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ERROR ESTIMATES OF FINITE DIFFERENCE TIME DOMAIN METHODS FOR THE KLEIN-GORDON-DIRAC SYSTEM IN THE NONRELATIVISTIC LIMIT REGIME*

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Abstract. In this paper, we establish error estimates of finite difference time domain (FDTD) methods for the Klein-Gordon-Dirac (KGD) system in the nonrelativistic limit regime, involving a small dimensionless parameter $0<\varepsilon\ll 1$ inversely proportional to the speed of light. In this limit regime, the solution of the KGD system propagates waves with $O(\varepsilon^2)$ and $O(1)$-wavelength in time and space respectively. The high oscillation and the nonlinear coupling between the real scalar Klein-Gordon field and the complex Dirac vector field bring great challenges to the analysis of the numerical methods for the KGD system in the nonrelativistic limit regime. Four implicit/semi-implicit/explicit FDTD methods are rigorously analyzed. By applying the energy method and cut-off technique, we obtain the error bounds for the FDTD methods at $O(\tau^2/\varepsilon^6+h^2/\varepsilon)$ with time step τ and mesh size h. Thus, in order to compute 'correct' solutions when $0<\varepsilon\ll 1$, the estimates suggest that the meshing strategy requirement of the FDTD methods is $\tau=O(\varepsilon^3)$ and $h=O(\sqrt{\varepsilon})$. In addition, numerical results are reported to support our conclusions. Our approach is valid in one, two and three dimensions.

Keywords. Klein-Gordon-Dirac system; nonrelativistic limit regime; Yukawa interaction; finite difference time domain (FDTD) methods; error estimates.

AMS subject classifications. 35Q55; 65N12; 81Q05.

1. Introduction

In quantum electrodynamics and/or particle physics, the Klein-Gordon-Dirac (KGD) system describes the nuclear force between nucleons through the Yukawa potential [13, 23, 24, 29, 32], and is a fundamental model to describe the dynamics of a complex-valued Dirac vector field, $\Psi(t,\mathbf{x})=(\psi_1(t,\mathbf{x}),\psi_2(t,\mathbf{x}),\ \psi_3(t,\mathbf{x}),\psi_4(t,\mathbf{x}))^T\in\mathbb{C}^4$, interacting with a neutral real-valued meson scalar field $\phi(t,\mathbf{x})\in\mathbb{R}$. The KGD system is given in three-dimensions (3D) [13, 19, 32] as:

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

where $0<\lambda\in\mathbb{R}$ is the coupling constant, c is the speed of light, $\hbar$ is the Planck's constant, $m_1>0$ is the mass of the meson and $m_2>0$ is the mass of the electron. Here, $i=\sqrt{-1}$ 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 $\mathbf{x}=(x_1,x_2,x_3)^T$ (equivalently written as $\mathbf{x}=(x,y,z)^T$), $\partial_j=\partial/\partial x_j\ (j=1,2,3)$ and $\Delta=\sum_{j=1}^3\partial_j^2$ in 3D. In addition, $\Psi^*=\overline{\Psi}^T$ is the conjugate transpose, α_1, α_2, α_3 and β are 4×4 matrices given as

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

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

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

In order to nondimensionalize the KGD (1.1), we introduce

$$\tilde{t}=\frac{t}{t_s},\quad \tilde{\mathbf{x}}=\frac{\mathbf{x}}{x_s},\quad \tilde{\Psi}(\tilde{t},\tilde{\mathbf{x}})=x_s^{3/2}\Psi(t,\mathbf{x}),\quad \tilde{\phi}(\tilde{t},\tilde{\mathbf{x}})=\frac{\phi(t,\mathbf{x})}{\phi_s}, \tag{1.4}$$

where t_s, x_s, ϕ_s are the time unit, length unit and meson field unit, respectively, satisfying $t_s=m_1x_s^2/\hbar$ and $\phi_s=\sqrt{4\pi m_1}\hbar/(m_1x_s^{3/2})$ with the wave speed $v=x_s/t_s=\hbar/(m_1x_s)$. Plugging (1.4) into (1.1), after a simple computation and then removing all $\tilde{}$, the dimensionless KGD system can be expressed as

$$\begin{cases} \varepsilon^2\partial_{tt}\phi(t,\mathbf{x})-\Delta\phi(t,\mathbf{x})+\dfrac{1}{\varepsilon^2}\phi(t,\mathbf{x})=g\Psi^*\beta\Psi(t,\mathbf{x}),\\ i\partial_t\Psi(t,\mathbf{x})+\dfrac{i}{\varepsilon}\sum\limits_{j=1}^{3}\alpha_j\partial_j\Psi(t,\mathbf{x})-\dfrac{\omega}{\varepsilon^2}\beta\Psi(t,\mathbf{x})-g\phi\beta\Psi(t,\mathbf{x})=0, \end{cases} \tag{1.5}$$

where ε is a dimensionless parameter inversely proportional to the speed of light given by

$$0<\varepsilon:=\frac{v}{c}=\frac{x_s}{t_sc}=\frac{\hbar}{m_1cx_s}\le 1, \tag{1.6}$$

the coupling constant $g=\lambda\sqrt{4\pi m_1x_s}/\hbar\in\mathbb{R}$ and the ratio $0<\omega=\frac{m_2}{m_1}\le 1$ between the mass of the electron and the mass of the meson are two dimensionless constants independent of ε. Note that the choice of x_s determines the observation scale of the evolution of the particles. In fact, there are two important parameter regimes: one is $\varepsilon=O(1)$, then the KGD (1.5) describes the case that the wave speed is of the same order to the speed of light (i.e. the dimensionless length unit is chosen as $x_s=\hbar/(m_1c)$, then $t_s=x_s/c$ and $\phi_s=\sqrt{4\pi\hbar m_1}c^{3/2}/\hbar$ in (1.4)); the other one is $0<\varepsilon\ll 1$, then the KGD (1.5) is in the nonrelativistic limit regime.

