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Optimal error estimates of finite difference time domain methods for the Klein–Gordon–Dirac system

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We propose and analyze finite difference methods for solving the Klein–Gordon–Dirac (KGD) system. Due to the nonlinear coupling between the complex Dirac 'wave function' and the real Klein–Gordon field, it is a great challenge to design and analyze numerical methods for KGD. To overcome the difficulty induced by the nonlinearity, four implicit/semi-implicit/explicit finite difference time domain (FDTD) methods are presented, which are time symmetric or time reversible. By rigorous error estimates, the FDTD methods converge with second-order accuracy in both spatial and temporal discretizations, and numerical results in one dimension are reported to support our conclusion. The error analysis relies on the energy method, the special nonlinear structure in KGD and the mathematical induction. Thanks to tensor grids and discrete Sobolev inequalities, our approach and convergence results are valid in higher dimensions under minor modifications.

Keywords: Klein–Gordon–Dirac system; Yukawa interaction; finite difference time domain (FDTD); methods; energy conservation; error estimates.

1. Introduction

In this paper, we consider the Klein–Gordon–Dirac (KGD) system, which plays a fundamental role in quantum electrodynamics and also appears in the Yukawa models (Bjorken & Drell, 1965; Holten, 1991; Greiner, 1994; Slawianowski & Kovalchuk, 2002; Ohlsson, 2011). The KGD system is given in three dimensions (Bjorken & Drell, 1965; Slawianowski & Kovalchuk, 2002; Ding & Xu, 2014) as

$$\begin{cases} \dfrac{1}{c^2}\partial_{tt}\phi(t,\mathbf{x}) - \Delta\phi(t,\mathbf{x}) + \dfrac{m_1^2c^2}{\hbar^2}\phi(t,\mathbf{x}) = 4\pi\lambda\Psi^*\beta\Psi(t,\mathbf{x}), \\ i\hbar\partial_t\Psi(t,\mathbf{x}) + i\hbar c\displaystyle\sum_{j=1}^{3}\alpha_j\partial_j\Psi(t,\mathbf{x}) - m_2c^2\beta\Psi(t,\mathbf{x}) - \lambda\phi\beta\Psi(t,\mathbf{x}) = 0, \end{cases} \quad \mathbf{x}\in\mathbb{R}^3, \quad t>0, \tag{1.1}$$

which describes a complex-valued Dirac vector field $\Psi(t,\mathbf{x})\in\mathbb{C}^4$ interacting with a neutral real-valued scalar meson field $\phi(t,\mathbf{x})\in\mathbb{R}$ through the Yukawa interaction, with a coupling constant $0<\lambda\in\mathbb{R}$. The coupling terms in this system, which come from the the Yukawa potential, describe the nuclear force between the meson field and the fermion field and give a closer description of many particles found in the real world. Here c is the speed of light, $\hbar$ is Planck's constant, $m_1, m_2 > 0$ are the masses of the meson and the electron, respectively; $\mathrm{i}=\sqrt{-1}$ is the imaginary unit, $(t,\mathbf{x})\in\mathbb{R}\times\mathbb{R}^3$, t is time, $\mathbf{x}$ is the spatial coordinate vector as $\mathbf{x}=(x_1,x_2,x_3)^{\mathrm{T}}$ (equivalently written as $\mathbf{x}=(x,y,z)^{\mathrm{T}}$), $\partial_j=\partial/\partial x_j$ $(j=1,2,3)$,

$\Delta = \sum_{j=1}^{3} \partial_j^2$ in three dimensions. In addition, $\Psi^* = \overline{\Psi}^{\mathrm{T}}$ is the conjugate transpose, α_1, α_2, α_3 and β are the 4×4 matrices given as

$$\alpha_j = \begin{pmatrix} \mathbf{0} & \sigma_j \\ \sigma_j & \mathbf{0} \end{pmatrix}, \quad j = 1, 2, 3, \quad \beta = \begin{pmatrix} I & \mathbf{0} \\ \mathbf{0} & -I \end{pmatrix}, \tag{1.2}$$

with σ_j ($j = 1, 2, 3$) being the Pauli matrices and I being the 2×2 identity matrix as

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1.3}$$

There are two important regimes for the KGD system (1.1): the relativistic case $c = \mathcal{O}(1)$ and the nonrelativistic case $c \gg 1$. In this paper we focus on the relativistic case, i.e., $c = \mathcal{O}(1)$, and some discussions on the nonrelativistic case can be found in Remark 3.6. For simplicity we set $m_1 = 1$, $\hbar = 1$, $c = 1$ and the coupling parameter in (1.1) as (by a proper scaling of space, time and the wave function)

$$\begin{cases} \partial_{tt}\phi(t, \mathbf{x}) - \Delta\phi(t, \mathbf{x}) + \phi(t, \mathbf{x}) = g\Psi^*(t, \mathbf{x})\beta\Psi(t, \mathbf{x}), \\ i\partial_t\Psi(t, \mathbf{x}) + i\sum\limits_{j=1}^{3} \alpha_j\partial_j\Psi(t, \mathbf{x}) - \omega\beta\Psi(t, \mathbf{x}) = g\phi(t, \mathbf{x})\beta\Psi(t, \mathbf{x}), \end{cases} \quad \mathbf{x} \in \mathbb{R}^3, \ t > 0, \tag{1.4}$$

with $\omega = m_2/m_1$, $g > 0$ and initial data

$$\phi(0, \mathbf{x}) = \phi^0(\mathbf{x}), \quad \partial_t\phi(0, \mathbf{x}) = \gamma(\mathbf{x}), \quad \Psi(0, \mathbf{x}) = \Psi^0(\mathbf{x}) = \left(\psi_1^0(\mathbf{x}), \psi_2^0(\mathbf{x}), \psi_3^0(\mathbf{x}), \psi_4^0(\mathbf{x})\right)^{\mathrm{T}}, \tag{1.5}$$

where $\phi^0(\mathbf{x}), \gamma(\mathbf{x}) \in \mathbb{R}$ and $\Psi^0(\mathbf{x}) \in \mathbb{C}^4$.

Introducing the density ρ_j for the j-th component ($j = 1, 2, 3, 4$) and the total electron density ρ, as well as the current density $\mathbf{J}(t, \mathbf{x}) = (J_1(t, \mathbf{x}), J_2(t, \mathbf{x}), J_3(t, \mathbf{x}))^{\mathrm{T}}$ defined as

$$\rho(t, \mathbf{x}) = \sum_{j=1}^{4} \rho_j(t, \mathbf{x}) = \Psi^*\Psi, \quad \rho_j(t, \mathbf{x}) = |\psi_j(t, \mathbf{x})|^2, \quad J_l(t, \mathbf{x}) = \Psi^*\alpha_l\Psi, \quad 1 \leqslant l \leqslant 3, \tag{1.6}$$

the following conservation law holds:

$$\partial_t\rho(t, \mathbf{x}) + \nabla \cdot \mathbf{J}(t, \mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^3, \ t \geqslant 0. \tag{1.7}$$

As a consequence, the KGD system (1.4) conserves the total electron mass

$$\|\Psi(t, \cdot)\|^2 := \int_{\mathbb{R}^3} |\Psi(t, \mathbf{x})|^2 \,\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \sum_{j=1}^{4} |\psi_j(t, \mathbf{x})|^2 \,\mathrm{d}\mathbf{x} \equiv \|\Psi(0, \cdot)\|^2 = \|\Psi^0\|^2. \tag{1.8}$$

In addition, (1.4) conserves the *energy*

$$
\begin{aligned}
\mathcal{E}(t) \;:=\; & \frac{1}{2}\int_{\mathbb{R}^3} |\partial_t \phi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} + \frac{1}{2}\int_{\mathbb{R}^3} |\nabla \phi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} + \frac{1}{2}\int_{\mathbb{R}^3} |\phi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} \\
& + \int_{\mathbb{R}^3} \left[i\Psi^*(t,\mathbf{x}) \sum_{j=1}^{3} \alpha_j \partial_j \Psi(t,\mathbf{x}) - \omega \Psi^*(t,\mathbf{x})\beta\Psi(t,\mathbf{x}) - g\phi(t,\mathbf{x})\Psi^*(t,\mathbf{x})\beta\Psi(t,\mathbf{x}) \right] \mathrm{d}\mathbf{x} \\
\equiv\; & \mathcal{E}(0), \quad t \geqslant 0.
\end{aligned} \tag{1.9}
$$

Similar to the dimension reduction of the nonlinear Schrödinger equation and Dirac equation (Bao & Cai, 2012a, 2013; Bao *et al.*, 2017), when the initial data $\phi^0(\mathbf{x})$ and $\Psi^0(\mathbf{x})$ are homogenous or strongly confined in the z-direction, ϕ and Ψ are formally assumed to be homogenous in the z-direction or concentrated on the xy–plane, then the KGD system (1.4) in three dimensions can be reduced to a two-dimensional system with $\mathbf{x} = (x,y)^{\mathrm{T}} \in \mathbb{R}^2$ that has a similar structure to (1.4). Furthermore, when the initial data $\phi^0(\mathbf{x})$ and $\Psi^0(\mathbf{x})$ are homogenous or strongly confined in the y-, z-directions, the KGD system (1.4) in three dimensions can be reduced to a one-dimensional system with $\mathbf{x} = x$. In lower dimensions ($d = 2, 1$), the two-component Dirac vector fields are usually adopted as in the (nonlinear) Dirac equation case (Bao *et al.*, 2015; Bao *et al.*, 2016). Accordingly, KGD (1.4) can be reduced to a simplified form in d dimensions ($d = 1, 2$) as

$$
\begin{cases}
\partial_{tt}\phi(t,\mathbf{x}) - \Delta\phi(t,\mathbf{x}) + \phi(t,\mathbf{x}) = g\Psi^*(t,\mathbf{x})\sigma_3\Psi(t,\mathbf{x}), \\
i\partial_t\Psi(t,\mathbf{x}) + i\sum_{j=1}^{d} \sigma_j\partial_j\Psi(t,\mathbf{x}) - \omega\sigma_3\Psi(t,\mathbf{x}) = g\phi(t,\mathbf{x})\sigma_3\Psi(t,\mathbf{x}),
\end{cases} \tag{1.10}
$$

where $\phi := \phi(t,\mathbf{x}) \in \mathbb{R}$ and $\Psi := \Psi(t,\mathbf{x}) \in \mathbb{C}^2$. Because of its simplicity, the two-component form (1.10) is widely used in one dimension and two dimensions. Analogously to the four-component case, (1.10) conserves the total mass

$$
\|\Psi(t,\cdot)\|^2 := \int_{\mathbb{R}^d} |\Psi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} \equiv \|\Psi(0,\cdot)\|^2 \tag{1.11}
$$

and the energy

$$
\begin{aligned}
\widehat{\mathcal{E}}(t) \;:=\; & \frac{1}{2}\int_{\mathbb{R}^d} |\partial_t \phi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} + \frac{1}{2}\int_{\mathbb{R}^d} |\nabla \phi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} + \frac{1}{2}\int_{\mathbb{R}^d} |\phi(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} \\
& + \int_{\mathbb{R}^d} \left[i\Psi^*(t,\mathbf{x}) \sum_{j=1}^{d} \sigma_j \partial_j \Psi(t,\mathbf{x}) - \omega \Psi^*(t,\mathbf{x})\sigma_3\Psi(t,\mathbf{x}) - g\phi(t,\mathbf{x})\Psi^*(t,\mathbf{x})\sigma_3\Psi(t,\mathbf{x}) \right] \mathrm{d}\mathbf{x} \\
\equiv\; & \widehat{\mathcal{E}}(0), \quad t \geqslant 0.
\end{aligned} \tag{1.12}
$$

The KGD system (1.4) ((1.10)) has been extensively studied theoretically in the literature, such as the existences of bound state solutions and the local and global well-posedness of the Cauchy problem, and we refer to Chadam & Glassey (1974), Bachelot (1989), Bournaveas (1999, 2001), Esteban *et al.* (1996), Fang (2004), Selberg & Tesfahun (2006), Machihara & Omoso (2007) and references therein for more details. While in the numerical aspect, recently, various numerical methods including the finite difference time domain (FDTD) methods and spectral methods have been proposed and analyzed for efficient computations of wave propagation in classical/relativistic quantum physics, i.e., dispersive waves in the Gross–Pitaevskii equation (Bao & Cai, 2013), the Klein–Gordon equation (Jiménez & Vázquez, 1990; Pascual *et al.*, 1995; Bao & Dong, 2012), the Dirac equation (Alvarez, 1992; Xu *et al.*, 2012; Hammer *et al.*, 2014; Bao *et al.*, 2016; Bao *et al.*, 2017), the Klein–Gordon–Schrödinger equations (Bao & Yang, 2007; Dehghan & Taleei, 2012), the Klein–Gordon–Zakharov equations (Cai & Liang, 2012) and the Maxwell–Dirac equations (Bao & Li, 2004; Lorin & Bandrauk, 2011), etc. To the best of our knowledge there has not been any numerical work on the KGD system (1.4) (or (1.10)). Thus, the main purpose of this paper is to design FDTD methods for the KGD system (1.4) (or (1.10)) and analyze their efficiencies and accuracies. The main difficulty in the error analysis is that the corresponding energy functional, which lacks a lower bound, is indefinite. Meanwhile, the nonlinear coupling terms bring new challenges for the numerical simulation and analysis. We detail the analysis and the comparison of several conservative/nonconservative implicit/semi-implicit/explicit FDTD schemes and pay particular attention to how the nonlinear terms affect the implementation and the convergence analysis. Based on our results, the conservative FDTD method performs the best in terms of computational efficiency, accuracy and stability.

This paper is organized as follows. In Section 2, four second-order conservative/nonconservative implicit/explicit FDTD methods are proposed. Then the error estimates are established in Section 3. Section 4 is devoted to the numerical tests. Finally, we give some concluding remarks in Section 5. Throughout this paper we use $p \lesssim q$ to represent that there exists a generic constant C that is independent of h and τ such that $|p| \leqslant Cq$.

