	1.64
$\|\theta^n\|_\infty$	3.14E-02	2.04E-02	1.43E-02	8.20E-03	5.30E-03
	rate	1.92	1.95	1.94	1.96
$\||e^n\||_2$	5.41E-02	3.52E-02	2.47E-02	1.45E-02	9.61E-03
	rate	1.93	1.95	1.84	1.85
$\||\theta^n\||_2$	1.33E-01	8.67E-02	6.09E-02	3.49E-02	2.26E-02
	rate	1.91	1.94	1.93	1.95

Table 2 Temporal error analysis of the DIFD scheme at time $t = 1.2$ with time step τ under mesh size $h = \pi/128$

τ	$\tau = 0.3$	$\tau = 0.24$	$\tau = 0.2$	$\tau = 0.15$	$\tau = 0.12$
$\|e^n\|_\infty$	3.07E-02	1.86E-02	1.53E-02	9.04E-03	5.90E-03
	rate	2.24	1.07	1.84	1.91
$\|\theta^n\|_\infty$	3.14E-02	1.96E-02	1.36E-02	7.45E-03	4.69E-03
	rate	2.11	2.02	2.08	2.07
$\||e^n\||_2$	2.10E-01	1.39E-01	1.07E-01	6.33E-02	4.15E-02
	rate	1.87	1.42	1.82	1.89
$\||\theta^n\||_2$	1.31E-01	8.51E-02	5.95E-02	3.35E-02	2.14E-02
	rate	2.01	1.96	2.00	2.00

Table 3 Temporal error analysis of the ZHFD scheme at time $t = 1.2$ with time step τ under mesh size $h = \pi/128$

τ	$\tau = 0.3$	$\tau = 0.24$	$\tau = 0.2$	$\tau = 0.15$	$\tau = 0.12$
$\|e^n\|_\infty$	1.43E-02	9.15E-03	6.32E-03	3.53E-03	2.24E-03
	rate	2.01	2.03	2.03	2.03
$\|\theta^n\|_\infty$	3.00E-03	1.89E-03	1.31E-03	7.42E-04	4.80E-04
	rate	2.06	2.02	1.98	1.95
$\||e^n\||_2$	9.29E-02	6.09E-02	4.28E-02	2.44E-02	1.57E-02
	rate	1.89	1.93	1.96	1.96
$\||\theta^n\||_2$	1.60E-02	1.05E-02	7.46E-03	4.32E-03	2.84E-03
	rate	1.87	1.89	1.90	1.90

Table 4 Spatial error analysis of the CIFD scheme at time $t = 1.2$ with different mesh size h under time step $\tau = 0.003$

h	$h = \pi/4$	$h = \pi/5$	$h = \pi/8$	$h = \pi/10$	$h = \pi/16$
$\|e^n\|_\infty$	5.96E-02	3.44E-02	1.55E-02	9.97E-03	3.90E-03
	rate	2.46	1.70	1.96	2.00
$\|\theta^n\|_\infty$	1.22E-02	7.72E-03	3.14E-03	2.02E-03	7.93E-04
	rate	2.06	1.94	1.96	1.97
$\|\|e^n\|\|_2$	2.29E-01	1.51E-01	6.07E-02	3.91E-02	1.54E-02
	rate	1.87	1.94	1.97	1.98
$\|\|\theta^n\|\|_2$	6.25E-02	4.14E-02	1.67E-02	1.08E-02	4.25E-03
	rate	1.85	1.93	1.95	1.96

Table 5 Spatial error analysis of the DIFD scheme at time $t = 1.2$ with different mesh size h under time step $\tau = 0.003$

h	$h = \pi/4$	$h = \pi/5$	$h = \pi/8$	$h = \pi/10$	$h = \pi/16$
$\|e^n\|_\infty$	5.96E-02	3.44E-02	1.55E-02	9.97E-03	3.90E-03
	rate	2.46	1.70	1.96	2.00
$\|\theta^n\|_\infty$	1.23E-02	7.74E-03	3.14E-03	2.02E-03	7.95E-04
	rate	2.10	1.94	1.96	1.96
$\|\|e^n\|\|_2$	2.29E-01	1.51E-01	6.07E-02	3.91E-02	1.54E-02
	rate	1.87	1.94	1.97	1.98
$\|\|\theta^n\|\|_2$	6.25E-02	4.14E-02	1.67E-02	1.08E-02	4.26E-03
	rate	1.85	1.93	1.95	1.96