To study the dynamics of the KGD (1.5), the initial data is usually assigned as

$$\phi(0,\mathbf{x})=\phi^0(\mathbf{x}),\ \partial_t\phi(0,\mathbf{x})=\frac{1}{\varepsilon^2}\gamma(\mathbf{x}),\ \Psi(0,\mathbf{x})=\Psi^0(\mathbf{x})=(\psi_1^0(\mathbf{x}),\psi_2^0(\mathbf{x}),\psi_3^0(\mathbf{x}),\psi_4^0(\mathbf{x}))^T, \tag{1.7}$$

where the functions $\phi^0(\mathbf{x})$, $\gamma(\mathbf{x})\in\mathbb{R}$ and $\Psi^0(\mathbf{x})\in\mathbb{C}^4$ are independent of ε. Similar to the dimension reduction of the nonlinear Schrödinger equation and the (nonlinear) Dirac equation [2, 3, 6, 37], under proper assumptions on the initial data, the KGD (1.5) can be reduced to a 2D (or 1D) system with $\mathbf{x}=(x,y)^T\in\mathbb{R}^2$ (or $\mathbf{x}=x$). In fact, they can be written in a unified way in d-dimensions $(d=1,2,3)$ as

$$\begin{cases} \varepsilon^2\partial_{tt}\phi(t,\mathbf{x})-\Delta\phi(t,\mathbf{x})+\dfrac{1}{\varepsilon^2}\phi(t,\mathbf{x})=g\Psi^*\beta\Psi(t,\mathbf{x}),\\ i\partial_t\Psi(t,\mathbf{x})+\dfrac{i}{\varepsilon}\sum\limits_{j=1}^{d}\alpha_j\partial_j\Psi(t,\mathbf{x})-\dfrac{\omega}{\varepsilon^2}\beta\Psi(t,\mathbf{x})-g\phi\beta\Psi(t,\mathbf{x})=0. \end{cases} \tag{1.8}$$

The KGD (1.8) is dispersive and conserves the total electron mass, i.e.

$$\|\Psi(t,\cdot)\|^2_{L^2(\mathbb{R}^d)}:=\int_{\mathbb{R}^d}|\Psi(t,\mathbf{x})|^2d\mathbf{x}=\int_{\mathbb{R}^d}\sum_{j=1}^{4}|\psi_j(t,\mathbf{x})|^2d\mathbf{x}\equiv\|\Psi^0\|^2_{L^2(\mathbb{R}^d)}. \tag{1.9}$$

In addition, the energy is conserved

$$\begin{aligned}\mathcal{E}(t) &:= \frac{\varepsilon^2}{2}\int_{\mathbb{R}^d} |\partial_t\phi(t,\mathbf{x})|^2 d\mathbf{x} + \frac{1}{2}\int_{\mathbb{R}^d} |\nabla\phi(t,\mathbf{x})|^2 d\mathbf{x} + \frac{1}{2\varepsilon^2}\int_{\mathbb{R}^d} \phi^2(t,\mathbf{x}) d\mathbf{x} \\ &\quad + \int_{\mathbb{R}^d}\left[\frac{i}{\varepsilon}\Psi^*\sum_{j=1}^{d}\alpha_j\partial_j\Psi(t,\mathbf{x}) - \frac{\omega}{\varepsilon^2}\Psi^*\beta\Psi(t,\mathbf{x}) - g\phi\Psi^*\beta\Psi(t,\mathbf{x})\right] d\mathbf{x} \\ &\equiv \mathcal{E}(0), \quad t\geq 0. \end{aligned} \tag{1.10}$$

It is easy to check that the energy $\mathcal{E}(t) = O(\varepsilon^{-2})$ is unbounded when $\varepsilon \to 0^+$.

In lower dimensions ($d=1,2$), two components of the Dirac vector fields are usually adopted as in the (nonlinear) Dirac equation cases [5, 7]. Accordingly, the KGD (1.8) can be reduced to a simplified form in 1D and 2D as

$$\begin{cases} \varepsilon^2\partial_{tt}\phi(t,\mathbf{x}) - \Delta\phi(t,\mathbf{x}) + \dfrac{1}{\varepsilon^2}\phi(t,\mathbf{x}) = g\Psi^*\sigma_3\Psi(t,\mathbf{x}), \\ i\partial_t\Psi(t,\mathbf{x}) + \dfrac{i}{\varepsilon}\sum\limits_{j=1}^{d}\sigma_j\partial_j\Psi(t,\mathbf{x}) - \dfrac{\omega}{\varepsilon^2}\sigma_3\Psi(t,\mathbf{x}) - g\phi\sigma_3\Psi(t,\mathbf{x}) = 0, \end{cases} \tag{1.11}$$

where $\phi(t,\mathbf{x}) \in \mathbb{R}$ and $\Psi(t,\mathbf{x}) \in \mathbb{C}^2$. Because of its simplicity, the KGD (1.11) with a two-vector form of the Dirac field is widely used in 1D and 2D.

For the KGD (1.8)((1.11)), there are extensive analytical results in the literature, such as the existence and multiplicity of bound state solutions and the well-posedness of the Cauchy problem, for which we refer to [1, 14, 15, 17, 18, 21, 22, 28, 31] and references therein. For the numerical part, when $\varepsilon = 1$, i.e. $O(1)$-speed of light regime, in our recent work [37], four conservative/non-conservative implicit/semi-implicit/explicit FDTD methods have been analyzed for the KGD system. We have proved discrete-H^1 error estimates for the Klein-Gordon component and l^2 error estimates for the Dirac component of these FDTD discretizations by employing energy methods and mathematical induction. However, in the nonrelativistic regime, i.e. $0 < \varepsilon \ll 1$, the analysis and efficient computation are mathematically and numerically rather complicated issues. Besides the challenges brought by the Dirac part and the nonlinear interaction terms, one of the main difficulties is due to that there exist highly oscillatory waves with wavelength of $O(\varepsilon^2)$ in time. To illustrate the oscillations further, Figures 1.1-1.2 show the solutions in 1D for different ε, obtained numerically, on a bounded interval $[-128,128]$ with $\phi^0(x) = e^{-x^2/2}$, $\gamma(x) = \frac{3}{2}e^{-x^2/2}$, $\Psi^0(x) = (e^{-x^2/2}, e^{-(x-1)^2/2})^T$ under periodic boundary conditions.