2. FDTD methods and their properties

In this section, we present four FDTD methods for the KGD system (1.10). For simplicity of notation, we shall illustrate the numerical methods and their analysis in one dimension only. Generalization to higher dimensions and the KGD system (1.10) (or (1.4)) are straightforward for tensor grids, and results remain valid under minor modifications. In practical computation, we truncate the whole space problem onto an interval $\Omega = (a, b)$ with periodic boundary conditions, which is large enough such that the truncation error is negligible. The KGD system (1.10) in the bounded domain Ω reads

$$\begin{cases} \partial_{tt}\phi(t,x) - \partial_{xx}\phi(t,x) + \phi(t,x) = g\Psi^*(t,x)\sigma_3\Psi(t,x), \quad x \in \Omega, \quad t > 0, \\ i\partial_t\Psi(t,x) + i\sigma_1\partial_x\Psi(t,x) - \omega\sigma_3\Psi(t,x) = g\phi(t,x)\sigma_3\Psi(t,x), \quad x \in \Omega, \quad t > 0, \\ \phi(t,a) = \phi(t,b), \quad \partial_x\phi(t,a) = \partial_x\phi(t,b), \quad t \geqslant 0, \\ \Psi(t,a) = \Psi(t,b), \quad \partial_x\Psi(t,a) = \partial_x\Psi(t,b), \quad t \geqslant 0, \\ \phi(0,x) = \phi^0(x), \quad \partial_t\phi(0,x) = \gamma(x), \quad \Psi(0,x) = \Psi^0(x), \quad x \in \bar{\Omega}, \end{cases} \tag{2.1}$$

where $\phi := \phi(t,x) \in \mathbb{R}$ and $\Psi := \Psi(t,x) = (\psi_1(t,x), \psi_2(t,x))^{\mathrm{T}} \in \mathbb{C}^2$.

2.1 *FDTD methods*

Choose spatial mesh size $h := \Delta x = \frac{b-a}{M}$ with M being an even positive integer, temporal step size $\tau := \Delta t > 0$ and the grid points and time steps are

$$x_j := a + jh, \quad j = 0, 1, 2, \ldots, M; \quad t_n := n\tau, \quad n = 0, 1, 2, \ldots. \tag{2.2}$$

Denote $X_M = \{U = (U_0, U_1, \ldots, U_M)^{\mathrm{T}} | U_j \in \mathbb{C}^2,\ j = 0, 1, 2, \ldots, M,\ U_0 = U_M\}$, $\widetilde{X}_M = \{U = (U_0, U_1, \ldots, U_M)^{\mathrm{T}} | U_j \in \mathbb{R},\ j = 0, 1, 2, \ldots, M,\ U_0 = U_M\}$ and we always use $U_{-1} = U_{M-1}$ and $U_{M+1} = U_1$ if they are involved. The Fourier transform of $U \in X_M$ (or $U \in \widetilde{X}_M$) is given as

$$U_j = \sum_{l=-M/2}^{M/2-1} \widetilde{U}_l e^{i\mu_l(x_j - a)}, \quad x_j \in \bar{\Omega},\ j = 0, 1, 2, \ldots, M, \tag{2.3}$$

with $\widetilde{U}_l \in \mathbb{C}^2$ (or $\widetilde{U}_l \in \mathbb{C}$) being the Fourier transform coefficients defined as

$$\widetilde{U}_l = \frac{1}{M} \sum_{j=0}^{M-1} U_j e^{-i\mu_l(x_j - a)}, \quad \mu_l = \frac{2l\pi}{b - a}, \quad -M/2 \leqslant l \leqslant M/2 - 1.$$

Let (ϕ_j^n, Ψ_j^n) be the numerical approximation of $(\phi(t_n, x_j), \Psi(t_n, x_j))$ for $j = 0, 1, 2, \ldots, M$ and $n = 0, 1, 2, \ldots$, and denote $\phi^n = (\phi_0^n, \phi_1^n, \ldots, \phi_M^n)^{\mathrm{T}} \in \widetilde{X}_M$ and $\Psi^n = (\Psi_0^n, \Psi_1^n, \ldots, \Psi_M^n)^{\mathrm{T}} \in X_M$ as the solution vectors at $t = t_n$. We introduce some finite difference operators for $U \in X_M$ or $\widetilde{X}_M$,

$$\delta_t^+ U_j^n = \frac{U_j^{n+1} - U_j^n}{\tau}, \qquad \delta_t U_j^n = \frac{U_j^{n+1} - U_j^{n-1}}{2\tau}, \qquad U_j^{n+1/2} = \frac{U_j^{n+1} + U_j^n}{2},$$
$$\delta_x^+ U_j^n = \frac{U_{j+1}^n - U_j^n}{h}, \qquad \delta_x U_j^n = \frac{U_{j+1}^n - U_{j-1}^n}{2h}, \qquad \mathcal{A} U_j^n = \frac{U_j^{n+1} + U_j^{n-1}}{2},$$
$$\delta_x^2 U_j^n = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{h^2}, \qquad \delta_t^2 U_j^n = \frac{U_j^{n+1} - 2U_j^n + U_j^{n-1}}{\tau^2}.$$

The standard discrete l^2-norm, H^1-seminorm and l^∞-norm for $U \in X_M$ (or $U \in \widetilde{X}_M$) are defined as

$$\|U\|_{l^2}^2 := h \sum_{j=0}^{M-1} |U_j|^2, \quad \|\delta_x^+ U\|_{l^2}^2 = h \sum_{j=0}^{M-1} |\delta_x^+ U_j|^2, \quad \|U\|_{l^\infty} := \max_{0 \leqslant j \leqslant M-1} |U_j|.$$

Here we consider several frequently used FDTD methods to discretize KGD (2.1) for $j = 0, 1, \ldots, M$:

- Crank–Nicolson finite difference (CNFD) method

$$\delta_t^2 \phi_j^n - \delta_x^2 \mathcal{A} \phi_j^n + \mathcal{A} \phi_j^n = g (\Psi_j^n)^* \sigma_3 \Psi_j^n, \quad n \geqslant 1, \tag{2.4}$$

$$i \delta_t^+ \Psi_j^n = \left[-i\sigma_1 \delta_x + \omega \sigma_3\right] \Psi_j^{n+1/2} + g \phi_j^{n+1/2} \sigma_3 \Psi_j^{n+1/2}, \quad n \geqslant 0; \tag{2.5}$$

- a semi-implicit energy conservative finite difference (SIFD1) method

$$\delta_t^2 \phi_j^n - \delta_x^2 \phi_j^n + \mathcal{A} \phi_j^n = g (\Psi_j^n)^* \sigma_3 \Psi_j^n, \quad n \geqslant 1, \tag{2.6}$$

$$i \delta_t \Psi_j^n = \left[-i\sigma_1 \delta_x + \omega \sigma_3\right] \mathcal{A} \Psi_j^n + g \phi_j^n \sigma_3 \mathcal{A} \Psi_j^n, \quad n \geqslant 1; \tag{2.7}$$

- another semi-implicit finite difference (SIFD2) method

$$\delta_t^2\phi_j^n - \delta_x^2\mathcal{A}\phi_j^n + \mathcal{A}\phi_j^n = g(\Psi_j^n)^*\sigma_3\Psi_j^n, \quad n \geqslant 1, \tag{2.8}$$

$$i\delta_t\Psi_j^n = -i\sigma_1\delta_x\Psi_j^n + \omega\sigma_3\mathcal{A}\Psi_j^n + g\mathcal{A}\phi_j^n\sigma_3\mathcal{A}\Psi_j^n, \quad n \geqslant 1; \tag{2.9}$$

- leap-frog finite difference (LFFD) method

$$\delta_t^2\phi_j^n - \delta_x^2\phi_j^n + \phi_j^n = g(\Psi_j^n)^*\sigma_3\Psi_j^n, \quad n \geqslant 1, \tag{2.10}$$

$$i\delta_t\Psi_j^n = \left[-i\sigma_1\delta_x + \omega\sigma_3\right]\Psi_j^n + g\phi_j^n\sigma_3\Psi_j^n, \quad n \geqslant 1. \tag{2.11}$$

Meanwhile, the initial and boundary conditions in (2.1) are discretized for $j = 0, 1, \ldots, M$ and $n \geq 0$ as

$$\phi_j^0 \;=\; \phi^0(x_j), \quad \phi_M^{n+1} = \phi_0^{n+1}, \quad \phi_{-1}^{n+1} = \phi_{M-1}^{n+1}, \tag{2.12}$$

$$\Psi_j^0 \;=\; \Psi^0(x_j), \quad \Psi_M^{n+1} = \Psi_0^{n+1}, \quad \Psi_{-1}^{n+1} = \Psi_{M-1}^{n+1}, \tag{2.13}$$

where the initial velocity $\gamma(x)$ of the Klein–Gordon field is employed to update the first step ϕ_j^1 by Taylor expansion and (2.1) as

$$\phi_j^1 = \phi_j^0 + \tau\gamma(x_j) + \frac{\tau^2}{2}\left[\left(\phi^0\right)''(x_j) - \phi_j^0 + g\left(\Psi_j^0\right)^*\sigma_3\Psi_j^0\right], \quad j = 0, 1, \ldots, M. \tag{2.14}$$

In addition, Taylor expansion can be applied to compute the first step for the Dirac fields for SIFD1 (2.7), SIFD2 (2.9) and LFFD (2.11) ($j = 0, 1, \ldots, M$) as

$$\Psi_j^1 = \Psi_j^0 - \tau\left[\sigma_1\left(\Psi^0\right)'(x_j) + i\omega\sigma_3\Psi_j^0 + ig\phi_j^0\sigma_3\Psi_j^0\right]. \tag{2.15}$$

Clearly, the above four FDTD methods are time symmetric and time reversible, i.e., CNFD (2.4–2.5) is unchanged if interchanging $n + 1 \leftrightarrow n$, $\tau \leftrightarrow -\tau$ and taking complex conjugates, whereas the others are unchanged if interchanging $n + 1 \leftrightarrow n - 1$, $\tau \leftrightarrow -\tau$ and taking complex conjugates. Moreover, LFFD (2.10–2.11) is explicit, and its computational cost per time step is $\mathcal{O}(M)$. In fact, it might be the simplest and the most efficient discretization for the KGD system. The others are implicit schemes. However, at each time step t_n, the computations of CNFD (2.4–2.5), SIFD1 (2.6–2.7) and SIFD2 (2.8–2.9) can be decoupled into two linear systems, i.e., one first updates the Klein–Gordon part ϕ_j^{n+1} by solving the linear system (2.4) or (2.6) or (2.8), and then updates the Dirac part Ψ_j^{n+1} by solving the other linear system (2.5) or (2.7) or (2.9).

In detail, for the Klein–Gordon part, (2.4) in CNFD and (2.8) in SIFD2 can be solved efficiently by the Thomas algorithm in one dimension that needs only $\mathcal{O}(M)$ operations. Meanwhile, the solutions to (2.4) and (2.8) can be explicitly updated in Fourier space for $l = -M/2, \ldots, M/2 - 1$ as

$$\widetilde{\phi_l^{n+1}} = \left[\frac{1}{\tau^2} + \frac{1}{h^2}\left(1 - \cos(\mu_l h)\right) + \frac{1}{2}\right]^{-1} \cdot \left[\widetilde{G_l^n} + \frac{2}{\tau^2}\widetilde{\phi_l^n}\right] - \widetilde{\phi_l^{n-1}}, \quad n \geqslant 1, \tag{2.16}$$

where $\widetilde{G_l^n} = (g\widetilde{(\Psi^n)^*\sigma_3\Psi^n})_l$ with $\mathcal{O}(M\ln M)$ computational cost per time step, and such an approach is valid in higher dimensions. For SIFD1, the solution of the Klein–Gordon component (2.6) can be explicitly written as

$$\phi_j^{n+1} = \frac{2\tau^2}{\tau^2+2}\left[G_j^n + \left(\frac{2}{\tau^2} - \frac{2}{h^2}\right)\phi_j^n + \frac{1}{h^2}\left(\phi_{j+1}^n + \phi_{j-1}^n\right)\right] - \phi_j^{n-1}, \quad n \geqslant 1, \tag{2.17}$$

and $G_j^n = g(\Psi_j^n)^*\sigma_3\Psi_j^n$ $(j = 0, 1, \ldots, M-1)$.

In addition, the Dirac component (2.9) in the SIFD2 scheme can be solved explicitly for $j = 0, 1, \ldots, M-1$ and $n \geqslant 1$ as

$$\Psi_j^{n+1} = \left[\frac{i}{\tau} - \omega\sigma_3 - g(\mathcal{A}\phi_j^n)\sigma_3\right]^{-1} \cdot \left[\left(\frac{i}{\tau} + \omega\sigma_3 + g(\mathcal{A}\phi_j^n)\sigma_3\right)\Psi_j^{n-1} + \frac{i}{h}\sigma_1\left(\Psi_{j-1}^n - \Psi_{j+1}^n\right)\right]. \tag{2.18}$$

Nevertheless, the corresponding Dirac components for CNFD and SIFD1 in (2.4–2.7) can be solved via either a direct solver or an iterative solver with the computational cost per time step, depending on the linear system solver, which is usually larger than $\mathcal{O}(M)$, especially in two dimensions and three dimensions. Overall, the computational costs for CNFD, SIFD1 and SIFD2 are usually $\mathcal{O}(M)$ in one dimension (by the Thomas algorithm) and larger than $\mathcal{O}(M)$ in two dimensions and three dimensions.

REMARK 2.1 Following the von Neumann linear stability analysis of the classical FDTD methods for the Dirac equation and Klein–Gordon equation (Bao & Dong, 2012; Bao *et al.*, 2017) we can conclude that for the linear stability, e.g., $g = 0$, CNFD (2.4–2.5) is unconditionally stable for any $\tau, h > 0$; SIFD1, SIFD2 and LFFD (2.6–2.11) are stable under the condition $0 < \tau \lesssim h$. The nonlinear stability of FDTD methods can be deduced partially through the error estimates in Section 3.

2.2 *Mass and energy conservation*

For CNFD (2.4–2.5), we have the following conservation laws on the discrete level.

LEMMA 2.2 CNFD (2.4–2.5) conserves the mass, i.e.,

$$\|\Psi^n\|_{l^2}^2 = h\sum_{j=0}^{M-1}\left|\Psi_j^n\right|^2 \equiv h\sum_{j=0}^{M-1}\left|\Psi^0(x_j)\right|^2 = \|\Psi^0\|_{l^2}^2, \quad n \geqslant 0 \tag{2.19}$$

and the energy

$$\begin{aligned}\mathcal{E}^n := {} & \frac{1}{2}\|\delta_t^+\phi^n\|_{l^2}^2 + \frac{1}{4}(\|\delta_x^+\phi^{n+1}\|_{l^2}^2 + \|\delta_x^+\phi^n\|_{l^2}^2) + \frac{1}{4}(\|\phi^{n+1}\|_{l^2}^2 + \|\phi^n\|_{l^2}^2) \\ & + ih\sum_{j=0}^{M-1}(\Psi_j^{n+1})^*\sigma_1\delta_x\Psi_j^{n+1} - \omega h\sum_{j=0}^{M-1}(\Psi_j^{n+1})^*\sigma_3\Psi_j^{n+1} \\ & - \frac{gh}{2}\sum_{j=0}^{M-1}(\phi_j^n + \phi_j^{n+1})(\Psi_j^{n+1})^*\sigma_3\Psi_j^{n+1} \equiv \mathcal{E}^0, \quad n \geqslant 0.\end{aligned} \tag{2.20}$$

Proof. (i) The mass conservation (2.19) is easy to obtain following the standard computations for the Dirac equation case (Bao *et al.*, 2017), and we omit the details here.