Table 6 Spatial error analysis of the ZHFD scheme at time $t = 1.2$ with different mesh size h under time step $\tau = 0.003$

h	$h = \pi/4$	$h = \pi/5$	$h = \pi/8$	$h = \pi/10$	$h = \pi/16$
$\|e^n\|_\infty$	5.96E-02	3.44E-02	1.55E-02	9.96E-03	3.90E-03
	rate	2.46	1.69	1.99	2.00
$\|\theta^n\|_\infty$	1.22E-02	7.72E-03	3.13E-03	2.01E-03	7.90E-04
	rate	2.06	1.92	1.98	1.99
$\|\|e^n\|\|_2$	2.29E-01	1.51E-01	6.07E-02	3.91E-02	1.54E-02
	rate	1.87	1.94	1.97	1.99
$\|\|\theta^n\|\|_2$	6.25E-02	4.14E-02	1.67E-02	1.08E-02	4.24E-03
	rate	1.85	1.93	1.97	1.98

Table 7 Error analysis of the CIFD scheme, the DIFD scheme and the ZHFD scheme at time $t = 1.5$

scheme	h, τ	$\|e^n\|_\infty + \|\theta^n\|_\infty$	$\|e^n\|_\infty$	$\|\theta^n\|_\infty$
CIFD	$h = \pi/50, \tau = 0.01$	5.2354e-4	4.0635e-4	1.1720e-4
DIFD	$h = \pi/50, \tau = 0.01$	5.2226e-4	4.1035e-4	1.1191e-4
MZFD	$h = \pi/50, \tau = 0.015$	5.1365e-4	4.1336e-4	1.0028e-4

The initial-boundary value problem (5.1)–(5.4) has an exact solution as follows

$$\psi(x, y, t) = \sin(x)\sin(y)\exp(-2it), \quad \phi(x, y, t) = \sin(x)\sin(y)\sin(\mu t).$$

In running the CIFD scheme and the DIFD scheme, we choose the Gauss - Seidel iteration method as our linear solver. In running the ZHFD scheme, we adopt the (outside) nonlinear iterative algorithm given in [22] with tolerance number of the iteration 10^{-8}, and also choose the Gauss-Seidel iteration method as the (inner) linear solver. Thanks to the unconditional stability, we study the temporal error and the spatial error of the proposed numerical methods separately. For the temporal error analysis, we use mesh size $h = \pi/128$ which is small enough to ignore the spatial discretization error. For the spatial error analysis, we use $\tau = 0.003$ to ignore the temporal error. The error (2.13) is presented at time $t = 1.2$ and measured under the norms with exactly the same form as given in the theoretical estimates (2.14). Tables 1, 2 and 3 and Tables 4, 5 and 6 show the results of the temporal and spatial errors of the CIFD scheme, DIFD scheme and ZHFD scheme, respectively (Table 7).

For comparing the efficiency of the ZHFD scheme, the CIFD scheme and the DIFD scheme, we also demonstrate the computational (CPU) time of the three schemes in computing the given example in Table 8. All experiments are carried out via MATLAB software on a PC with 4G RAM. Here, due to the limit of the computer, we do not run the DIFD scheme by using any parallel computing method, and all methods are programmed in sequential way. To show clearer comparison of the efficiency of the three schemes, we plot the CPU time used by the CIFD and DIFD schemes into a percentage bar chart in Fig. 1 where we use the CPU time of ZHFD as benchmark unit. In addition, we show the necessary step size of the three methods to reach in the same order of accuracy in Table 7. In order to test the conservation laws conserved by the CIFD scheme and the DIFD scheme, we let $f = 0$, $g = 0$ in (5.1)–(5.2), and display the discrete mass and energy in Figs. 2 and 3.