This highly temporal oscillatory nature of the solution causes severe numerical burdens, making the numerical approximations of the KGD (1.8)((1.11)) extremely challenging and costive, especially in the nonrelativistic limit regime ($0 < \varepsilon \ll 1$). Recently, the FDTD methods and spectral methods have been proposed and analyzed for the efficient computation of the wave propagation in quantum physics with/without the highly oscillatory behavior in time, i.e. dispersive waves in the Dirac equation (see, e.g., [5–7,25,27] and references therein), Klein-Gordon equation (see, e.g., [8,9,12,20] and references therein) and/or dispersive PDEs (see, e.g., [10,11,33] and references therein). To the best of our knowledge, so far there are very few works addressing the efficiency of the numerics for the KGD (1.8)((1.11)) as $\varepsilon \to 0^+$. The aim of this paper is to carry out rigorous error analysis of the FDTD methods for the KGD (1.8)((1.11)) in the nonrelativistic limit regime. We will establish the error bounds of several conservative/non-conservative implicit/semi-implicit/explicit FDTD discretizations and focus on how the

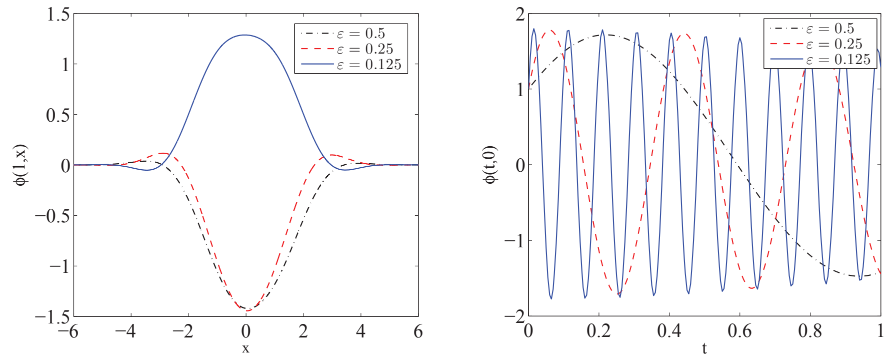

Fig. 1.1. *The solution $\phi(t=1,x)$ and $\phi(t,x=0)$ of the KGD* (1.11) *with $d=1$ for different ε.*

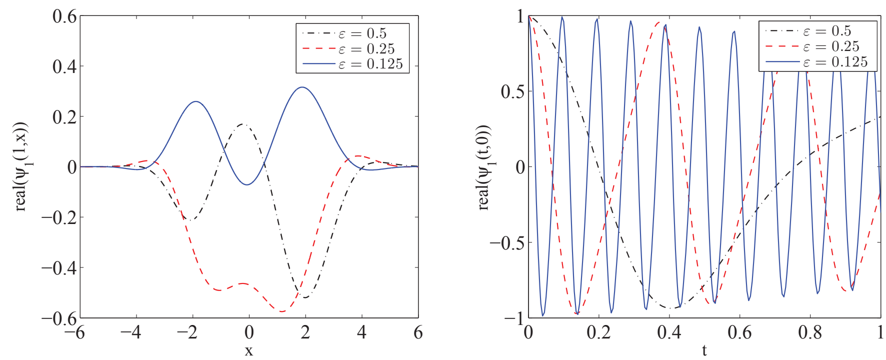

Fig. 1.2. *The solution $\psi_1(t=1,x)$ and $\psi_1(t,x=0)$ of the KGD* (1.11) *with $d=1$ for different ε. real(f) denotes the real part of f.*

errors depend explicitly on the small parameter ε in addition to the time step τ and mesh size h. Different from the $\varepsilon=1$ case [37], in the nonrelativistic regime, there is no optimal control on the nonlinear terms by directly generalizing the mathematical induction approach employed in [37] due to the ε-dependence of the wave operator in the Klein-Gordon part. Instead, we use the cut-off technique and energy methods for the error analysis.

The rest of the paper is organized as follows. In Section 2, four second-order conservative/non-conservative implicit/explicit FDTD methods are revisited and analyzed. Section 3 is devoted to the main results of this paper and details the rigorous error analysis. Numerical comparison results are reported in Section 4. Finally, some concluding remarks are drawn in Section 5. Throughout this paper, we adopt the standard notations for Sobolev spaces and use $p \lesssim q$ to represent that there exists a generic constant C which is independent of τ, h and ε, such that $|p| \leq Cq$. C denotes some constant independent of τ, h and ε, which may change from line to line.

2. FDTD methods and their analysis

In this section, we present four FDTD methods for the KGD (1.11) in the nonrelativistic limit regime. For simplicity of notations, we shall only illustrate the numerical methods and their analysis in 1D. Generalizations to higher dimensions and the KGD (1.11) (or (1.8)) 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 (1.11), on the bounded domain Ω, reads

$$\begin{cases} \varepsilon^2\partial_{tt}\phi(t,x)-\partial_{xx}\phi(t,x)+\dfrac{1}{\varepsilon^2}\phi(t,x)=g\Psi^*\sigma_3\Psi(t,x), \quad x\in\Omega, \quad t>0,\\ i\partial_t\Psi(t,x)+\dfrac{i}{\varepsilon}\sigma_1\partial_x\Psi(t,x)-\dfrac{\omega}{\varepsilon^2}\sigma_3\Psi(t,x)-g\phi\sigma_3\Psi(t,x)=0, \quad x\in\Omega, \quad t>0,\\ \phi(t,a)=\phi(t,b),\ \partial_x\phi(t,a)=\partial_x\phi(t,b),\ \Psi(t,a)=\Psi(t,b),\ \partial_x\Psi(t,a)=\partial_x\Psi(t,b),\\ \phi(0,x)=\phi^0(x), \quad \partial_t\phi(0,x)=\dfrac{1}{\varepsilon^2}\gamma(x), \quad \Psi(0,x)=\Psi^0(x), \quad x\in\bar{\Omega}, \quad t\geq 0, \end{cases} \tag{2.1}$$

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

2.1. FDTD methods. Choose the space mesh size $h:=\Delta x=\frac{b-a}{M}$ with M being an even positive integer and time step size $\tau:=\Delta t>0$, the index sets $\mathscr{T}_M^0=\{j|j=0,1,\cdots,M\}$, $\mathscr{T}_{M-1}^0=\{j|j=0,1,\cdots,M-1\}$, the grid points and time steps are:

$$x_j:=a+jh, \quad j\in\mathscr{T}_M^0; \quad t_n:=n\tau, \quad n=0,1,2,\cdots. \tag{2.2}$$