(ii) We show the energy conservation (2.20). Multiplying both sides of (2.4) by $h(\phi_j^{n+1}-\phi_j^{n-1})$, summing over j and using the summation by parts formula, we obtain

$$\begin{aligned}&\left(\|\delta_t^+\phi^n\|_{l^2}^2-\|\delta_t^+\phi^{n-1}\|_{l^2}^2\right)+\frac{1}{2}\left(\|\delta_x^+\phi^{n+1}\|_{l^2}^2-\|\delta_x^+\phi^{n-1}\|_{l^2}^2\right)+\frac{1}{2}\left(\|\phi^{n+1}\|_{l^2}^2-\|\phi^{n-1}\|_{l^2}^2\right)\\&\quad-gh\sum_{j=0}^{M-1}(\phi_j^{n+1}-\phi_j^{n-1})(\Psi_j^n)^*\sigma_3\Psi_j^n=0.\end{aligned}\tag{2.21}$$

Next multiplying both sides of (2.5) from the left by $2h(\Psi_j^{n+1}-\Psi_j^n)^*$, summing over j and taking the real parts will yield

$$\begin{aligned}&ih\sum_{j=0}^{M-1}\left[\left(\Psi_j^{n+1}\right)^*\sigma_1\delta_x\Psi_j^{n+1}-\left(\Psi_j^n\right)^*\sigma_1\delta_x\Psi_j^n\right]-\omega h\sum_{j=0}^{M-1}\left[\left(\Psi_j^{n+1}\right)^*\sigma_3\Psi_j^{n+1}-\left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right]\\&\quad-\frac{gh}{2}\sum_{j=0}^{M-1}\left(\phi_j^n+\phi_j^{n+1}\right)\left[\left(\Psi_j^{n+1}\right)^*\sigma_3\Psi_j^{n+1}-\left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right]=0.\end{aligned}\tag{2.22}$$

Combining (2.21) with (2.22) leads to $\mathcal{E}^n\equiv\mathcal{E}^{n-1}$, and the energy conservation (2.20) holds. □

SIFD1 (2.6–2.7) has similar conservation laws on the discrete level, and the proof is similar to that of Lemma 2.2, which will be skipped.

LEMMA 2.3 SIFD1 (2.6–2.7) conserves the mass

$$\left\|\Psi^{n+1}\right\|_{l^2}^2+\|\Psi^n\|_{l^2}^2=h\sum_{j=0}^{M-1}\left(\left|\Psi_j^n\right|^2+\left|\Psi_j^{n+1}\right|^2\right)\equiv\left\|\Psi^1\right\|_{l^2}^2+\left\|\Psi^0\right\|_{l^2}^2,\quad n\geqslant 0\tag{2.23}$$

and the energy

$$\begin{aligned}\widetilde{\mathcal{E}}^n:=&\frac{1}{2}\|\delta_t^+\phi^n\|_{l^2}^2+\frac{h}{2}\sum_{j=0}^{M-1}\delta_x^+\phi_j^n\cdot\delta_x^+\phi_j^{n+1}+\frac{1}{4}\left(\left\|\phi^{n+1}\right\|_{l^2}^2+\|\phi^n\|_{l^2}^2\right)\\&+\frac{ih}{2}\sum_{j=0}^{M-1}\left[\left(\Psi_j^{n+1}\right)^*\sigma_1\delta_x\Psi_j^{n+1}+\left(\Psi_j^n\right)^*\sigma_1\delta_x\Psi_j^n\right]-\frac{\omega h}{2}\sum_{j=0}^{M-1}\left[\left(\Psi_j^{n+1}\right)^*\sigma_3\Psi_j^{n+1}+\left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right]\\&-\frac{gh}{2}\sum_{j=0}^{M-1}\left[\phi_j^n\left(\Psi_j^{n+1}\right)^*\sigma_3\Psi_j^{n+1}+\phi_j^{n+1}\left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right]\equiv\widetilde{\mathcal{E}}^0,\quad n\geqslant 0.\end{aligned}\tag{2.24}$$

We remark here that SIFD2 and LFFD (2.8–2.11) do not conserve the mass and energy, but according to the error estimates in Section 3 the losses of the mass and energy for these two schemes are at $\mathcal{O}(\tau^2+h^2)$. See Lemma 3.7 for more details.

3. Error estimates

Let $0 < T < T^*$ with T^* being the maximal existence time of the solution to the KGD system (2.1); following the theoretical studies on the KGD system (Chadam & Glassey, 1974; Bachelot, 1989; Bournaveas, 1999, 2001; Fang, 2004; Selberg & Tesfahun, 2006; Machihara & Omoso, 2007), we make the following assumptions on the exact solution $(\phi(t,x), \Psi(t,x))$ of the KGD system (2.1):

$$\begin{aligned}
\phi(t,x) \in\ & C^5([0,T];L^\infty) \cap C^4\big([0,T];W_p^{1,\infty}\big) \cap C^3\big([0,T];W_p^{2,\infty}\big) \cap C^2\big([0,T];W_p^{3,\infty}\big)\\
&\cap C^1\big([0,T];W_p^{4,\infty}\big) \cap C\big([0,T];W_p^{5,\infty}\big),\\
\Psi(t,x) \in\ & C^4\big([0,T];[L^\infty]^2\big) \cap C^3\big([0,T];\big[W_p^{1,\infty}\big]^2\big) \cap C^2\big([0,T];\big[W_p^{2,\infty}\big]^2\big)\\
&\cap C^1\big([0,T];\big[W_p^{3,\infty}\big]^2\big) \cap C\big([0,T];\big[W_p^{4,\infty}\big]^2\big),
\end{aligned} \tag{A}$$

where $W_p^{m,\infty} = \{u | u \in W_p^{m,\infty}(\Omega),\ \partial_x^l u(a) = \partial_x^l u(b), l = 0, 1, \ldots, m-1\}$ for $m \geqslant 1$, and the boundary values are understood in the trace sense.

Denote

$$N_\phi = \|\phi(t,x)\|_{L^\infty([0,T];L^\infty)}, \quad N_\Psi = \|\Psi(t,x)\|_{L^\infty([0,T];[L^\infty]^2)}, \tag{3.1}$$

and the grid error functions $\eta^n = (\eta_0^n, \eta_1^n, \ldots, \eta_M^n)^{\mathrm{T}}$ and $\mathbf{e}^n = (e_0^n, e_1^n, \ldots, e_M^n)^{\mathrm{T}}$ as

$$\eta_j^n = \phi\big(t_n, x_j\big) - \phi_j^n \in \mathbb{R}, \quad \mathbf{e}_j^n = \Psi\big(t_n, x_j\big) - \Psi_j^n \in \mathbb{C}^2, \quad j = 0, 1, \ldots, M-1, \ \ n \geqslant 0, \tag{3.2}$$

where ϕ_j^n and Ψ_j^n are the numerical approximations obtained from the FDTD methods.

For CNFD (2.4–2.5), the following error bounds can be established (see the proof in Section 3.1).

THEOREM 3.1 (Error bounds of CNFD). Under assumption (A), there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that for any $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, we have the following error estimates for CNFD (2.4–2.5) with (2.12) and (2.13):

$$\|\eta^n\|_{l^2} + \|\delta_x^+ \eta^n\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\mathbf{e}^n\|_{l^2} \lesssim h^2 + \tau^2, \tag{3.3}$$

$$\|\phi^n\|_{l^\infty} \leqslant 1 + N_\phi, \quad \|\Psi^n\|_{l^\infty} \leqslant 1 + N_\Psi, \quad 0 \leqslant n \leqslant \frac{T}{\tau}. \tag{3.4}$$

For LFFD (2.10–2.11), we assume the stability condition

$$\tau < \min\{\sqrt{2}/2, \sqrt{3}h/2\}, \quad h > 0 \tag{3.5}$$

and establish the following error estimates (see the proof in Section 3.2).

THEOREM 3.2 (Error bounds of LFFD). Under the assumption (A) and the stability condition $\tau \leqslant \alpha \min\{\sqrt{2}/2, \sqrt{3}h/2\}$ $(0 < \alpha < 1)$, there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that for any $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, we have the following error estimates for LFFD (2.10–2.11) with (2.12) and (2.13):

$$\|\eta^n\|_{l^2} + \|\delta_x^+ \eta^n\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\mathbf{e}^n\|_{l^2} \lesssim h^2 + \tau^2, \tag{3.6}$$

$$\|\phi^n\|_{l^\infty} \leqslant 1 + N_\phi, \quad \|\Psi^n\|_{l^\infty} \leqslant 1 + N_\Psi, \quad 0 \leqslant n \leqslant \frac{T}{\tau}. \tag{3.7}$$

REMARK 3.3 The above Theorem 3.2 is still valid in higher dimensions (two dimensions and three dimensions), while Theorem 3.1 holds in two dimensions ($d = 2$) and three dimensions ($d = 3$) under the technical condition $\tau = o(h^{d/4})$. See more discussions in Remarks 3.10 and 3.11.

As is the case with CNFD (2.4–2.5) or LFFD (2.10–2.11), error estimates for SIFD1 (2.6–2.7) and SIFD2 (2.8–2.9) can be derived under the stability condition (3.5), with the details omitted for brevity.

THEOREM 3.4 (Error bounds of SIFD1). Under assumption (A) and the stability condition $\tau \leqslant \alpha \min\{\sqrt{2}/2, \sqrt{3}h/2\}$ $(0 < \alpha < 1)$, there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that for any $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, we have the following error estimates for SIFD1 (2.6–2.7) with (2.12) and (2.13):

$$\|\eta^n\|_{l^2} + \|\delta_x^+ \eta^n\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\mathbf{e}^n\|_{l^2} \lesssim h^2 + \tau^2, \tag{3.8}$$

$$\|\phi^n\|_{l^\infty} \leqslant 1 + N_\phi, \quad \|\Psi^n\|_{l^\infty} \leqslant 1 + N_\Psi, \quad 0 \leqslant n \leqslant \frac{T}{\tau}. \tag{3.9}$$

THEOREM 3.5 (Error bounds of SIFD2). Under assumption (A) and the stability condition $\tau \leqslant \alpha \min\{\sqrt{2}/2, \sqrt{3}h/2\}$ $(0 < \alpha < 1)$, there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that for any $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, we have the following error estimates for SIFD2 (2.8–2.9) with (2.12) and (2.13):

$$\|\eta^n\|_{l^2} + \|\delta_x^+ \eta^n\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\mathbf{e}^n\|_{l^2} \lesssim h^2 + \tau^2, \tag{3.10}$$

$$\|\phi^n\|_{l^\infty} \leqslant 1 + N_\phi, \quad \|\Psi^n\|_{l^\infty} \leqslant 1 + N_\Psi, \quad 0 \leqslant n \leqslant \frac{T}{\tau}. \tag{3.11}$$

REMARK 3.6 While we focus on the relativistic case $c = \mathcal{O}(1)$, Theorems 3.1, 3.2, 3.4, 3.5 can be extended to the nonrelativistic case $c \gg 1$, e.g., $\hbar = m_1 = 1$ in (1.1). However, as in the nonrelativistic case for the nonlinear Klein–Gordon equation and the (nonlinear) Dirac equation (Bao & Dong, 2012; Bao *et al.*, 2016; Bao *et al.*, 2017), the error estimates explicitly involve c, and there are extra difficulties in the analysis. The main difficulty is that the solution of the KGD system oscillates with wavelength $\mathcal{O}(c^{-2})$ and $\mathcal{O}(1)$ in time and space, respectively. When $c \gg 1$, the stability constraints for explicit/semiimplicit schemes LFFD, SIFD1 and SIFD2 become $\tau = \mathcal{O}(c^{-2})$ as those in Bao & Dong (2012), Bao *et al.* (2016), Bao *et al.* (2017), and the estimates for the FDTD methods are expected to be of the order $\mathcal{O}(ch^2 + c^6\tau^2)$, following the Klein–Gordon equation and the Dirac equation cases (Bao & Dong, 2012; Bao *et al.*, 2016; Bao *et al.*, 2017). However, the arguments shown in the current paper for the KGD system in the relativistic case $c = \mathcal{O}(1)$ cannot be directly generalized to cover the whole range of the relativistic and the nonrelativistic cases, where speed of light $c \geqslant 1$ and other techniques and tools have to be introduced for dealing with c-dependent estimates for $c \gg 1$. In addition, when $c \gg 1$, the solution of the KGD equation depends on c, which has to be taken into account. We will discuss the c-dependent estimates for the FDTD methods in detail elsewhere.

Based on the above theorems, the four FDTD methods studied here share the same second-order accuracy in temporal/spatial discretization. In particular, we can draw the following conclusions on the energy and mass preservations for the nonconservative FDTD schemes including LFFD and SIFD2.

LEMMA 3.7 Under the assumptions of Theorem 3.2 for LFFD (2.10–2.11), or the assumptions of Theorem 3.4 for SIFD2 (2.8–2.9), for the numerical solutions (ϕ^n, Ψ^n) $(0 \le n \le \frac{T}{\tau} - 1)$ to LFFD or SIFD2, we have the mass error as

$$\left| \|\Psi^n\|_{l^2}^2 - \|\Psi(0,\cdot)\|^2 \right| \lesssim \tau^2 + h^2. \tag{3.12}$$

For the energy of the numerical solution defined as (discretization of energy functional (1.12))

$$\begin{aligned}\widehat{\mathscr{E}}^n := &\frac{1}{2}\|\delta_t^+\phi^n\|_{l^2}^2 + \frac{1}{4}\left(\|\delta_x^+\phi^n\|_{l^2}^2 + \|\delta_x^+\phi^{n+1}\|_{l^2}^2\right) + \frac{1}{4}\left(\|\phi^n\|_{l^2}^2 + \|\phi^{n+1}\|_{l^2}^2\right)\\ &+ \frac{ih}{2}\sum_{j=0}^{M-1}\left[\left(\Psi_j^{n+1}\right)^*\sigma_1\delta_x\Psi_j^{n+1} + \left(\Psi_j^n\right)^*\sigma_1\delta_x\Psi_j^n\right] - \frac{\omega h}{2}\sum_{j=0}^{M-1}\left[\left(\Psi_j^{n+1}\right)^*\sigma_3\Psi_j^{n+1} + \left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right]\\ &- \frac{gh}{2}\sum_{j=0}^{M-1}\left[\phi_j^{n+1}\left(\Psi_j^{n+1}\right)^*\sigma_3\Psi_j^{n+1} + \phi_j^n\left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right],\end{aligned} \tag{3.13}$$

the error between $\widehat{\mathscr{E}}^n$ and the energy $\widehat{\mathscr{E}}(0)$ of the exact solution $(\phi(t,x), \Psi(t,x))$ given in (1.12) (restricted on bounded interval Ω) is bounded as

$$\left|\widehat{\mathscr{E}}^n - \widehat{\mathscr{E}}(0)\right| \lesssim \tau^2 + h^2. \tag{3.14}$$

We note that the proof of Lemma 3.7 is essentially contained in the proof of Theorem 3.2, where the error bounds on $\delta_t^+\phi^n$ are also derived. For simplicity of presentation we omit the proof of Lemma 3.7 here.