Table 8 CPU time (seconds) spent by the three schemes at time $t = 1.5$ with different mesh size h and time step

scheme	$h = \pi/8$ $\tau = 0.008$	$h = \pi/16$ $\tau = 0.004$	$h = \pi/32$ $\tau = 0.002$	$h = \pi/64$ $\tau = 0.001$
CIFD	0.0936s	0.9173s	8.3472s	73.4558s
DIFD	0.1092s	1.0592s	9.6391s	80.0044s
ZHFD	0.3732s	3.6540s	33.1396s	325.1841s

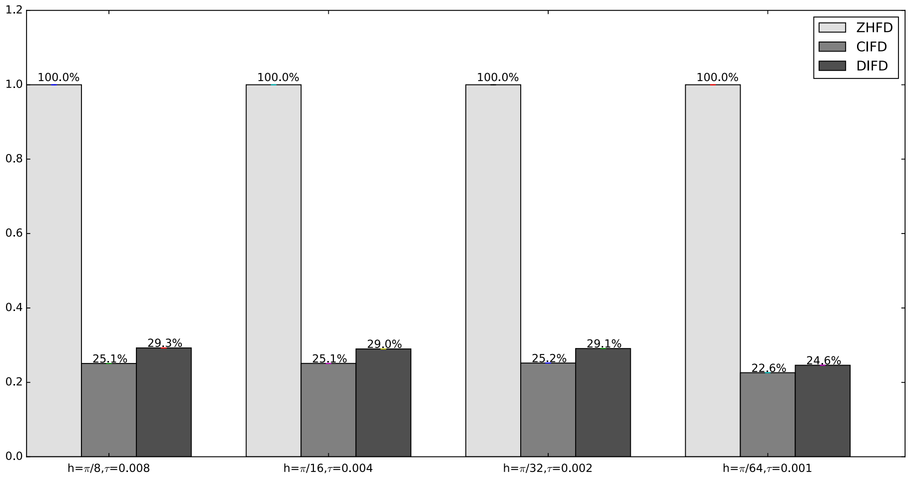

Fig. 1 Percentage bar charts of the CPU time used by the ZHFD scheme, the CIFD scheme and the DIFD scheme in computing Example 5.1 at $t = 1.5$

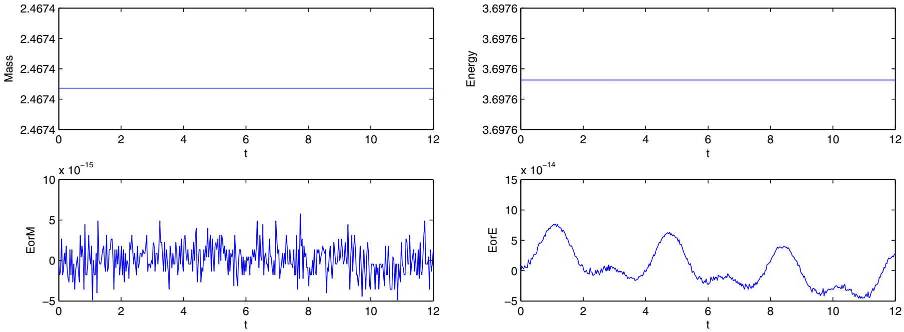

Fig. 2 Total mass (*left*) and energy (*right*) of the CIFD scheme in computing Example 5.1 with $f = g = 0$

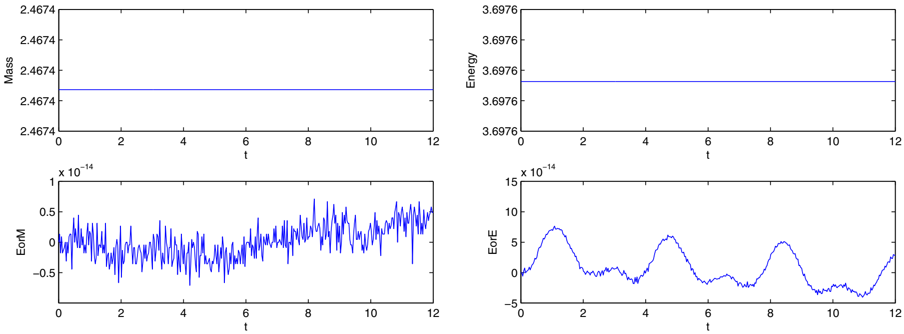

Fig. 3 Total mass (*left*) and energy (*right*) of the DIFD scheme in computing Example 5.1 with $f = g = 0$