Denote $X_M=\{U=(U_j)_{j\in\mathscr{T}_M^0}|U_j\in\mathbb{C}^2,U_0=U_M\}\subset\mathbb{C}^{(M+1)\times 2}$, $\widetilde{X}_M=\{U=(U_j)_{j\in\mathscr{T}_M^0}|U_j\in\mathbb{R},U_0=U_M\}\subset\mathbb{R}^{M+1}$ and we always use $U_{-1}=U_{M-1}$ and $U_{M+1}=U_1$ if they are involved. The standard discrete l^2-norm, semi-H^1-norm and l^∞-norm for $U\in X_M$ (or $U\in\widetilde{X}_M$) are defined as

$$\|U\|^2:=h\sum_{j\in\mathscr{T}_{M-1}^0}|U_j|^2, \quad \|\delta_x^+U\|^2=h\sum_{j\in\mathscr{T}_{M-1}^0}|\delta_x^+U_j|^2, \quad \|U\|_\infty:=\sup_{j\in\mathscr{T}_M^0}|U_j|.$$

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

$$\delta_t^+U_j^n=\frac{U_j^{n+1}-U_j^n}{\tau},\ \delta_tU_j^n=\frac{U_j^{n+1}-U_j^{n-1}}{2\tau},\ \delta_xU_j^n=\frac{U_{j+1}^n-U_{j-1}^n}{2h},\ U_j^{n+1/2}=\frac{U_j^{n+1}+U_j^n}{2},$$

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

Here we consider several frequently used FDTD methods to discretize the KGD (2.1) for $j\in\mathscr{T}_M^0$.

- Crank-Nicolson finite difference (CNFD) method

$$\varepsilon^2\delta_t^2\phi_j^n-\delta_x^2\mathcal{A}\phi_j^n+\frac{1}{\varepsilon^2}\mathcal{A}\phi_j^n=g(\Psi_j^n)^*\sigma_3\Psi_j^n, \quad n\geq 1, \tag{2.3}$$

$$i\delta_t^+\Psi_j^n=\left[-\frac{i}{\varepsilon}\sigma_1\delta_x+\frac{\omega}{\varepsilon^2}\sigma_3\right]\Psi_j^{n+1/2}+g\phi_j^{n+1/2}\sigma_3\Psi_j^{n+1/2}, \quad n\geq 0; \tag{2.4}$$

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

$$\varepsilon^2\delta_t^2\phi_j^n-\delta_x^2\phi_j^n+\frac{1}{\varepsilon^2}\mathcal{A}\phi_j^n=g(\Psi_j^n)^*\sigma_3\Psi_j^n, \quad n\geq 1, \tag{2.5}$$

$$i\delta_t\Psi_j^n=\left[-\frac{i}{\varepsilon}\sigma_1\delta_x+\frac{\omega}{\varepsilon^2}\sigma_3\right]\mathcal{A}\Psi_j^n+g\phi_j^n\sigma_3\mathcal{A}\Psi_j^n, \quad n\geq 1; \tag{2.6}$$

- Another semi-implicit finite difference (SIFD2) method

$$\varepsilon^2\delta_t^2\phi_j^n-\delta_x^2\mathcal{A}\phi_j^n+\frac{1}{\varepsilon^2}\mathcal{A}\phi_j^n=g(\Psi_j^n)^*\sigma_3\Psi_j^n,\quad n\geq 1, \tag{2.7}$$

$$i\delta_t\Psi_j^n=-\frac{i}{\varepsilon}\sigma_1\delta_x\Psi_j^n+\frac{\omega}{\varepsilon^2}\sigma_3\mathcal{A}\Psi_j^n+g\mathcal{A}\phi_j^n\sigma_3\mathcal{A}\Psi_j^n,\quad n\geq 1; \tag{2.8}$$

- Leap-frog finite difference (LFFD) method

$$\varepsilon^2\delta_t^2\phi_j^n-\delta_x^2\phi_j^n+\frac{1}{\varepsilon^2}\phi_j^n=g(\Psi_j^n)^*\sigma_3\Psi_j^n,\quad n\geq 1, \tag{2.9}$$

$$i\delta_t\Psi_j^n=\left[-\frac{i}{\varepsilon}\sigma_1\delta_x+\frac{\omega}{\varepsilon^2}\sigma_3\right]\Psi_j^n+g\phi_j^n\sigma_3\Psi_j^n,\quad n\geq 1. \tag{2.10}$$

The initial and boundary conditions in (2.1) are discretized for $j\in\mathscr{T}_M^0$ and $n\geq 0$ as

$$\phi_j^0=\phi^0(x_j),\ \phi_M^{n+1}=\phi_0^{n+1},\ \phi_{-1}^{n+1}=\phi_{M-1}^{n+1},\ \Psi_j^0=\Psi^0(x_j),\ \Psi_M^{n+1}=\Psi_0^{n+1},\ \Psi_{-1}^{n+1}=\Psi_{M-1}^{n+1}, \tag{2.11}$$

and the first step for the Dirac field Ψ^1 can be updated for the SIFD1 (2.6), SIFD2 (2.8) and LFFD (2.10) as

$$\Psi_j^1=\Psi_j^0-\tau\left[\frac{1}{\tau}\sin(\frac{\tau}{\varepsilon})\sigma_1(\Psi^0)'(x_j)+i\left(\frac{\omega}{\tau}\sin(\frac{\tau}{\varepsilon^2})+g\phi_j^0\right)\sigma_3\Psi_j^0\right],\quad j\in\mathscr{T}_M^0. \tag{2.12}$$

Meanwhile, the first step for the Klein-Gordon field ϕ^1 is computed as

$$\phi_j^1=\phi_j^0+\sin(\frac{\tau}{\varepsilon^2})\gamma(x_j)+2\sin^2(\frac{\tau}{2\varepsilon})\left[(\phi^0)''(x_j)+g(\Psi_j^0)^*\sigma_3\Psi_j^0\right]-2\sin^2(\frac{\tau}{2\varepsilon^2})\phi_j^0,\quad j\in\mathscr{T}_M^0. \tag{2.13}$$

REMARK 2.1.