3.1 *The proof of Theorem* 3.1

Due to the indefiniteness of the Dirac operator $-i\sigma_1\partial_x + \omega\sigma_3$, the energy conservation of CNFD does not yield any *a priori* bound on the H^1 norm of the Dirac spinor fields Ψ^n. Thus, there is no control on the l^∞ norm of the numerical solution Ψ^n and the nonlinear term in one dimension by the Sobolev inequality and energy conservation, which is quite different from the classical conservative FDTD methods for nonlinear Schrödinger-type equations (Bao & Cai, 2012b, 2013; Wang *et al.*, 2013; Wang & Huang, 2015). However, we observe that the computations of the Dirac field Ψ_j^{n+1} and the Klein–Gordon field ϕ_j^{n+1} from time t_n to t_{n+1} in CNFD (2.4–2.5) can be decoupled, i.e., one first updates ϕ_j^{n+1} by solving (2.4), and then updates Ψ_j^{n+1} by solving (2.5). Hence, we can use mathematical induction to establish the error estimates of CNFD, where at each step only a single equation needs to be considered, and the nonlinear term depends only on the previous steps. The nonlinear part is then controlled by the l^∞ norms of the error functions from previous steps by means of the discrete Sobolev inequality and the inverse inequality.

We start with the local truncation errors of CNFD (2.4–2.5) $\zeta^n = (\zeta_0^n, \zeta_1^n, \ldots, \zeta_M^n)^{\mathrm{T}} \in \widetilde{X}_M$ and $\theta^n = (\theta_0^n, \theta_1^n, \ldots, \theta_M^n)^{\mathrm{T}} \in X_M$ given as

$$\zeta_j^0 := \delta_t^+ \phi^0(x_j) - \gamma(x_j) - \frac{\tau}{2}\left[\delta_x^2 \phi^0(x_j) - \phi^0(x_j) + g\big(\Psi^0(x_j)\big)^* \sigma_3 \Psi^0\big(x_j\big)\right], \tag{3.15}$$

$$\begin{aligned}\zeta_j^n &:= \delta_t^2 \phi\big(t_n, x_j\big) - \frac{1}{2}\delta_x^2\big(\phi\big(t_{n+1}, x_j\big) + \phi\big(t_{n-1}, x_j\big)\big) + \frac{1}{2}\big(\phi\big(t_{n+1}, x_j\big) + \phi\big(t_{n-1}, x_j\big)\big) \\ &\quad - g\Psi^*\big(t_n, x_j\big)\sigma_3 \Psi\big(t_n, x_j\big), \quad 1 \leqslant n \leqslant \frac{T}{\tau},\end{aligned} \tag{3.16}$$

$$\begin{aligned}\theta_j^n &:= i\delta_t^+ \Psi\big(t_n, x_j\big) + \frac{i}{2}\sigma_1 \delta_x\big(\Psi\big(t_{n+1}, x_j\big) + \Psi\big(t_n, x_j\big)\big) - \frac{\omega}{2}\sigma_3\big(\Psi\big(t_{n+1}, x_j\big) + \Psi\big(t_n, x_j\big)\big) \\ &\quad - \frac{g}{4}\big(\phi\big(t_{n+1}, x_j\big) + \phi\big(t_n, x_j\big)\big)\sigma_3\big(\Psi\big(t_{n+1}, x_j\big) + \Psi\big(t_n, x_j\big)\big), \quad 0 \leqslant n \leqslant \frac{T}{\tau}.\end{aligned} \tag{3.17}$$

The following estimates hold for ζ^n and θ^n.

LEMMA 3.8 (Local truncation errors of CNFD). Let $(\phi(t,x), \Psi(t,x))$ be the exact solution of KGD (2.1). Under assumption (A) there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that for any $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, the local truncation errors (3.15–3.17) satisfy

$$\|\zeta^n\|_{l^2} + \|\delta_x^+ \zeta^n\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\theta^n\|_{l^2} + \|\delta_x^+ \theta^n\|_{l^2} \lesssim h^2 + \tau^2, \quad 0 \leqslant n \leqslant \frac{T}{\tau}. \tag{3.18}$$

Proof. The essential tool is Taylor expansion. Under assumption (A) and noting (2.1), with the help of the triangle inequality and the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}
\big|\zeta_j^0\big| &\leqslant \frac{\tau^2}{6}\|\partial_{ttt}\phi\|_{L^\infty} + \frac{h\tau}{6}\big\|(\phi^0)'''\big\|_{L^\infty}, \\
\big|\delta_x^+\zeta_j^0\big| &\leqslant \frac{\tau^2}{6}\big\|\partial_{tttx}\phi\big\|_{L^\infty} + \frac{h\tau}{6}\big\|(\phi^0)''''\big\|_{L^\infty}, \\
\big|\zeta_j^{n+1}\big| &\leqslant \frac{\tau^2}{12}\|\partial_{tttt}\phi\|_{L^\infty} + \frac{\tau^2}{2}\big(\big\|\partial_{ttxx}\phi\big\|_{L^\infty} + \big\|\partial_{tt}\phi\big\|_{L^\infty}\big) + \frac{h^2}{12}\big\|\partial_{xxxx}\phi\big\|_{L^\infty}, \\
\big|\delta_x^+\zeta_j^{n+1}\big| &\leqslant \frac{\tau^2}{12}\big\|\partial_{ttttx}\phi\big\|_{L^\infty} + \frac{\tau^2}{2}\big(\big\|\partial_{ttxxx}\phi\big\|_{L^\infty} + \big\|\partial_{ttx}\phi\big\|_{L^\infty}\big) + \frac{h^2}{12}\big\|\partial_{xxxxx}\phi\big\|_{L^\infty}, \\
\big|\theta_j^n\big| &\leqslant \frac{\tau^2}{6}\big\|\partial_{ttt}\Psi\big\|_{L^\infty} + \frac{h^2}{6}\big\|\partial_{xxx}\Psi\big\|_{L^\infty} + \frac{\tau^2}{4}\big(\big\|\partial_{xtt}\Psi\big\|_{L^\infty} + \big\|\partial_{tt}\Psi\big\|_{L^\infty}\big) \\
&\quad + \frac{\tau^2}{4}g\big(\|\phi\|_{L^\infty}\big\|\partial_{tt}\Psi\big\|_{L^\infty} + \big\|\Psi\big\|_{L^\infty}\big\|\partial_{tt}\phi\big\|_{L^\infty} + \big\|\partial_t\phi\big\|_{L^\infty}\big\|\partial_t\Psi\big\|_{L^\infty}\big), \\
|\delta_x^+\theta_j^n| &\leqslant \frac{\tau^2}{6}\big\|\partial_{tttx}\Psi\big\|_{L^\infty} + \frac{h^2}{6}\big\|\partial_{xxxx}\Psi\big\|_{L^\infty} + \frac{\tau^2}{4}\big(\big\|\partial_{xxtt}\Psi\big\|_{L^\infty} + \big\|\partial_{ttx}\Psi\big\|_{L^\infty}\big) \\
&\quad + \frac{\tau^2}{4}g\big(\|\phi\|_{L^\infty}\big\|\partial_{ttx}\Psi\big\|_{L^\infty} + \|\Psi\|_{L^\infty}\big\|\partial_{ttx}\phi\big\|_{L^\infty} + \big\|\partial_x\phi\big\|_{L^\infty}\big\|\partial_{tt}\Psi\big\|_{L^\infty}\big) \\
&\quad + \frac{\tau^2}{4}g\big(\big\|\partial_x\Psi\big\|_{L^\infty}\big\|\partial_{tt}\phi\big\|_{L^\infty} + \big\|\partial_{tx}\phi\big\|_{L^\infty}\big\|\partial_t\Psi\big\|_{L^\infty} + \big\|\partial_t\phi\big\|_{L^\infty}\big\|\partial_{tx}\Psi\big\|_{L^\infty}\big),
\end{aligned}$$

where $L^\infty = L^\infty([0,T];L^\infty)$ for ζ_j^n, $L^\infty = L^\infty([0,T];[L^\infty]^2)$ for θ_j^n, $j = 0,1,\ldots,M-1$ and $0 \leqslant n \leqslant \frac{T}{\tau}$. These immediately imply

$$\|\zeta_j^n\|_{l^\infty} + \|\delta_x^+\zeta_j^n\|_{l^\infty} + \|\theta_j^n\|_{l^\infty} + \|\delta_x^+\theta_j^n\|_{l^\infty} \leqslant C\big(h^2+\tau^2\big), \quad 0 \leqslant n \leqslant \frac{T}{\tau}, \tag{3.19}$$

where the constant C is independent of h and τ. The conclusions for the local truncation errors follow. □

Next we study the growth of the error functions. Subtracting (2.4), (2.5) and (2.14) from (3.16), (3.17) and (3.15), respectively, noting (3.2), we have the error equations of CNFD as

$$\delta_t^2\eta_j^n - \frac{1}{2}\big(\delta_x^2\eta_j^{n+1} + \delta_x^2\eta_j^{n-1}\big) + \frac{1}{2}\big(\eta_j^{n+1} + \eta_j^{n-1}\big) = \zeta_j^n + \lambda_j^n, \quad 1 \leqslant n \leqslant \frac{T}{\tau}, \tag{3.20}$$

$$i\delta_t^+\mathbf{e}_j^n + \frac{i}{2}\sigma_1(\delta_x\mathbf{e}_j^{n+1} + \delta_x\mathbf{e}_j^n) - \frac{\omega}{2}\sigma_3(\mathbf{e}_j^{n+1} + \mathbf{e}_j^n) = \theta_j^n + \chi_j^n, \quad 0 \leqslant n \leqslant \frac{T}{\tau}, \tag{3.21}$$

$$\eta_0^n = \eta_M^n, \quad \eta_{-1}^n = \eta_{M-1}^n, \quad \eta_j^0 = 0, \quad \eta_j^1 = \tau\zeta_j^0, \quad j = 0,1,\ldots,M-1, \tag{3.22}$$

$$\mathbf{e}_0^n = \mathbf{e}_M^n, \quad \mathbf{e}_{-1}^n = \mathbf{e}_{M-1}^n, \quad \mathbf{e}_j^0 = 0, \quad j = 0,1,\ldots,M-1, \tag{3.23}$$

where $\lambda^n = (\lambda_0^n, \lambda_1^n, \ldots, \lambda_M^n)^{\mathrm{T}} \in \widetilde{X}_M$ and $\chi^n = (\chi_0^n, \chi_1^n, \ldots, \chi_M^n)^{\mathrm{T}} \in X_M$ are the nonlinear terms, which can be expressed as

$$\lambda_j^n := g\left[\Psi^*(t_n,x_j)\sigma_3\Psi(t_n,x_j) - (\Psi_j^n)^*\sigma_3\Psi_j^n\right], \tag{3.24}$$

$$\chi_j^n := g\left[\frac{1}{4}\Big(\phi\big(t_{n+1},x_j\big) + \phi\big(t_n,x_j\big)\Big)\sigma_3\Big(\Psi\big(t_{n+1},x_j\big) + \Psi\big(t_n,x_j\big)\Big) - \phi_j^{n+1/2}\sigma_3\Psi_j^{n+1/2}\right]. \tag{3.25}$$

Since the first step calculations are different from the others we investigate the first step separately.

Lemma 3.9 (Error bounds at $n = 1$ for CNFD). Under assumption (A), there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, such that for any $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$, we have the following error estimates for CNFD (2.4–2.5) with (2.12) and (2.13) when $n = 1$:

$$\|\eta^1\|_{l^2} + \|\delta_x^+\eta^1\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\mathbf{e}^1\|_{l^2} + \|\delta_x^+\mathbf{e}^1\|_{l^2} \lesssim h^2 + \tau^2, \tag{3.26}$$

$$\|\phi^1\|_{l^\infty} \leqslant 1 + N_\phi, \qquad \|\Psi^1\|_{l^\infty} \leqslant 1 + N_\Psi. \tag{3.27}$$

Proof. When $n = 1$, from (2.14), we can get

$$\|\eta^1\|_{l^\infty} = \tau\|\zeta^0\|_{l^\infty} \leqslant C\tau\big(\tau^2\|\partial_{ttt}\phi(t,x)\|_{L^\infty([0,T];L^\infty)} + h\tau\|(\phi^0)'''(x)\|_{L^\infty}\big), \tag{3.28}$$

$$\|\delta_x^+\eta^1\|_{l^\infty} = \tau\|\delta_x^+\zeta^0\|_{l^\infty} \leqslant C\tau\big(\tau^2\|\partial_{tttx}\phi(t,x)\|_{L^\infty([0,T];L^\infty)} + h\tau\|(\phi^0)''''(x)\|_{L^\infty}\big), \tag{3.29}$$

where the constant C is independent of h and τ. The estimates on η^1 and ϕ^1 are then obvious for sufficiently small h and τ, with the additional bound

$$\|\delta_x^+\phi^1\|_{l^\infty} \leqslant \|\partial_x\phi(\tau,x)\|_{L^\infty([0,T];L^\infty)} + \|\delta_x^+\eta^1\|_{l^\infty} \lesssim 1. \tag{3.30}$$

Therefore, we have

$$\begin{aligned}
\left|\delta_x^+\chi_j^0\right| &= \frac{g}{4}\left|\delta_x^+(\eta_j^1\sigma_3(\Psi(\tau,x_j)+\Psi(0,x_j))) + \delta_x^+\left((\phi_j^1+\phi_j^0)\sigma_3\mathbf{e}_j^1\right)\right| \\
&\leqslant \frac{g}{4}\Big(2N_\Psi\left|\delta_x^+\eta_j^1\right| + 2\|\partial_x\Psi\|_{L^\infty([0,\tau];[L^\infty]^2)}\left|\eta_j^1\right| + \|\phi^1+\phi^0\|_{l^\infty}\left|\delta_x^+\mathbf{e}_j^1\right| \\
&\qquad + \|\delta_x^+(\phi^1+\phi^0)\|_{l^\infty}\left|\mathbf{e}_j^1\right|\Big) \\
&\leqslant C\left(\left|\eta_j^1\right| + \left|\delta_x^+\eta_j^1\right| + \left|\mathbf{e}_j^1\right| + \left|\delta_x^+\mathbf{e}_j^1\right|\right), \quad j=0,1,\ldots,M-1.
\end{aligned} \tag{3.31}$$