From Tables 1–8, Figs. 1, 2, 3, 4 and 5 and results not shown here for brevity, we can draw the following conclusions:

1. Both CIFD and DIFD scheme have second order accuracy in time and in space, which means that our theoretical error estimates are optimal. The CIFD

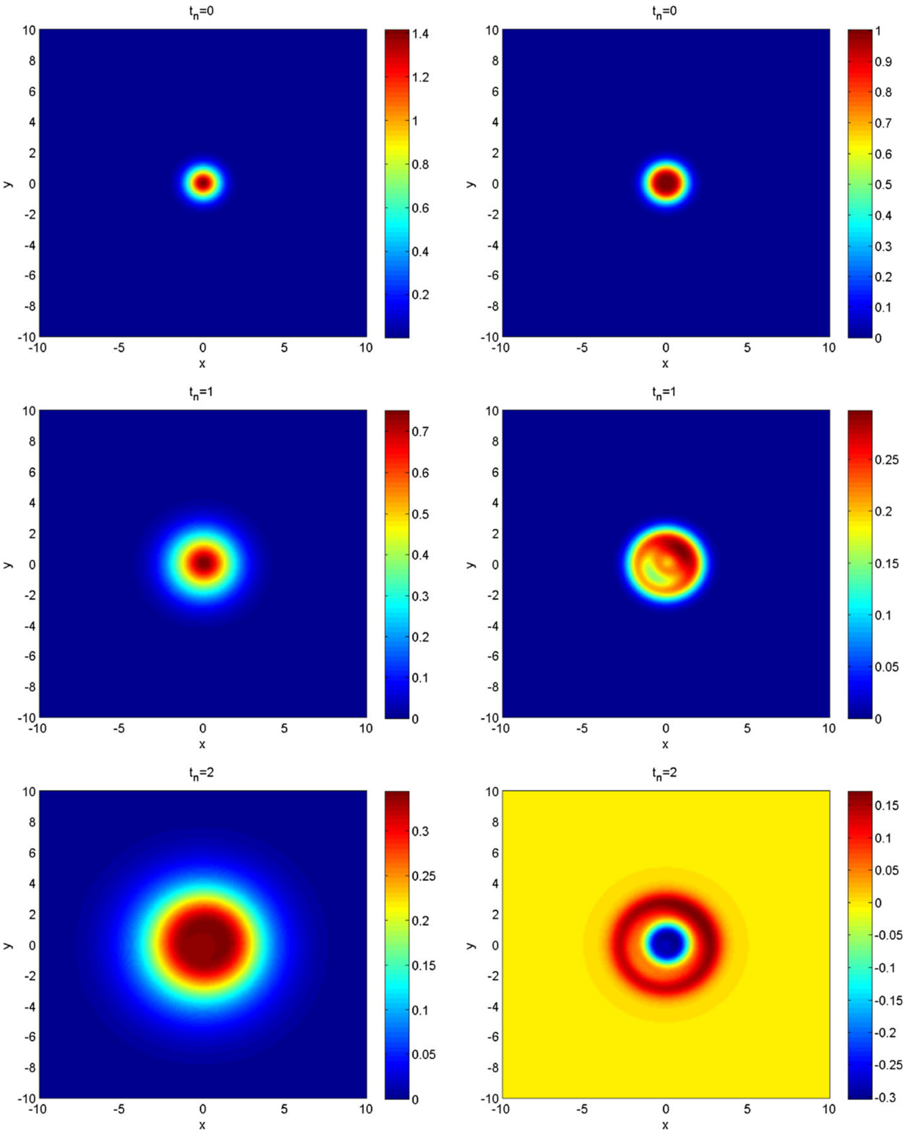

Fig. 4 Files of $|\psi^n|$ (*left*) and ϕ^n (*right*) computed by the CIFD scheme in solving Example 5.2 at $t_n = 0, 1, 2$