(1) By using Taylor expansion, the first step can be simply computed as

$$\phi_j^1=\phi_j^0+\frac{\tau}{\varepsilon^2}\gamma(x_j)+\frac{\tau^2}{2\varepsilon^2}\left[(\phi^0)''(x_j)-\frac{1}{\varepsilon^2}\phi_j^0+g(\Psi_j^0)^*\sigma_3\Psi_j^0\right],\quad j\in\mathscr{T}_M^0,$$

$$\Psi_j^1=\Psi_j^0-\tau\left[\frac{1}{\varepsilon}\sigma_1(\Psi^0)'(x_j)+\frac{i}{\varepsilon^2}\left(\omega+\varepsilon^2g\phi_j^0\right)\sigma_3\Psi_j^0\right],\quad j\in\mathscr{T}_M^0.$$

The above approximations are not appropriate if $\varepsilon\ll 1$, in which case, τ has to be very small to bound ϕ_j^1 and Ψ_j^1. In order to get the first step value (ϕ_j^1,Ψ_j^1) uniformly bounded for $\varepsilon\in(0,1]$, we adopt $\frac{1}{\tau}\sin(\frac{\tau}{\varepsilon})$ and $\frac{1}{\tau}\sin(\frac{\tau}{\varepsilon^2})$ instead of $\frac{1}{\varepsilon}$ and $\frac{1}{\varepsilon^2}$ such that the modified versions (2.12)-(2.13) are second order in terms of τ satisfying $\|\phi^1\|_\infty\lesssim 1$ and $\|\Psi^1\|_\infty\lesssim 1$ for any fixed $0<\varepsilon\leq 1$. We remark here that they can be simply replaced by 1 when $\varepsilon=O(1)$.

(2) The CNFD, SIFD1, SIFD2 and LFFD (2.3)-(2.10) are uniquely solvable at each time step. As illustrated in [37], all the schemes can be decoupled such that only linear systems need to be solved at each step and the solvability and uniqueness are straightforward.

The above four methods are all time-symmetric and time-reversible. The CNFD (2.3)-(2.4) conserves the mass $\|\Psi^n\|$ $(n\geq 0)$ and the energy at the discrete level,

$$\mathcal{E}^n:=\frac{1}{2}\varepsilon^2\|\delta_t^+\phi^n\|^2+\frac{1}{4}(\|\delta_x^+\phi^{n+1}\|^2+\|\delta_x^+\phi^n\|^2)+\frac{1}{4\varepsilon^2}(\|\phi^{n+1}\|^2+\|\phi^n\|^2)$$

$$+\frac{ih}{\varepsilon}\sum_{j\in\mathscr{T}_{M-1}^0}(\Psi_j^{n+1})^*\sigma_1\delta_x\Psi_j^{n+1}-\frac{\omega h}{\varepsilon^2}\sum_{j\in\mathscr{T}_{M-1}^0}(\Psi_j^{n+1})^*\sigma_3\Psi_j^{n+1}$$
$$-\frac{gh}{2}\sum_{j\in\mathscr{T}_{M-1}^0}(\phi_j^n+\phi_j^{n+1})(\Psi_j^{n+1})^*\sigma_3\Psi_j^{n+1}\equiv\mathcal{E}^0=O(\frac{1}{\varepsilon^2}),\quad n\geq 0.$$

In addition, the SIFD1 (2.5)-(2.6) conserves the mass $\|\Psi^{n+1}\|^2+\|\Psi^n\|^2$ $(n\geq 0)$ and the discrete energy

$$\widetilde{\mathcal{E}}^n:=\frac{1}{2}\varepsilon^2\|\delta_t^+\phi^n\|^2+\frac{h}{2}\sum_{j\in\mathscr{T}_{M-1}^0}\delta_x^+\phi_j^n\cdot\delta_x^+\phi_j^{n+1}+\frac{1}{4\varepsilon^2}(\|\phi^{n+1}\|^2+\|\phi^n\|^2)$$
$$+\frac{h}{2\varepsilon}\sum_{j\in\mathscr{T}_{M-1}^0,k=n,n+1}\Big[i(\Psi_j^k)^*\sigma_1\delta_x\Psi_j^k-\frac{\omega}{\varepsilon}(\Psi_j^k)^*\sigma_3\Psi_j^k\Big]$$
$$-\frac{gh}{2}\sum_{j\in\mathscr{T}_{M-1}^0}\big[\phi_j^n(\Psi_j^{n+1})^*\sigma_3\Psi_j^{n+1}+\phi_j^{n+1}(\Psi_j^n)^*\sigma_3\Psi_j^n\big]\equiv\widetilde{\mathcal{E}}^0=O(\frac{1}{\varepsilon^2}),\quad n\geq 0.$$

The proof is quite standard and similar to those for the $O(1)$ case [37]. We omit them for brevity.

Furthermore, following the linear stability analysis of the FDTD methods for the Dirac equation and Klein-Gordon equation via Von Neumann method [6, 9], we have the following lemma, with the proof omitted.

LEMMA 2.1.

(i). The CNFD (2.3)-(2.4) *is unconditionally stable for any* τ, $h>0$ *and* $0<\varepsilon\leq 1$.

(ii). The SIFD1, SIFD2 and LFFD (2.5)-(2.10) *are stable under the stability condition*

$$0<\tau<\varepsilon^2 h/\sqrt{h^2+\varepsilon^2},\quad h>0,\quad 0<\varepsilon\leq 1.$$