Next, by definition, $\mathbf{e}^0 = \mathbf{0} \in X_M$. For $n=1$, the error equation (3.21) collapses to

$$\frac{i}{\tau}\mathbf{e}_j^1 + \frac{i}{2}\sigma_1\delta_x\mathbf{e}_j^1 - \frac{\omega}{2}\sigma_3\mathbf{e}_j^1 = \theta_j^0 + \chi_j^0. \tag{3.32}$$

Multiplying $h\tau(\mathbf{e}_j^1)^*$ from the left on both sides of (3.32), summing over j and taking the imaginary parts, we can derive the estimate for $\|\mathbf{e}^1\|_{l^2}$ by Young's inequality and the triangle inequality,

$$\begin{aligned}
\|\mathbf{e}^1\|_{l^2}^2 &= \mathrm{Im}\left[h\tau\sum_{j=0}^{M-1}\left(\mathbf{e}_j^1\right)^*\left(\theta_j^0 + \frac{g}{4}\eta_j^1\sigma_3\left(\Psi(\tau,x_j)+\Psi(0,x_j)\right)\right)\right] \\
&\leqslant \frac{1}{2}\|\mathbf{e}^1\|_{l^2}^2 + \tau^2\left(\|\theta^0\|_{l^2}^2 + \frac{g^2}{4}N_\Psi^2\|\eta^1\|_{l^2}^2\right),
\end{aligned}$$

where $\mathrm{Im}(f)$ denotes the imaginary part of f. The above inequality results in

$$\|\mathbf{e}^1\|_{l^2}^2 \leqslant 2\tau^2\left(\|\theta^0\|_{l^2}^2 + \frac{g^2}{4}N_\Psi^2\|\eta^1\|_{l^2}^2\right) \lesssim \tau^2\left(\tau^2+h^2\right)^2. \tag{3.33}$$

Similarly to above, multiplying $h\tau(\delta_x^2\mathbf{e}_j^1)^*$ on both sides of (3.32) from the left, summing over j and taking the imaginary parts, noting (3.31), we have

$$\begin{aligned}
\|\delta_x^+\mathbf{e}^1\|_{l^2}^2 &= \mathrm{Im}\left[h\tau\sum_{j=0}^{M-1}\left(\delta_x^+\mathbf{e}_j^1\right)^*\delta_x^+(\theta_j^0+\chi_j^0)\right] \\
&\leqslant C\tau\left(\|\delta_x^+\mathbf{e}^1\|_{l^2}^2 + \|\delta_x^+\theta^0\|_{l^2}^2 + \|\eta^1\|_{l^2}^2 + \|\delta_x^+\eta^1\|_{l^2}^2 + \|\mathbf{e}^1\|_{l^2}^2\right),
\end{aligned}$$

and for sufficiently small τ, such that $C\tau \leqslant \frac{1}{2}$ in the above inequality, Lemma 3.8, (3.28), (3.29) and (3.33) will imply

$$\left\|\delta_x^+\mathbf{e}^1\right\|_{l^2}^2 \lesssim \tau\left(h^2+\tau^2\right)^2. \tag{3.34}$$

Thus, the error estimates on $\mathbf{e}^1$ are proved. It remains to show (3.27) for Ψ^1. Using the Sobolev inequality in one dimension we have, for sufficiently small τ and h,

$$\left\|\mathbf{e}^1\right\|_{l^\infty} \leqslant C\left\|\mathbf{e}^1\right\|_{l^2}^{1/2}\left(\left\|\delta_x^+\mathbf{e}^1\right\|_{l^2}+\left\|\mathbf{e}^1\right\|_{l^2}\right)^{1/2} \leqslant C\left(h^2+\tau^2\right) \leqslant 1,$$

and $\|\Psi^1\|_{l^\infty} \leqslant \|\Psi(t,x)\|_{L^\infty([0,T];[L^\infty]^2)} + \|\mathbf{e}^1\|_{l^\infty} \leqslant N_\Psi + 1$. □

We now proceed to prove Theorem 3.1 by mathematical induction, i.e., we will show for sufficiently small $\tau_0 > 0$ and $h_0 > 0$ to be specified later, when $0 < \tau < \tau_0$ and $0 < h < h_0$, the error bounds hold as

$$\|\eta^n\|_{l^2} + \left\|\delta_x^+\eta^n\right\|_{l^2} \leqslant C_1\left(h^2+\tau^2\right), \qquad \|\mathbf{e}^n\|_{l^2} \leqslant C_1\left(h^2+\tau^2\right), \tag{3.35}$$

$$\|\phi^n\|_{l^\infty} \leqslant 1 + N_\phi, \qquad \|\Psi^n\|_{l^\infty} \leqslant 1 + N_\Psi, \tag{3.36}$$

for all $0 \leqslant n \leqslant \frac{T}{\tau}$, where the constant C_1 will be determined later and depends only on T, g and the exact solution $(\phi(t,x), \Psi(t,x))$ but is independent of h and τ.

As the first step in the induction process, we need to prove that, under the hypothesis that (3.35–3.36) hold for all n satisfying $0 \leqslant n \leqslant m$ $(1 \leqslant m \leqslant \frac{T}{\tau} - 1)$, estimates (3.35–3.36) still hold for $n = m+1$. In order to verify this by the energy method we study the error of the nonlinear terms in advance. For $j = 0, 1, \ldots, M-1$, with the help of the triangle inequality and the induction hypothesis, (3.24) and (3.25) imply

$$\begin{aligned}\left|\lambda_j^n\right| &= g\left|\Psi^*(t_n,x_j)\sigma_3\mathbf{e}_j^n + \left(\mathbf{e}_j^n\right)^*\sigma_3\Psi_j^n\right| \leqslant g\left(\|\Psi(t,x)\|_{L^\infty([0,T];[L^\infty]^2)} + \|\Psi^n\|_{l^\infty}\right)\left|\mathbf{e}_j^n\right| \\ &\leqslant \tilde{C}_1|\mathbf{e}_j^n|, \quad 0 \leqslant n \leqslant m,\end{aligned} \tag{3.37}$$

$$\begin{aligned}|\chi_j^n| &= g\left|\frac{1}{2}\eta_j^{n+1/2}\sigma_3\left(\Psi\left(t_{n+1},x_j\right)+\Psi\left(t_n,x_j\right)\right) + \phi_j^{n+1/2}\sigma_3\mathbf{e}_j^{n+1/2}\right| \\ &\leqslant g\left[\|\Psi(t,x)\|_{L^\infty([0,T];[L^\infty]^2)}\left|\eta_j^{n+1/2}\right| + \frac{1}{2}\left(\|\phi^{n+1}\|_{l^\infty} + \|\phi^n\|_{l^\infty}\right)\left|\mathbf{e}_j^{n+1/2}\right|\right] \\ &\leqslant \tilde{C}_1\left(\left|\eta_j^{n+1/2}\right| + \left|\mathbf{e}_j^{n+1/2}\right|\right), \quad 0 \leqslant n \leqslant m-1,\end{aligned} \tag{3.38}$$

where $\tilde{C}_1$ depends only on g, N_Ψ and N_ϕ.

The error equations (3.20–3.21), together with (3.37) and (3.38), indicate that η^{m+1} can be estimated by (3.20) and the information of ζ^n, η^n, Ψ^n and $\mathbf{e}^n$ from the previous steps $0 \leqslant n \leqslant m$; meanwhile, $\mathbf{e}^{m+1}$ can be controlled by (3.21) and the estimates of ϕ^{m+1} and θ^n, $\mathbf{e}^n$, η^n, ϕ^n from the previous steps $0 \leqslant n \leqslant m$. Hence, we have to estimate η^{m+1} before $\mathbf{e}^{m+1}$.

Step 1. (Estimate $\|\eta^{m+1}\|_{l^2} + \|\delta_x^+\eta^{m+1}\|_{l^2}$ and $\|\phi^{m+1}\|_{l^\infty}$). Computing the product of (3.20) with $h(\eta_j^{n+1} - \eta_j^{n-1})$, summing over j, making use of (3.37), the summation by parts formula, the Cauchy inequality and Lemma 3.8, we obtain for $1 \leqslant n \leqslant m$,

$$\begin{aligned}
&\left(\|\delta_t^+\eta^n\|_{l^2}^2 - \|\delta_t^+\eta^{n-1}\|_{l^2}^2\right) + \frac{1}{2}\left(\|\delta_x^+\eta^{n+1}\|_{l^2}^2 - \|\delta_x^+\eta^{n-1}\|_{l^2}^2\right) + \frac{1}{2}\left(\|\eta^{n+1}\|_{l^2}^2 - \|\eta^{n-1}\|_{l^2}^2\right) \\
&\quad = h\sum_{j=0}^{M-1}\left(\zeta_j^n + \lambda_j^n\right)\left(\eta_j^{n+1} - \eta_j^{n-1}\right) \leqslant \tau\left(\|\zeta^n\|_{l^2}^2 + \|\delta_t^+\eta^n\|_{l^2}^2 + \|\delta_t^+\eta^{n-1}\|_{l^2}^2 + \|\lambda^n\|_{l^2}^2\right) \\
&\quad \leqslant \tau\left(\|\delta_t^+\eta^n\|_{l^2}^2 + \|\delta_t^+\eta^{n-1}\|_{l^2}^2\right) + \tau\tilde{C}_1^2\|\mathbf{e}^n\|_{l^2}^2 + \tilde{C}_2\tau\left(\tau^2 + h^2\right)^2, \qquad (3.39)
\end{aligned}$$

where the constant $\tilde{C}_2$ is independent of h and τ. Multiplying both sides of (3.21) from the left by $2h\tau(\mathbf{e}_j^{n+1/2})^*$, taking the imaginary parts and summing over j, using the triangle inequality, Young's inequality, together with (3.38) and Lemma 3.8, we derive for sufficiently small τ and $0 \leqslant n \leqslant m-1$,

$$\begin{aligned}
\|\mathbf{e}^{n+1}\|_{l^2}^2 - \|\mathbf{e}^n\|_{l^2}^2 &\leqslant h\tau\sum_{j=0}^{M-1}\left(|\theta_j^n| + |\chi_j^n|\right)\left(|\mathbf{e}_j^{n+1}| + |\mathbf{e}_j^n|\right) \\
&\leqslant \left(2\tilde{C}_1^2 + 1\right)\tau\left(\|\mathbf{e}^{n+1}\|_{l^2}^2 + \|\mathbf{e}^n\|_{l^2}^2 + \|\eta^{n+1}\|_{l^2}^2 + \|\eta^n\|_{l^2}^2\right) + \frac{\tau}{2}\|\theta^n\|_{l^2}^2 \\
&\leqslant \left(2\tilde{C}_1^2 + 1\right)\tau\sum_{k=n}^{n+1}\left(\|\mathbf{e}^k\|_{l^2}^2 + \|\eta^k\|_{l^2}^2\right) + \tilde{C}_3\tau\left(\tau^2 + h^2\right)^2, \qquad (3.40)
\end{aligned}$$

with $\tilde{C}_3$ being a constant independent of h and τ.

Denote

$$\mathscr{S}^n = \|\delta_t^+\eta^n\|_{l^2}^2 + \frac{1}{2}\left(\|\delta_x^+\eta^{n+1}\|_{l^2}^2 + \|\delta_x^+\eta^n\|_{l^2}^2\right) + \frac{1}{2}\left(\|\eta^{n+1}\|_{l^2}^2 + \|\eta^n\|_{l^2}^2\right) + \|\mathbf{e}^n\|_{l^2}^2, \quad n \geqslant 0. \quad (3.41)$$

Noticing the initial data (3.22–3.23) and Lemma 3.8, we get

$$\begin{aligned}
\mathscr{S}^0 &= \|\delta_t^+\eta^0\|_{l^2}^2 + \frac{1}{2}\|\delta_x^+\eta^1\|_{l^2}^2 + \frac{1}{2}\|\eta^1\|_{l^2}^2 = \|\zeta^0\|_{l^2}^2 + \frac{\tau^2}{2}\|\delta_x^+\zeta^0\|_{l^2}^2 + \frac{\tau^2}{2}\|\zeta^0\|_{l^2}^2 \\
&\leqslant \tilde{C}_4\left(\tau^2 + h^2\right)^2, \qquad (3.42)
\end{aligned}$$

where $\tilde{C}_4$ is independent of h and τ. Inequalities (3.39) and (3.40) lead to

$$\mathscr{S}^n - \mathscr{S}^{n-1} \leqslant \tau\tilde{C}_5\left(\mathscr{S}^n + \mathscr{S}^{n-1}\right) + \tau\tilde{C}_6\left(\tau^2 + h^2\right)^2, \quad 1 \leqslant n \leqslant m, \qquad (3.43)$$

where $\tilde{C}_5$ and $\tilde{C}_6$ are independent of h and τ. Summing the above inequality for time steps from 1 to n, we have

$$\mathscr{S}^n - \mathscr{S}^0 \leqslant 2\tilde{C}_5\tau\sum_{k=0}^{n}\mathscr{S}^k + \tilde{C}_6 T\left(\tau^2 + h^2\right)^2, \quad 1 \leqslant n \leqslant m \leqslant \frac{T}{\tau} - 1. \qquad (3.44)$$

Hence, the discrete Grönwall's inequality (Pachpatte, 2002; Holte, 2009) suggests that there exists a constant $\tau_1 > 0$, such that when $0 < \tau \leqslant \tau_1$, the following holds:

$$\mathscr{S}^n \leqslant \tilde{C}_7 e^{(n+1)\tilde{C}_8\tau}\big(\tau^2 + h^2\big)^2, \quad 0 \leqslant n \leqslant m \leqslant \frac{T}{\tau} - 1, \tag{3.45}$$

for some constants $\tilde{C}_7$ and $\tilde{C}_8$ independent of h and τ.

Choosing $n = m$ in (3.45), in view of (3.41) we obtain

$$\big\|\eta^{m+1}\big\|_{l^2}^2 + \big\|\delta_x^+\eta^{m+1}\big\|_{l^2}^2 \leqslant 2\tilde{C}_7 e^{(m+1)\tilde{C}_8\tau}\big(\tau^2 + h^2\big)^2, \quad 0 \leqslant m \leqslant \frac{T}{\tau} - 1 \tag{3.46}$$

and

$$\big\|\eta^{m+1}\big\|_{l^2} + \big\|\delta_x^+\eta^{m+1}\big\|_{l^2} \leqslant 2\sqrt{\tilde{C}_7} e^{\tilde{C}_8 T/2}\big(\tau^2 + h^2\big). \tag{3.47}$$

The discrete Sobolev inequality will imply

$$\big\|\eta^{m+1}\big\|_{l^\infty} \leqslant C\big\|\eta^{m+1}\big\|_{l^2}^{\frac{1}{2}} \cdot \big(\big\|\eta^{m+1}\big\|_{l^2} + \big\|\delta_x^+\eta^{m+1}\big\|_{l^2}\big)^{\frac{1}{2}} \leqslant 2C\sqrt{\tilde{C}_7} e^{T\tilde{C}_8/2}(\tau^2 + h^2). \tag{3.48}$$

Thus, there exist constants $h_1 > 0$ and $\tau_2 > 0$ sufficiently small depending on $\tilde{C}_7$ and $\tilde{C}_8$, such that when $0 < h \leqslant h_1$ and $0 < \tau \leqslant \min\{\tau_1, \tau_2\}$ we get

$$\big\|\phi^{m+1}\big\|_{l^\infty} \leqslant \big\|\phi(t_{m+1}, x)\big\|_{L^\infty([0,T];L^\infty)} + \big\|\eta^{m+1}\big\|_{l^\infty} \leqslant N_\phi + 1. \tag{3.49}$$

Now, we have proved the estimates for η^{m+1} and ϕ^{m+1} in (3.35) and (3.36). It remains to show the estimates on $\mathbf{e}^{m+1}$ and Ψ^{m+1}.