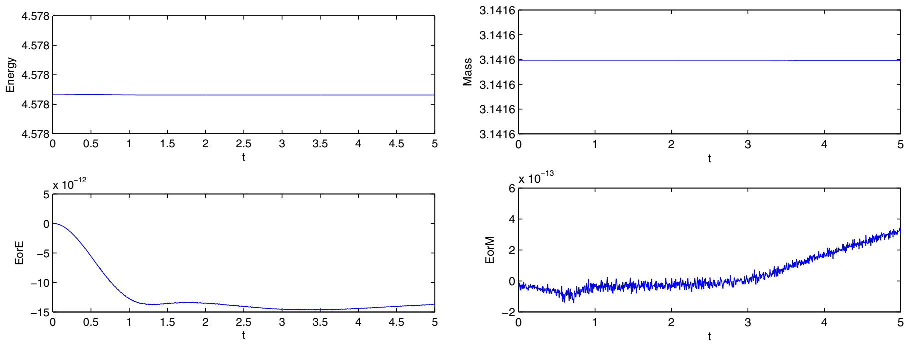

Fig. 5 Total mass (*left*) and energy (*right*) of the CIFD scheme in computing Example 5.2

and DIFD schemes are unconditionally stable. The time step can be chosen independent of the mesh size.

2. The CIFD and DIFD schemes have comparable accuracy with the ZHFD scheme (see Tables 1–3, 4–7) in computing the nucleon field ψ. ZHFD under the same step size is more accurate than CIFD or DIFD in computing the meson field ϕ (the error of ZHFD in ϕ is approximately ten time less that of CIFD or DIFD). However, CIFD and DIFD are more efficient than ZHFD (see Tables 7 and 8 and Fig. 1). The performance of CIFD and DIFD are similar in accuracy and efficiency under the sequential implementation.
3. The CIFD and DIFD scheme preserve well the total mass and energy in the discrete sense (see Figs. 2, 3, 5 and 6).

Example 5.2 At last but not least, we consider the dynamics of the waves in the 2D KGS (1.1)–(1.3) under a general initial localised data

$$\psi_0(\mathbf{x}) = (1+i)\mathrm{e}^{-|\mathbf{x}|^2}, \quad \phi_0(\mathbf{x}) = \mathrm{sech}(|\mathbf{x}|^2), \quad \phi_1(\mathbf{x}) = \sin(x+y)\mathrm{e}^{-2|\mathbf{x}|^2}. \tag{5.5}$$

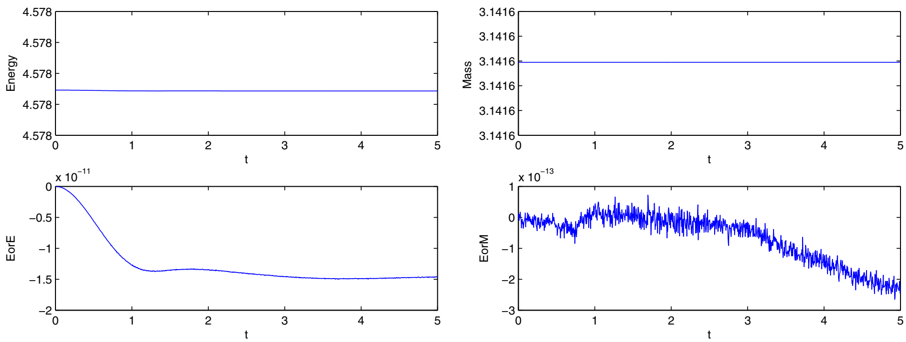

Fig. 6 Total mass (*left*) and energy (*right*) of the DIFD scheme in computing Example 5.2

6 Conclusion

In this paper, we propose and analyze two finite difference schemes for solving the initial-boundary value problem of the Klein-Gordon-Schrödinger equations in two dimensions or three dimensions. The two schemes conserve the discrete mass and energy in the discrete level. At each time step, only two systems of linear algebraic equations need to be solved, hence the two proposed schemes are efficient in the practical computation. Different from the analysis method used in [31] where they proved the stability and convergence of a nonlinear finite difference scheme for solving the dissipative KGS equations based on the $a\ priori$ estimates of the numerical solution, we here introduce an introduction argument as well as a 'lifting' technique to establish the optimal error estimates of the CIFD scheme and the DIFD scheme in H^2 norm without any restrictions on the grid ratios. The analysis method used in this paper can be applied to more general nonlinear Schrödinger-type equations and many other implicit finite difference schemes for which previous works often require certain restriction on the time-step size τ.

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