3. Error estimates

3.1. Main results. Motivated by the analytical studies on the nonlinear Dirac equation and Klein-Gordon equation [7,9](and references therein), we make the following assumptions on the exact solution of the KGD (2.1)

$$(A)\quad\begin{aligned}&\phi(t,x)\in C^5([0,T];L^\infty)\cap C^4([0,T];W_p^{1,\infty})\cap C^3([0,T];W_p^{2,\infty})\cap C^2([0,T];W_p^{3,\infty})\\&\qquad\cap C^1([0,T];W_p^{4,\infty})\cap C([0,T];W_p^{5,\infty});\\&\Psi(t,x)\in C^4([0,T];[L^\infty]^2)\cap C^3([0,T];[W_p^{1,\infty}]^2)\cap C^2([0,T];[W_p^{2,\infty}]^2)\\&\qquad\cap C^1([0,T];[W_p^{3,\infty}]^2)\cap C([0,T];[W_p^{4,\infty}]^2);\\&\left\|\frac{\partial^{r+s}}{\partial t^r\partial x^s}\phi(t,x)\right\|_{L^\infty}\lesssim\frac{1}{\varepsilon^{2r}},\quad\left\|\frac{\partial^{r+s}}{\partial t^r\partial x^s}\Psi(t,x)\right\|_{L^\infty}\lesssim\frac{1}{\varepsilon^{2r}},\ 0\leq r\leq 4,\ 0\leq r+s\leq 5,\end{aligned}$$

with $0<T<T^*$ (T^* the maximal common existence time of the solution), $W_p^{m,\infty}=\{u|u\in W_p^{m,\infty}(\Omega),\ \partial_x^l u(a)=\partial_x^l u(b),\ l=0,1,\cdots,m-1\}$ for $m\geq 1$, $L^\infty=L^\infty([0,T];L^\infty)$ for ϕ and $L^\infty=L^\infty([0,T];[L^\infty]^2)$ for Ψ.

Denote

$$N_\phi=\sup_{\varepsilon\in(0,1]}\|\phi(t,x)\|_{L^\infty},\quad N_\Psi=\sup_{\varepsilon\in(0,1]}\|\Psi(t,x)\|_{L^\infty},$$

and the grid error functions $\eta^n \in \widetilde{X}_M$ and $\mathbf{e}^n \in X_M$ as

$$\eta_j^n = \phi(t_n, x_j) - \phi_j^n, \quad \mathbf{e}_j^n = \Psi(t_n, x_j) - \Psi_j^n, \quad j \in \mathscr{T}_M^0, \quad n \geq 0,$$

where (ϕ_j^n, Ψ_j^n) is the numerical approximation obtained from the FDTD methods.

For the CNFD (2.3)-(2.4), the error estimates can be established as follows (see its proof in Section 3.1).

THEOREM 3.1 (Error bounds of CNFD). *Under the Assumption (A), there exist constants $\tau_0 > 0$ and $h_0 > 0$ sufficiently small and independent of ε, such that, for any $0 < \varepsilon \leq 1$, when $0 < \tau \leq \tau_0 \varepsilon^3$ and $0 < h \leq h_0 \varepsilon^{1/2}$, we have the error estimates for the CNFD* (2.3)-(2.4) *with* (2.11) *given as*

$$\|\eta^n\| + \|\delta_x^+ \eta^n\| \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon^6}, \quad \|\boldsymbol{e}^n\| + \|\delta_x^+ \boldsymbol{e}^n\| \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon^6}, \tag{3.1}$$

$$\|\phi^n\|_\infty \leq 1 + N_\phi, \qquad \|\Psi^n\|_\infty \leq 1 + N_\Psi, \qquad 0 \leq n \leq \frac{T}{\tau}. \tag{3.2}$$

For the SIFD1 (2.5)-(2.6), under the stability condition

$$\tau \leq \alpha \varepsilon^2 h / \sqrt{h^2 + \varepsilon^2}, \quad 0 < \alpha < 1, \quad h > 0, \tag{3.3}$$

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

THEOREM 3.2 (Error bounds of SIFD1). *Under the Assumption (A) and the stability condition* (3.3)*, there exist constants $\tau_0 > 0$ and $h_0 > 0$ sufficiently small and independent of ε, such that, for any $0 < \varepsilon \leq 1$, when $0 < \tau \leq \tau_0 \varepsilon^3$ and $0 < h \leq h_0 \varepsilon^{1/2}$, we have the error estimates for the SIFD1* (2.5)-(2.6) *with* (2.11) *given as*

$$\|\eta^n\| + \|\delta_x^+ \eta^n\| \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon^6}, \quad \|\boldsymbol{e}^n\| + \|\delta_x^+ \boldsymbol{e}^n\| \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon^6}, \tag{3.4}$$

$$\|\phi^n\|_\infty \leq 1 + N_\phi, \qquad \|\Psi^n\|_\infty \leq 1 + N_\Psi, \qquad 0 \leq n \leq \frac{T}{\tau}. \tag{3.5}$$

REMARK 3.1.

(1) In 2D ($d=2$) and 3D ($d=3$) cases, the above theorems are still valid under the technical conditions $0 < \tau \lesssim \varepsilon^3 / \sqrt{C_d(h)}$ and $0 < h \lesssim \varepsilon^{1/2} / \sqrt{C_d(h)}$. The key is to control $\|\eta^n\|_\infty$ and $\|\mathbf{e}^n\|_\infty$ by the discrete Sobolev inequality [3, 34] in 2D and 3D as

$$\|U\|_\infty \lesssim C_d(h) \left[\|U\| + \|\delta_x^+ U\| \right], \quad C_d(h) = \begin{cases} 1, & d=1, \\ |\ln h|, & d=2, \\ h^{-1/2}, & d=3, \end{cases}$$

when U is a periodic 2D/3D mesh function.

(2) The error bounds for the SIFD2 and LFFD (2.7)-(2.10) are the same as those in Theorem 3.1 and Theorem 3.2 under the stability condition $\tau \leq \alpha \varepsilon^2 h / \sqrt{h^2 + \varepsilon^2}$ $(0 < \alpha < 1)$, which can also be derived by proceeding in the analogous lines for the CNFD or SIFD1. The details are skipped.