Step 2. (Estimate $\|\mathbf{e}^{m+1}\|_{l^2}$). From Step 1, we have $\|\phi^{m+1}\|_{l^\infty} \leqslant N_\phi + 1$ and the control on χ^n (3.38) is now valid for all $0 \leqslant n \leqslant m$. As a consequence, (3.40) holds for $0 \leqslant n \leqslant m$.

Summing inequality (3.40) together for time steps $0, 1, \ldots, n$, noting $\mathbf{e}^0 = \mathbf{0}$ and (3.47), which also holds for all $0 \leqslant n \leqslant m + 1$, we have

$$\big\|\mathbf{e}^{n+1}\big\|_{l^2}^2 \leqslant \big(2\tilde{C}_1^2 + 1\big)\tau \sum_{k=0}^{n+1} \|\mathbf{e}^k\|_{l^2}^2 + \tilde{C}_9 T\big(\tau^2 + h^2\big)^2, \quad 1 \leqslant n \leqslant m, \tag{3.50}$$

where $\tilde{C}_9$ is independent of h and τ. Using the discrete Grönwall's inequality, we deduce that there exists $\tau_3 > 0$ sufficiently small, such that when $0 < \tau \leqslant \min\{\tau_1, \tau_2, \tau_3\}$,

$$\big\|\mathbf{e}^{n+1}\big\|_{l^2} \leqslant \tilde{C}_{10} e^{(n+1)\tilde{C}_{11}\tau}\big(\tau^2 + h^2\big), \quad 0 \leqslant n \leqslant m \leqslant \frac{T}{\tau} - 1 \tag{3.51}$$

and

$$\big\|\mathbf{e}^{m+1}\big\|_{l^2} \leqslant \tilde{C}_{10} e^{(m+1)\tilde{C}_{11}\tau}\big(\tau^2 + h^2\big), \quad m \leqslant \frac{T}{\tau} - 1, \tag{3.52}$$

where the constants $\tilde{C}_{10}$ and $\tilde{C}_{11}$ are independent of h and τ. Thus, we are left with the estimate of $\|\Psi^{m+1}\|_{l^\infty}$.

Step 3 (Estimate $\|\Psi^{m+1}\|_{l^\infty}$). By the inverse inequality in one dimension we can get for $m \leqslant \frac{T}{\tau} - 1$,

$$\left\|\mathbf{e}^{m+1}\right\|_{l^\infty} \leqslant \frac{1}{\sqrt{h}}\left\|\mathbf{e}^{m+1}\right\|_{l^2} \leqslant \tilde{C}_{10} e^{\tilde{C}_{11}T}\frac{\tau^2+h^2}{\sqrt{h}}. \tag{3.53}$$

On the other hand, by using the triangle inequality, the error equation (3.21) implies for $0 \leqslant n \leqslant m$,

$$\begin{aligned}\left\|\delta_x(\mathbf{e}^{n+1}+\mathbf{e}^n)\right\|_{l^2} &\leqslant \tilde{C}_{12}\left(\left\|\delta_t^+\mathbf{e}^n\right\|_{l^2}+\left\|\mathbf{e}^{n+1}\right\|_{l^2}+\|\mathbf{e}^n\|_{l^2}+\left\|\eta^{n+1}\right\|_{l^2}+\|\eta^n\|_{l^2}+\|\theta^n\|_{l^2}\right)\\ &\leqslant \tilde{C}_{12}\left(\frac{\left\|\mathbf{e}^{n+1}\right\|_{l^2}+\|\mathbf{e}^n\|_{l^2}}{\tau}+\tilde{C}_{13}\left(\tau^2+h^2\right)\right)\leqslant \tilde{C}_{14}\frac{\tau^2+h^2}{\tau}\end{aligned}$$

for sufficiently small τ and the constants $\tilde{C}_{12}, \tilde{C}_{13}, \tilde{C}_{14}$ are independent of h and τ. The Sobolev inequality gives that for $n \leqslant m$,

$$\begin{aligned}&\|\mathbf{e}^{n+1}\|_{l^\infty}-\|\mathbf{e}^n\|_{l^\infty} \leqslant \|\mathbf{e}^{n+1}+\mathbf{e}^n\|_{l^\infty}\\ &\qquad\leqslant C\left\|\mathbf{e}^{n+1}+\mathbf{e}^n\right\|_{l^2}^{\frac{1}{2}}\cdot\left(\left\|\mathbf{e}^{n+1}+\mathbf{e}^n\right\|_{l^2}+\left\|\delta_x\left(\mathbf{e}_j^{n+1}+\mathbf{e}_j^n\right)\right\|_{l^2}\right)^{\frac{1}{2}} \leqslant \tilde{C}_{15}\frac{\tau^2+h^2}{\sqrt{\tau}},\end{aligned} \tag{3.54}$$

with some constant $\tilde{C}_{15}$ that is independent of h and τ. Summing the above inequality together for $n = 0, \ldots, m$, we have

$$\left\|\mathbf{e}^{m+1}\right\|_{l^\infty} \leqslant \tilde{C}_{15}(m+1)\frac{\tau^2+h^2}{\sqrt{\tau}} \leqslant \tilde{C}_{15}T\frac{\tau^2+h^2}{\tau^{\frac{3}{2}}}. \tag{3.55}$$

Thus, for $m \leqslant \frac{T}{\tau} - 1$, in view of (3.53) and (3.55), we have

$$\begin{aligned}\left\|\mathbf{e}^{m+1}\right\|_{l^\infty} &\leqslant \tilde{C}_{16}\min\left\{\frac{\tau^2+h^2}{\tau^{\frac{3}{2}}}, \frac{\tau^2+h^2}{\sqrt{h}}\right\} \leqslant \tilde{C}_{16}\min\left\{\frac{h^2}{\tau^{\frac{3}{2}}}+\tau^{\frac{1}{2}}, \frac{\tau^2}{\sqrt{h}}+h^{\frac{3}{2}}\right\}\\ &\leqslant \tilde{C}_{16}\left(2\tau^{\frac{1}{4}}h^{\frac{3}{4}}+\tau^{\frac{1}{2}}+h^{\frac{3}{2}}\right),\end{aligned} \tag{3.56}$$

where $\tilde{C}_{16} = \max\{\tilde{C}_{15}T, \tilde{C}_{10}e^{\tilde{C}_{11}T}\}$. Therefore, it is easy to find that there exist constants $h_2 > 0$ and $\tau_4 > 0$, such that when $0 < h \leqslant \min\{h_1, h_2\}$ and $0 < \tau \leqslant \min\{\tau_1, \tau_2, \tau_3, \tau_4\}$, $\|\mathbf{e}^{m+1}\|_{l^\infty} \leqslant 1$ and

$$\left\|\Psi^{m+1}\right\|_{l^\infty} \leqslant \left\|\Psi(t_{m+1}, x)\right\|_{L^\infty([0,T];[L^\infty]^2)} + \left\|\mathbf{e}^{m+1}\right\|_{l^\infty} \leqslant N_\Psi + 1. \tag{3.57}$$

Now, we have all the estimates in (3.35–3.36) at $n = m+1$, if $C_1 \geqslant \max\{2\sqrt{\tilde{C}_7}e^{\tilde{C}_8T/2}, \tilde{C}_{10}e^{\tilde{C}_{11}T}\}$.

To complete the proof we need only to verify the $m = 1$ case, i.e., (3.35–3.36) holds for $n = 0, 1$. This has been done in Lemma 3.9 ($n = 0$ is obvious), i.e., there exist constants $\tilde{C}_{17}$ (independent of

h and τ), $\tau_5 > 0$ and $h_3 > 0$, such that for $0 < \tau \leqslant \tau_5$ and $0 < h \leqslant h_3$,

$$\|\eta^1\|_{l^2} + \|\delta_x^+\eta^1\|_{l^2} + \|\mathbf{e}^1\|_{l^2} \leqslant \tilde{C}_{17}(\tau^2 + h^2), \quad \|\phi^1\|_{l^\infty} \leqslant N_\phi + 1, \quad \|\Psi^1\|_{l^\infty} \leqslant N_\Psi + 1. \tag{3.58}$$

Therefore, by selecting $C_1 = \max\{2\sqrt{\tilde{C}_7}e^{\tilde{C}_8 T/2}, \tilde{C}_{10}e^{\tilde{C}_{11}T}, \tilde{C}_{17}\}$ in (3.35–3.36), we complete the mathematical induction process, and (3.35–3.36) are valid for all $0 \leqslant n \leqslant \frac{T}{\tau}$ with $h_0 = \min\{h_1, h_2, h_3\}$ and $\tau_0 = \min\{\tau_1, \tau_2, \tau_3, \tau_4, \tau_5\}$. The proof is finished.

REMARK 3.10 In the two-dimensional ($d = 2$) and three-dimensional ($d = 3$) cases the above proof still works with minor modifications. The key is to control $\|\eta^n\|_{l^\infty}$ in (3.48) by the discrete Sobolev inequalities (Thomée, 2006) in two dimensions and three dimensions as

$$\|f_h\|_{l^\infty} \lesssim C_d(h)\, \|f_h\|_{H^1}, \quad d = 2, 3, \tag{3.59}$$

where $C_d(h) = |\ln h|$ when $d = 2$ and $C_d(h) = h^{-1/2}$ when $d = 3$, f_h is a periodic two-dimensional/three-dimensional mesh function. For $\|\mathbf{e}^n\|_{l^\infty}$, the inverse inequality used in (3.53) in two dimensions and three dimensions becomes

$$\|f_h\|_{l^\infty} \leqslant h^{-d/2}\|f_h\|_{l^2}. \tag{3.60}$$

Thus, by assuming the additional conditions $\tau = o(h^{1/2})$ in two dimensions and $\tau = o(h^{3/4})$ in three dimensions, a similar proof will give the conclusions in Theorem 3.1.

3.2 *The proof of Theorem* 3.2

For the explicit LFFD (2.10–2.11) we can establish the error estimates in Theorem 3.2. Here we sketch the proof and omit those parts similar to the proof of Theorem 3.1 for CNFD. Throughout this section, the stability condition (3.5) is assumed. We use similar notation to that in Section 3.1.

Define the local truncation errors $\zeta^n = (\zeta_0^n, \zeta_1^n, \ldots, \zeta_M^n)^{\mathrm{T}} \in \widetilde{X}_M$ and $\theta^n = (\theta_0^n, \theta_1^n, \ldots, \theta_M^n)^{\mathrm{T}} \in X_M$ ($n \geqslant 0$) of LFFD (2.10–2.11) as

$$\zeta_j^0 := \delta_t^+\phi^0(x_j) - \gamma(x_j) - \frac{\tau}{2}\left[\delta_x^2\phi^0(x_j) - \phi^0(x_j) + g\big(\Psi^0(x_j)\big)^*\sigma_3\Psi^0(x_j)\right], \tag{3.61}$$

$$\zeta_j^n := \delta_t^2\phi(t_n, x_j) - \delta_x^2\phi(t_n, x_j) + \phi(t_n, x_j) - g\Psi^*(t_n, x_j)\sigma_3\Psi(t_n, x_j), \quad n \geqslant 1, \tag{3.62}$$

$$\theta_j^0 := \delta_t^+\Psi^0(x_j) + \sigma_1\delta_x^+\Psi^0(x_j) + i\left[\omega + g\phi^0(x_j)\right]\sigma_3\Psi^0(x_j), \tag{3.63}$$

$$\theta_j^n := i\delta_t\Psi(t_n, x_j) + \left[i\sigma_1\delta_x - \omega\sigma_3\right]\Psi(t_n, x_j) - g\phi(t_n, x_j)\sigma_3\Psi(t_n, x_j), \quad n \geqslant 1, \tag{3.64}$$

for $j = 0, 1, \ldots, M-1$. The error equations for LFFD (2.10–2.11) can be derived as

$$\delta_t^2\eta_j^n - \delta_x^2\eta_j^n + \eta_j^n = \zeta_j^n + \lambda_j^n, \quad \eta_0^n = \eta_M^n, \quad \eta_{-1}^n = \eta_{M-1}^n, \quad \eta_j^0 = 0, \quad \eta_j^1 = \tau\zeta_j^0, \tag{3.65}$$

$$i\delta_t\mathbf{e}_j^n + i\sigma_1\delta_x\mathbf{e}_j^n - \omega\sigma_3\mathbf{e}_j^n = \theta_j^n + \chi_j^n, \quad \mathbf{e}_0^n = \mathbf{e}_M^n, \quad \mathbf{e}_{-1}^n = \mathbf{e}_{M-1}^n, \quad \mathbf{e}_j^0 = 0, \quad \mathbf{e}_j^1 = \tau\theta_j^0, \tag{3.66}$$

where $j = 0, 1, \ldots, M-1$, $n \geqslant 1$, $\lambda^n = (\lambda_0^n, \lambda_1^n, \ldots, \lambda_M^n)^{\mathrm{T}} \in \widetilde{X}_M$ and $\chi^n = (\chi_0^n, \chi_1^n, \ldots, \chi_M^n)^{\mathrm{T}} \in X_M$ are the errors of the nonlinear terms in LFFD (2.10–2.11) where

$$\lambda_j^n := g\left[\Psi^*\left(t_n, x_j\right)\sigma_3\Psi\left(t_n, x_j\right) - \left(\Psi_j^n\right)^*\sigma_3\Psi_j^n\right], \quad n \geqslant 1, \tag{3.67}$$

$$\chi_j^n := g\left[\phi\left(t_n, x_j\right)\sigma_3\Psi\left(t_n, x_j\right) - \phi_j^n\sigma_3\Psi_j^n\right], \quad n \geqslant 1. \tag{3.68}$$

Similarly to Lemma 3.8, under assumption (A), we have estimates on the local truncation errors of LFFD (2.10–2.11):

$$\|\zeta^n\|_{l^2} + \left\|\delta_x^+\zeta^n\right\|_{l^2} \lesssim h^2 + \tau^2, \quad \|\theta^n\|_{l^2} + \left\|\delta_x^+\theta^n\right\|_{l^2} \lesssim h^2 + \tau^2, \quad 0 \leqslant n \leqslant \frac{T}{\tau}. \tag{3.69}$$

For $n = 1$, the error equations (3.65–3.66) imply

$$\left\|\eta^1\right\|_{l^2}^2 = \tau^2\left\|\zeta^0\right\|_{l^2}^2, \quad \left\|\delta_x^+\eta^1\right\|_{l^2}^2 = \tau^2\left\|\delta_x^+\zeta^0\right\|_{l^2}^2 \quad \text{and} \quad \left\|\mathbf{e}^1\right\|_{l^2}^2 = \tau^2\left\|\theta^0\right\|_{l^2}^2,$$

and

$$\left\|\eta^1\right\|_{l^2}^2 + \left\|\delta_x^+\eta^1\right\|_{l^2}^2 + \left\|\mathbf{e}^1\right\|_{l^2}^2 \leqslant \tilde{C}_1\left(h^2 + \tau^2\right)^2, \tag{3.70}$$

i.e., (3.6) holds. Under the stability condition (3.5), the inverse inequality then yields

$$\left\|\mathbf{e}^1\right\|_{l^\infty} \leqslant h^{-1/2}\left\|\mathbf{e}^1\right\|_{l^2} \leqslant \sqrt{\tilde{C}_1}\left(h^{3/2} + 3/4h^{3/2}\right), \quad \left\|\eta^1\right\|_{l^\infty} \leqslant \sqrt{\tilde{C}_1}\left(h^{3/2} + 3/4h^{3/2}\right),$$

and there exists a constant $h_1 > 0$, such that when $0 < h \leqslant h_1$, $\|\mathbf{e}^1\|_{l^\infty} \leqslant 1$ and $\|\eta^1\|_{l^\infty} \leqslant 1$, which verifies (3.7) in view of the triangle inequality and assumption (A). In other words, the conclusions in Theorem 3.2 hold for $n = 1$.