Based on the above theorems, the four FDTD methods studied here share the same temporal/spatial resolution capacity in the nonrelativistic limit regime. In fact, given an accuracy bound ϱ, the ε-scalability of the FDTD methods should be

$$\tau = O(\varepsilon^3 \sqrt{\varrho}) = O(\varepsilon^3), \quad h = O(\sqrt{\varrho \varepsilon}) = O(\sqrt{\varepsilon}), \quad 0 < \varepsilon \leq 1.$$

3.2. The proof of Theorem 3.1. For the CNFD (2.3)-(2.4), we establish the error estimates in Theorem 3.1. The proof is quite different from the conservative FDTD methods for the KGD system in the $O(1)$-speed of light regime [37] and the nonlinear Schrödinger type equations [3, 4, 35, 36]. In fact, due to the ε-dependence of the wave operator ∂_{tt} and the indefiniteness of the 'free' Dirac operator $-\frac{i}{\varepsilon}\sigma_1\partial_x+\frac{\omega}{\varepsilon^2}\sigma_3$ in the KGD (2.1), there is no control on the l^∞ norm of the numerical solution (ϕ^n,Ψ^n) and the nonlinear terms $((\Psi^n)^*\sigma_3\Psi^n$ and $\phi^{n+1/2}\sigma_3\Psi^{n+1/2})$ in 1D by the Sobolev inequality and the energy conservation. Thus, the main difficulty is to show that the numerical solution (ϕ^n,Ψ^n) is uniformly bounded, i.e. $\|\phi^n\|_\infty\lesssim 1$ and $\|\Psi^n\|_\infty\lesssim 1$. There is a good news, in [7, 16, 33], a similar difficulty was tackled by truncating the nonlinearity to a global Lipschitz function with compact support in d-dimensions. Here, we use the same cut-off idea. Choosing a function $\rho(s)\in C_0^\infty(\mathbb{R})$ such that

$$\rho(s)=\begin{cases}1, & |s|\le 1,\\ \in[0,1], & |s|\le 2,\\ 0, & |s|\ge 2.\end{cases}$$

Denote $N_1=(1+N_\Psi)^2>0$, $N_2=(1+N_\phi)^2>0$ and define

$$\mathbf{F}_{N_1}(\Psi)=\rho(|\Psi|^2/N_1)\Psi,\quad \widetilde{F}_{N_2}(\phi)=\rho(|\phi|^2/N_2)\phi,\quad \Psi\in\mathbb{C}^2,\quad \phi\in\mathbb{R},$$

then $\mathbf{F}_{N_1}(\Psi)$ and $\widetilde{F}_{N_2}(\phi)$ have compact support and are smooth and global Lipschitz, i.e there exist $C_{N_1}>0$ and $C_{N_2}>0$, such that $\forall\,\Psi_1,\Psi_2\in\mathbb{C}^2,\phi_1,\phi_2\in\mathbb{R}$,

$$|\mathbf{F}_{N_1}(\Psi_1)-\mathbf{F}_{N_1}(\Psi_2)|\le C_{N_1}|\Psi_1-\Psi_2|,\quad |\widetilde{F}_{N_2}(\phi_1)-\widetilde{F}_{N_2}(\phi_2)|\le C_{N_2}|\phi_1-\phi_2|.\tag{3.6}$$

Set $\widehat{\phi}^0=\phi^0$, $\widehat{\phi}^1=\phi^1$, $\widehat{\Psi}^0=\Psi^0$ and determine $\widehat{\phi}^n\in\widetilde{X}_M$ and $\widehat{\Psi}^n\in X_M$ as follows

$$\varepsilon^2\delta_t^2\widehat{\phi}_j^n-\delta_x^2\mathcal{A}\widehat{\phi}_j^n+\frac{1}{\varepsilon^2}\mathcal{A}\widehat{\phi}_j^n=g(\widehat{\Psi}_j^n)^*\sigma_3\mathbf{F}_{N_1}(\widehat{\Psi}_j^n),\quad j\in\mathscr{T}_M^0,\quad n\ge 1,\tag{3.7}$$

$$i\delta_t^+\widehat{\Psi}_j^n=\left[-\frac{i}{\varepsilon}\sigma_1\delta_x+\frac{\omega}{\varepsilon^2}\sigma_3\right]\widehat{\Psi}_j^{n+1/2}+g\widetilde{F}_{N_2,j}^{n+1/2}\sigma_3\mathbf{F}_{N_1,j}^{n+1/2},\quad j\in\mathscr{T}_M^0,\quad n\ge 0,\tag{3.8}$$

where $\mathbf{F}_{N_1,j}^{n+1/2}=(\mathbf{F}_{N_1}(\widehat{\Psi}_j^{n+1})+\mathbf{F}_{N_1}(\widehat{\Psi}_j^n))/2$ and $\widetilde{F}_{N_2,j}^{n+1/2}=(\widetilde{F}_{N_2}(\widehat{\phi}_j^{n+1})+\widetilde{F}_{N_2}(\widehat{\phi}_j^n))/2$. In fact, we can view $(\widehat{\phi}_j^n,\widehat{\Psi}_j^n)$ as another approximation to $(\phi(t_n,x_j),\Psi(t_n,x_j))$. It is easy to verify that the above scheme (3.7)-(3.8) is uniquely solvable, for sufficiently small τ, using the properties of ρ and standard techniques [3]. Define the corresponding errors as

$$\widehat{\eta}_j^n=\phi(t_n,x_j)-\widehat{\phi}_j^n,\quad \widehat{\mathbf{e}}_j^n=\Psi(t_n,x_j)-\widehat{\Psi}_j^n,\quad j\in\mathscr{T}_M^0,\quad n\ge 0.\tag{3.9}$$

Regarding the error bounds on $(\widehat{\eta}^n,\widehat{\mathbf{e}}^n)$, we have the following estimates.

THEOREM 3.3. *Under the Assumption (A), there exist constants $\tau_0>0$ and $h_0>0$ sufficiently small and independent of ε, such that, for any $0<\varepsilon\le 1$, when $0<\tau\le\tau_0\varepsilon^3$ and $0<h\le h_0\varepsilon^{1/2}$, (3.7)-(3.8) have the error bounds as*

$$\|\widehat{\eta}^n\|+\|\delta_x^+\widehat{\eta}^n\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6},\quad \|\widehat{\mathbf{e}}^n\|+\|\delta_x^+\widehat{\mathbf{e}}^n\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6},\tag{3.10}$$

$$\|\widehat{\phi}^n\|_\infty\le 1+N_\phi,\qquad \|\widehat{\Psi}^n\|_\infty\le 1+N_\Psi,\qquad 0\le n\le\frac{T}{\tau}.\tag{3.11}$$