We adopt mathematical induction to prove Theorem 3.2, i.e., we want to show that there exist $h_0 > 0$ and $\tau_0 > 0$, such that when $0 < h \leqslant h_0$ and $0 < \tau \leqslant \tau_0$ under the stability condition $\tau \leqslant \alpha\min\{\sqrt{2}/2, \sqrt{3}h/2\}$, the error bounds hold as

$$\|\eta^n\|_{l^2} + \left\|\delta_x^+\eta^m\right\|_{l^2} \leqslant C_1\left(h^2 + \tau^2\right), \quad \|\mathbf{e}^n\|_{l^2} \leqslant C_1\left(h^2 + \tau^2\right), \tag{3.71}$$

$$\|\phi^n\|_{l^\infty} \leqslant 1 + N_\phi, \qquad \|\Psi^n\|_{l^\infty} \leqslant 1 + N_\Psi, \tag{3.72}$$

for all $0 \leqslant n \leqslant \frac{T}{\tau}$, where C_1, τ_0 and h_0 will be classified later. It has been shown that (3.71–3.72) are true for $n = 0, 1$ ($n = 0$ is trivial) if $h_0 \leqslant h_1$ and $C_1 \geqslant \sqrt{\tilde{C}_1}$.

We need to prove only that (3.71–3.72) are still valid for LFFD (2.10–2.11) when $n = m + 1$ ($1 \leqslant m \leqslant \frac{T}{\tau} - 1$) under the hypothesis that (3.71–3.72) are valid for all n satisfying $0 \leqslant n \leqslant m$. For the time steps $0 \leqslant n \leqslant m$, the errors of the nonlinear terms can be controlled as

$$\|\lambda^n\|_{l^2}^2 \leqslant \tilde{C}_2\|\mathbf{e}^n\|_{l^2}^2, \quad \|\chi^n\|_{l^2}^2 \leqslant \tilde{C}_2\left(\|\mathbf{e}^n\|_{l^2}^2 + \|\eta^n\|_{l^2}^2\right), \quad 1 \leqslant n \leqslant m \leqslant \frac{T}{\tau} - 1, \tag{3.73}$$

where the constant $\tilde{C}_2$ depends only on g, N_Ψ and N_ϕ. Unlike the proof for the CNFD case we can now estimate $\mathbf{e}^{m+1}$ and η^{m+1} at the same time by using (3.73) to bound the nonlinear terms, which is mainly due to the explicit property of LFFD (2.10–2.11).

Firstly, we estimate $\|\eta^{m+1}\|_{l^2}$, $\|\delta_x^+\eta^{m+1}\|_{l^2}$ and $\|\mathbf{e}^{m+1}\|_{l^2}$. Multiplying both sides of (3.65) by $h(\eta_j^{n+1}-\eta_j^{n-1})$, summing over j, using the summation by parts formula, (3.69) and (3.73), we obtain for $1\leqslant n\leqslant m$,

$$
\begin{aligned}
&\left(1-\frac{\tau^2}{2}-\frac{\tau^2}{h^2}\right)\left(\|\delta_t^+\eta^n\|_{l^2}^2-\|\delta_t^+\eta^{n-1}\|_{l^2}^2\right)+\frac{1}{2}\left(\|\eta^{n+1}\|_{l^2}^2-\|\eta^{n-1}\|_{l^2}^2\right)\\
&\quad+\frac{1}{2h}\sum_{j=0}^{M-1}\left[\left(\eta_{j+1}^{n+1}-\eta_j^n\right)^2+\left(\eta_{j+1}^n-\eta_j^{n+1}\right)^2-\left(\eta_{j+1}^n-\eta_j^{n-1}\right)^2-\left(\eta_{j+1}^{n-1}-\eta_j^n\right)^2\right]\\
&\quad=h\sum_{j=0}^{M-1}\left(\zeta_j^n+\lambda_j^n\right)\left(\eta_j^{n+1}-\eta_j^{n-1}\right)\leqslant 2\tau\left(\|\zeta^n\|_{l^2}^2+\|\lambda^n\|_{l^2}^2+\|\delta_t^+\eta^n\|_{l^2}^2+\|\delta_t^+\eta^{n-1}\|_{l^2}^2\right)\\
&\quad\leqslant\tilde{C}_3\tau\left(\|\delta_t^+\eta^n\|_{l^2}^2+\|\delta_t^+\eta^{n-1}\|_{l^2}^2+\|\mathbf{e}^n\|_{l^2}^2\right)+\tilde{C}_4\tau\left(\tau^2+h^2\right)^2,
\end{aligned}
\tag{3.74}
$$

with some constants $\tilde{C}_3$ and $\tilde{C}_4$ independent of h and τ. Multiplying both sides of (3.66) from the left by $4h\tau(\mathcal{A}\mathbf{e}_j^n)^*$, taking the imaginary parts, summing over j, in view of (3.69) and (3.73), we can get for $1\leqslant n\leqslant m$,

$$
\begin{aligned}
&\|\mathbf{e}^{n+1}\|_{l^2}^2-\|\mathbf{e}^{n-1}\|_{l^2}^2+2\mathrm{Re}\left[\tau h\sum_{j=0}^{M-1}\left((\mathbf{e}_j^{n+1})^*\sigma_1\delta_x\mathbf{e}_j^n-(\mathbf{e}_j^n)^*\sigma_1\delta_x\mathbf{e}_j^{n-1}\right)\right]\\
&\leqslant 2\tau\left(\|\theta^n\|_{l^2}^2+\|\chi^n\|_{l^2}^2+\sum_{k=n-1}^{n+1}\|\mathbf{e}^k\|_{l^2}^2\right)\leqslant\tilde{C}_5\tau\left(\sum_{k=n-1}^{n+1}\|\mathbf{e}^k\|_{l^2}^2+\|\eta^n\|_{l^2}^2\right)+\tilde{C}_6\tau\left(\tau^2+h^2\right)^2,
\end{aligned}
\tag{3.75}
$$

where we have employed the triangle inequality and the Cauchy inequality, $\mathrm{Re}(f)$ denotes the real part of f, $\tilde{C}_5$ and $\tilde{C}_6$ are independent of h and τ.

Denote

$$
\begin{aligned}
\mathscr{S}^n=&\|\mathbf{e}^{n+1}\|_{l^2}^2+\|\mathbf{e}^n\|_{l^2}^2+2\mathrm{Re}\left(\tau h\sum_{j=0}^{M-1}(\mathbf{e}_j^{n+1})^*\sigma_1\delta_x\mathbf{e}_j^n\right)+\left(1-\frac{\tau^2}{2}-\frac{\tau^2}{h^2}\right)\|\delta_t^+\eta^n\|_{l^2}^2\\
&+\frac{1}{2}\left(\|\eta^{n+1}\|_{l^2}^2+\|\eta^n\|_{l^2}^2\right)+\frac{1}{2h}\sum_{j=0}^{M-1}\left[\left(\eta_{j+1}^{n+1}-\eta_j^n\right)^2+\left(\eta_{j+1}^n-\eta_j^{n+1}\right)^2\right],\quad n\geqslant 0.
\end{aligned}
\tag{3.76}
$$

Under the stability assumption that $\tau \leqslant \alpha \min\{\sqrt{2}/2, \sqrt{3}h/2\}$ $(0 < \alpha < 1)$, $1 - \dfrac{\tau^2}{2} - \dfrac{\tau^2}{h^2} \geqslant 1 - \alpha^2 > 0$. Since

$$\|\delta_x^+ \eta^{n+1}\|_{l^2}^2 = \frac{1}{h} \sum_{j=0}^{M-1} \left(\eta_{j+1}^{n+1} - \eta_j^n - \tau \delta_t^+ \eta_j^n\right)^2 \leqslant \frac{2}{h} \sum_{j=0}^{M-1} \left(\eta_{j+1}^{n+1} - \eta_j^n\right)^2 + \frac{2\tau^2}{h^2} \|\delta_t^+ \eta^n\|_{l^2}^2,$$

$$\begin{aligned} 2\left|\mathrm{Re}\left(\tau h \sum_{j=0}^{M-1} \left(\mathbf{e}_j^{n+1}\right)^* \sigma_1 \delta_x \mathbf{e}_j^n\right)\right| &\leqslant \frac{\sqrt{3}}{2}\alpha h \sum_{j=0}^{M-1} \left|\mathbf{e}_j^{n+1}\right| \cdot \left|\mathbf{e}_{j+1}^n - \mathbf{e}_{j-1}^n\right| \\ &\leqslant \frac{\sqrt{3}}{2}\alpha \left(\|\mathbf{e}^{n+1}\|_{l^2}^2 + \|\mathbf{e}^n\|_{l^2}^2\right), \end{aligned}$$

we can conclude that for $C_b = \min\left\{\frac{1}{4}, \frac{2(1-\alpha^2)}{3\alpha^2}\right\}$ (using the stability assumption to get $\tau^2/h^2 \leqslant 3\alpha^2/4$),

$$\mathscr{S}^n \geqslant \left(1 - \frac{\sqrt{3}}{2}\alpha\right)\left(\|\mathbf{e}^{n+1}\|_{l^2}^2 + \|\mathbf{e}^n\|_{l^2}^2\right) + C_b \|\delta_x^+ \eta^{n+1}\|_{l^2}^2 + \frac{1}{2}\left(\|\eta^{n+1}\|_{l^2}^2 + \|\eta^n\|_{l^2}^2\right). \tag{3.77}$$

Together with (3.74), (3.75) and (3.76) imply

$$\mathscr{S}^n - \mathscr{S}^{n-1} \leqslant \tilde{C}_7 \tau (\mathscr{S}^n + \mathscr{S}^{n-1}) + \tilde{C}_8 \tau \left(\tau^2 + h^2\right)^2, \quad 1 \leqslant n \leqslant m, \tag{3.78}$$

and $\tilde{C}_8 = \tilde{C}_4 + \tilde{C}_6$ and $\tilde{C}_7 = \max\{(\tilde{C}_3 + \tilde{C}_5)/(1 - \frac{\sqrt{3}}{2}\alpha), 2\tilde{C}_5, \tilde{C}_3/(1 - \alpha^2)\}$. Summing the above inequality for time steps $1, \ldots, n$ we arrive at

$$\mathscr{S}^n \leqslant 2\tilde{C}_7 \tau \sum_{k=0}^{n} \mathscr{S}^n + \mathscr{S}^0 + \tilde{C}_8 T \left(\tau^2 + h^2\right)^2, \quad 0 \leqslant n \leqslant m \leqslant \frac{T}{\tau} - 1, \tag{3.79}$$

where

$$\begin{aligned} \mathscr{S}^0 &= \|\mathbf{e}^1\|_{l^2}^2 + \left(1 - \frac{\tau^2}{2} - \frac{\tau^2}{h^2}\right) \|\delta_t^+ \eta^0\|_{l^2}^2 + \left(\frac{1}{2} + \frac{1}{h^2}\right) \|\eta^1\|_{l^2}^2 \\ &= \tau^2 \|\theta^0\|_{l^2}^2 + \|\zeta^0\|_{l^2}^2 \lesssim (\tau^2 + h^2)^2. \end{aligned} \tag{3.80}$$

By Grönwall's inequality (Pachpatte, 2002; Holte, 2009) there exists a constant $\tau_1 > 0$ such that when $0 < \tau \leqslant \tau_1$,

$$\mathscr{S}^n \leqslant \tilde{C}_9 e^{n\tilde{C}_{10}\tau} \left(\tau^2 + h^2\right)^2 \leqslant \tilde{C}_9 e^{\tilde{C}_{10}T} \left(\tau^2 + h^2\right)^2, \quad 0 \leqslant n \leqslant m \leqslant \frac{T}{\tau} - 1, \tag{3.81}$$

where $\tilde{C}_9$ and $\tilde{C}_{10}$ depend on T, g, ω, the exact solution $(\phi(t,x), \Psi(t,x))$ and the parameter $\alpha \in (0,1)$ in the stability assumption. Letting $n = m$ in (3.81) we have

$$\mathscr{S}^m \leqslant \tilde{C}_9 e^{\tilde{C}_{10}T}(\tau^2 + h^2)^2, \tag{3.82}$$

and (3.77) leads to

$$\left\|\mathbf{e}^{m+1}\right\|_{l^2}^2 + \left\|\delta_x^+ \eta^{m+1}\right\|_{l^2}^2 + \left\|\eta^{m+1}\right\|_{l^2}^2 \leqslant \tilde{C}_{11}\left(\tau^2 + h^2\right)^2, \tag{3.83}$$

with $\tilde{C}_{11}$ depending only on T, g, ω, the exact solution $(\phi(t,x), \Psi(t,x))$ and the parameter $\alpha \in (0,1)$. Thus, (3.71) is true for $n = m+1$ if $C_1 \geqslant \sqrt{\tilde{C}_{11}}$. It remains to show that (3.72) holds at $n = m+1$.

Now we will show the estimates on $\|\Psi^{m+1}\|_{l^\infty}$ and $\|\phi^{m+1}\|_{l^\infty}$. In fact, the inverse inequality in one dimension, together with the stability condition $\tau \leqslant \alpha \min\{\sqrt{2}/2, \sqrt{3}h/2\}$, implies

$$\left\|\mathbf{e}^{m+1}\right\|_{l^\infty} \leqslant \frac{1}{\sqrt{h}}\left\|\mathbf{e}^{m+1}\right\|_{l^2} \leqslant \sqrt{\tilde{C}_{11}}\frac{\tau^2 + h^2}{\sqrt{h}} \leqslant \sqrt{\tilde{C}_{11}}\left(3\alpha^2 h^{3/2}/4 + h^{3/2}\right), \tag{3.84}$$

$$\left\|\eta^{m+1}\right\|_{l^\infty} \leqslant \frac{1}{\sqrt{h}}\left\|\eta^{m+1}\right\|_{l^2} \leqslant \sqrt{\tilde{C}_{11}}\left(3\alpha^2 h^{3/2}/4 + h^{3/2}\right). \tag{3.85}$$

Thus, there exists $h_2 > 0$ sufficiently small, when $0 < h \leqslant h_2$ and τ satisfies the stability requirement, we have

$$\left\|\mathbf{e}^{m+1}\right\|_{l^\infty} \leqslant 1, \quad \left\|\eta^{m+1}\right\|_{l^\infty} \leqslant 1, \tag{3.86}$$

and the triangle inequality gives

$$\begin{aligned}
\left\|\Psi^{m+1}\right\|_{l^\infty} &\leqslant \left\|\Psi(t_{m+1}, x)\right\|_{L^\infty([0,T];[L^\infty]^2)} + \left\|\mathbf{e}^{m+1}\right\|_{l^\infty} \leqslant N_\Psi + 1, \\
\left\|\phi^{m+1}\right\|_{l^\infty} &\leqslant \left\|\phi(t_{m+1}, x)\right\|_{L^\infty([0,T];L^\infty)} + \left\|\eta^{m+1}\right\|_{l^\infty} \leqslant N_\Phi + 1,
\end{aligned}$$

which verifies (3.72) at $n = m+1$.

Under the stability condition and the choices of $\tau_0 = \tau_1$, $h_0 = \min\{h_1, h_2\}$, $C_1 = \max\{\sqrt{\tilde{C}_1}, \sqrt{\tilde{C}_{11}}\}$, the estimates (3.6–3.7) are valid when $n = m+1$. Hence, the induction process is done, and the proof of Theorem 3.2 is complete.

REMARK 3.11 The proof of Theorem 3.2 can be directly generalized to higher dimensions ($d = 2, 3$). The key observation is that the l^∞ norms can be estimated by the inverse inequality as in (3.84–3.85) for two-dimensional and three-dimensional cases, under the stability condition $\tau \lesssim h$ (cf. Remark 3.10).

4. Numerical examples

In this section we apply FDTD methods presented in Section 2 for KGD (1.10) and report numerical results to verify our error analysis. The computational interval Ω is chosen large enough such that the periodic boundary conditions do not introduce a significant aliasing error relative to the whole space problem.

TABLE 1 *Spatial errors of CNFD at $t = 1$*

Spatial error	$h_0 = 1/8$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
e_Ψ	6.92E–3	1.74E–3	4.35E–04	1.09E–4	2.71E–5
Order	—	1.99	2.00	2.00	2.00
e_ϕ	5.41E–3	1.36E–3	3.39E–4	8.49E–5	2.13E–5
Order	—	2.00	2.00	2.00	2.00
$\Vert\phi(t_n) - \phi^n_{\tau,h}\Vert_{l^\infty}$	2.20E–3	5.51E–4	1.38E–4	3.48E–5	8.34E–6
Order	—	2.00	2.00	1.99	2.06

TABLE 2 *Spatial errors of SIFD1 at $t = 1$*

Spatial error	$h_0 = 1/8$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
e_Ψ	6.92E–3	1.74E–3	4.35E–4	1.09E–4	2.72E–5
Order	—	1.99	2.00	2.00	2.00
e_ϕ	5.41E–3	1.36E–3	3.39E–4	8.45E–5	2.09E–5
Order	—	2.00	2.00	2.00	2.01
$\Vert\phi(t_n) - \phi^n_{\tau,h}\Vert_{l^\infty}$	2.20E–3	5.50E–4	1.37E–4	3.40E–5	7.57E–6
Order	—	2.00	2.01	2.01	2.17

TABLE 3 *Spatial errors of SIFD2 at $t = 1$*

Spatial error	$h_0 = 1/8$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
e_Ψ	6.92E–3	1.74E–3	4.35E–4	1.09E–4	2.71E–5
Order	—	1.99	2.00	2.00	2.00
e_ϕ	5.41E–3	1.36E–3	3.39E–4	8.49E–5	2.13E–5
Order	—	2.00	2.00	2.00	2.00
$\Vert\phi(t_n) - \phi^n_{\tau,h}\Vert_{l^\infty}$	2.20E–3	5.51E–4	1.38E–4	3.48E–5	8.33E–6
Order	—	2.00	2.00	1.99	2.06

TABLE 4 *Spatial errors of LFFD at $t = 1$*

Spatial error	$h_0 = 1/8$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
e_Ψ	6.92E–3	1.74E–3	4.35E–4	1.09E–4	2.72E–5
Order	—	1.99	2.00	2.00	2.00
e_ϕ	5.41E–3	1.36E–3	3.39E–4	8.40E–5	2.08E–5
Order	—	1.99	2.00	2.01	2.01
$\Vert\phi(t_n) - \phi^n_{\tau,h}\Vert_{l^\infty}$	2.20E–3	5.52E–4	1.38E–4	3.29E–5	7.29E–6
Order	—	1.99	2.01	2.06	2.17

In the computation, the problem is solved numerically with coefficients $g = 1$ and $\omega = 1$ on an interval $\Omega = [-128, 128]$, i.e., $a = -128$ and $b = 128$ with periodic boundary conditions. The 'reference' solution $(\phi(t,x), \Psi(t,x))$ is obtained numerically by CNFD with a very small time step and a very fine mesh size, e.g., $\tau_e = 5 \times 10^{-6}$ and $h_e = 1/2048$. Denote $(\phi^n_{\tau,h}, \Psi^n_{\tau,h})$ as the numerical solution obtained by a numerical method with time step τ and mesh size h. In order to quantify the

TABLE 5 *Temporal errors of CNFD at $t = 1$*

Temporal error	$\tau_0 = 1/20$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$
e_Ψ	3.75E–3	9.83E–4	2.46E–4	6.14E–5	1.53E–5
Order	—	1.93	2.00	2.00	2.00
e_ϕ	5.35E–3	1.34E–3	3.35E–4	8.38E–5	2.13E–5
Order	—	2.00	2.00	2.00	1.98
$\\|\phi(t_n) - \phi^n_{\tau,h}\\|_{l^\infty}$	3.05E–3	7.68E–4	1.92E–4	4.81E–5	1.21E–5
Order	—	1.99	2.00	2.00	1.99

TABLE 6 *Temporal errors of SIFD1 at $t = 1$*

Temporal error	$h_0 = 1/16$, $\tau_0 = 1/20$	$h_0/2$, $\tau_0/2$	$h_0/2^2$, $\tau_0/2^2$	$h_0/2^3$, $\tau_0/2^3$	$h_0/2^4$, $\tau_0/2^4$
e_Ψ	4.50E–3	1.13E–3	2.81E–4	7.03E–5	1.75E–5
Order	—	2.00	2.00	2.00	2.00
e_ϕ	1.51E–3	3.79E–4	9.48E–5	2.39E–5	7.08E–6
Order	—	1.98	2.00	1.99	1.76
$\\|\phi(t_n) - \phi^n_{\tau,h}\\|_{l^\infty}$	8.24E–4	2.06E–4	5.16E–5	1.29E–5	3.26E–6
Order	—	2.00	2.00	2.00	1.99

TABLE 7 *Temporal errors of SIFD2 at $t = 1$*

Temporal error	$h_0 = 1/16$, $\tau_0 = 1/20$	$h_0/2$, $\tau_0/2$	$h_0/2^2$, $\tau_0/2^2$	$h_0/2^3$, $\tau_0/2^3$	$h_0/2^4$, $\tau_0/2^4$
e_Ψ	4.28E–3	1.07E–3	2.68E–4	6.70E–5	1.67E–5
Order	—	2.00	2.00	2.00	2.00
e_ϕ	1.66E–3	4.13E–4	1.03E–4	2.59E–5	7.44E–6
Order	—	2.00	2.00	1.99	1.80
$\\|\phi(t_n) - \phi^n_{\tau,h}\\|_{l^\infty}$	6.92E–4	1.72E–4	4.29E–5	1.07E–5	2.71E–6
Order	—	2.00	2.00	2.00	1.99

numerical results we define the error functions (l^2-error, discrete H^1-error and l^∞-error) as

$$\begin{aligned} e_\Psi(t_n) &= \|\Psi(t_n,\cdot) - \Psi^n_{\tau,h}\|_{l^2}, \\ e_\phi(t_n) &= \sqrt{\|\phi(t_n,\cdot) - \phi^n_{\tau,h}\|^2_{l^2} + \|\delta^+_x(\phi(t_n,\cdot) - \phi^n_{\tau,h})\|^2_{l^2}}, \\ \|\phi(t_n) - \phi^n_{\tau,h}\|_{l^\infty} &= \max_{0\leqslant j\leqslant M} \left|\phi\left(t_n, x_j\right) - \phi^n_{\tau,h}\left(x_j\right)\right|. \end{aligned}$$

The initial data is set as

$$\phi^0(x) = e^{-x^2/2}, \quad \gamma(x) = \frac{3}{2}e^{-x^2/2}, \quad \Psi^0(x) = (e^{-x^2/2}, e^{-(x-1)^2/2})^{\mathrm{T}}.$$

We first test the spatial discretization errors. In order to do this, we choose a very small time step, e.g., $\tau = \tau_e = 5 \times 10^{-6}$, such that the errors from time discretization are negligible, and solve KGD with

TABLE 8 *Temporal errors of LFFD at $t = 1$*

Temporal error	$h_0 = 1/16$ $\tau_0 = 1/20$	$h_0/2$ $\tau_0/2$	$h_0/2^2$ $\tau_0/2^2$	$h_0/2^3$ $\tau_0/2^3$	$h_0/2^4$ $\tau_0/2^4$
e_Ψ	2.33E–3	5.81E–4	1.45E–4	3.63E–5	9.11E–6
Order	—	2.00	2.00	2.00	2.00
e_ϕ	1.22E–3	3.05E–4	7.64E–5	1.94E–5	5.10E–6
Order	—	2.00	2.00	2.00	1.92
$\\|\phi(t_n) - \phi^n_{\tau,h}\\|_{l^\infty}$	5.90E–3	1.48E–4	3.69E–5	9.26E–6	2.34E–6
Order	—	2.00	2.00	1.99	1.98

TABLE 9 *Comparison of properties of different FDTD methods for solving KGD (M is the total number of the spatial grid points)*

Method	CNFD	SIFD1	SIFD2	LFFD
Time symmetric	Yes	Yes	Yes	Yes
Mass conservation	Yes	Yes	No	No
Energy conservation	Yes	Yes	No	No
Unconditionally stable	Yes	No	No	No
Explicit scheme	No	No	No	Yes
Temporal accuracy	2nd	2nd	2nd	2nd
Spatial accuracy	2nd	2nd	2nd	2nd
Memory cost	$\mathcal{O}(M)$	$\mathcal{O}(M)$	$\mathcal{O}(M)$	$\mathcal{O}(M)$

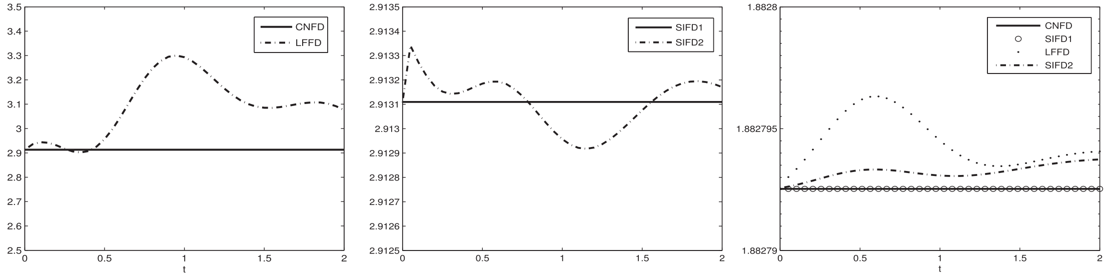

FIG. 1. The discrete energy $\mathcal{E}(t)$ obtained by CNFD and LFFD (left), the discrete energy $\widetilde{\mathcal{E}}(t)$ obtained by SIFD1 and SIFD2 (middle) and the electron mass $\\|\Psi(t)\\|_{l^2}$ (right) with $\tau = 0.001$ and $h = 1/128$.

FDTD methods under different mesh sizes h. Table 1 lists the numerical errors e_Ψ, e_ϕ and $\\|\phi(t_n) - \phi^n_{\tau,h}\\|_{l^\infty}$ at $t = 1$ with different mesh sizes h for CNFD (2.4–2.5). Tables 2–4 show similar results for the spatial errors for SIFD1 (2.6–2.7), SIFD2 (2.8–2.9) and LFFD (2.10–2.11), respectively.

Next we check the temporal errors at $t = 1$, listed in Tables 5–8. Due to the stability constraints for SIFD1 (2.6–2.7), SIFD2 (2.8–2.9) and LFFD (2.10–2.11), we set $0 < \tau < \min\{\sqrt{2}/2, \sqrt{3}h/2\}$ in Tables 6–8.

Finally, Fig. 1 displays the discrete energy and mass at different times with $h = 1/128$ and τ_e for different FDTD methods, which confirms the mass and energy conservation of CNFD and SIFD1. We summarize the properties of the FDTD methods in Table 9.

5. Conclusion

Four conservative/nonconservative implicit/semi-implicit/explicit FDTD methods were analyzed and compared numerically for solving the KGD system coupled through the Yukawa interaction. The nonlinear Yukawa interaction term and the Dirac part bring significant difficulties in the convergence analysis of the FDTD methods. By utilizing mathematical induction, the energy method and the special coupling structure, the error estimates were rigorously established, which showed that these FDTD methods are all second-order accurate in both space and time. Based on the convergence, stability and computational results, we conclude that CNFD performs best in terms of the stability, and it conserves both mass and energy. But in view of the implementation, computational cost and memory cost, LFFD is the simplest and the most efficient discretization for the KGD system.

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