We begin with the local truncation errors of (3.7)-(3.8) ($\widehat{\zeta}^n$,$\widehat{\theta}^n$) given as

$$\begin{aligned}\widehat{\zeta}_j^n :=& \varepsilon^2\delta_t^2\phi(t_n,x_j) - \frac{1}{2}\delta_x^2(\phi(t_{n+1},x_j)+\phi(t_{n-1},x_j)) + \frac{1}{2\varepsilon^2}(\phi(t_{n+1},x_j)+\phi(t_{n-1},x_j))\\ &- g\Psi^*(t_n,x_j)\sigma_3\Psi(t_n,x_j), \quad j\in\mathscr{T}_M^0, \quad 1\le n\le\frac{T}{\tau}-1, \end{aligned}\tag{3.12}$$

$$\begin{aligned}\widehat{\theta}_j^n :=& i\delta_t^+\Psi(t_n,x_j) + \frac{i}{2\varepsilon}\sigma_1\delta_x(\Psi(t_{n+1},x_j)+\Psi(t_n,x_j)) - \frac{\omega}{2\varepsilon^2}\sigma_3(\Psi(t_{n+1},x_j)+\Psi(t_n,x_j))\\ &- \frac{g}{4}(\phi(t_{n+1},x_j)+\phi(t_n,x_j))\sigma_3(\Psi(t_{n+1},x_j)+\Psi(t_n,x_j)), \quad j\in\mathscr{T}_M^0, \quad 0\le n\le\frac{T}{\tau}-1. \end{aligned}\tag{3.13}$$

The following estimates hold for $\widehat{\zeta}^n$ and $\widehat{\theta}^n$.

LEMMA 3.1 (Local truncation errors $\widehat{\zeta}^n$ and $\widehat{\theta}^n$). *Under the Assumption (A), there exist constants $\tau_0>0$ and $h_0>0$ sufficiently small and independent of ε, s.t., for any $0<\varepsilon\le 1$, when $0<\tau\le\tau_0$ and $0<h\le h_0$, the local truncation errors* (3.12)-(3.13) *satisfy*

$$\|\widehat{\zeta}^n\|+\|\delta_x^+\widehat{\zeta}^n\|\lesssim h^2+\frac{\tau^2}{\varepsilon^6}, 1\le n\le\frac{T}{\tau}-1; \|\widehat{\theta}^n\|+\|\delta_x^+\widehat{\theta}^n\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}, 0\le n\le\frac{T}{\tau}-1. \tag{3.14}$$

Proof. Under the Assumption (A) and noticing (2.1), applying Taylor expansion to the local truncation errors (3.12)-(3.13), we derive that

$$\begin{aligned}|\widehat{\zeta}_j^n| &\le \frac{\tau^2}{12}\varepsilon^2\|\partial_{tttt}\phi\|_{L^\infty} + \frac{\tau^2}{2}\|\partial_{ttxx}\phi\|_{L^\infty} + \frac{\tau^2}{2\varepsilon^2}\|\partial_{tt}\phi\|_{L^\infty} + \frac{h^2}{12}\|\partial_{xxxx}\phi\|_{L^\infty},\\
|\delta_x^+\widehat{\zeta}_j^n| &\le \frac{\tau^2}{12}\varepsilon^2\|\partial_{ttttx}\phi\|_{L^\infty} + \frac{\tau^2}{2}\|\partial_{ttxxx}\phi\|_{L^\infty} + \frac{\tau^2}{2\varepsilon^2}\|\partial_{ttx}\phi\|_{L^\infty} + \frac{h^2}{12}\|\partial_{xxxxx}\phi\|_{L^\infty},\\
|\widehat{\theta}_j^n| &\le \frac{h^2}{6\varepsilon}\|\partial_{xxx}\Psi\|_{L^\infty} + \frac{\tau^2}{6}\|\partial_{ttt}\Psi\|_{L^\infty} + \frac{\tau^2}{4\varepsilon^2}(\varepsilon\|\partial_{xtt}\Psi\|_{L^\infty} + \|\partial_{tt}\Psi\|_{L^\infty})\\
&\quad + \frac{\tau^2}{4}g(\|\phi\|_{L^\infty}\|\partial_{tt}\Psi\|_{L^\infty} + \|\Psi\|_{L^\infty}\|\partial_{tt}\phi\|_{L^\infty} + \|\partial_t\phi\|_{L^\infty}\|\partial_t\Psi\|_{L^\infty}),\\
|\delta_x^+\widehat{\theta}_j^n| &\le \frac{h^2}{6\varepsilon}\|\partial_{xxxx}\Psi\|_{L^\infty} + \frac{\tau^2}{6}\|\partial_{tttx}\Psi\|_{L^\infty} + \frac{\tau^2}{4\varepsilon^2}(\varepsilon\|\partial_{xxtt}\Psi\|_{L^\infty} + \|\partial_{ttx}\Psi\|_{L^\infty})\\
&\quad + \frac{\tau^2}{4}g(\|\phi\|_{L^\infty}\|\partial_{ttx}\Psi\|_{L^\infty} + \|\partial_x\phi\|_{L^\infty}\|\partial_{tt}\Psi\|_{L^\infty} + \|\Psi\|_{L^\infty}\|\partial_{ttx}\phi\|_{L^\infty}\\
&\quad + \|\partial_x\Psi\|_{L^\infty}\|\partial_{tt}\phi\|_{L^\infty} + \|\partial_t\phi\|_{L^\infty}\|\partial_{tx}\Psi\|_{L^\infty} + \|\partial_{tx}\phi\|_{L^\infty}\|\partial_t\Psi\|_{L^\infty}),\end{aligned}$$

with the help of the triangle inequality and the Cauchy-Schwartz inequality.

These immediately imply

$$\|\widehat{\zeta}^n\|_\infty+\|\delta_x^+\widehat{\zeta}^n\|_\infty\lesssim h^2+\frac{\tau^2}{\varepsilon^6}, 1\le n\le\frac{T}{\tau}-1; \|\widehat{\theta}^n\|_\infty+\|\delta_x^+\widehat{\theta}^n\|_\infty\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}, 0\le n\le\frac{T}{\tau}-1.$$

Thus, the conclusions for the local truncation errors follow. ∎

Since the first step is calculated differently from the others, we investigate the first step separately and illustrate the error estimates in the following lemma.

LEMMA 3.2 (Error bounds at $n=1$). *Under the Assumption (A), there exist constants $\tau_0>0$ and $h_0>0$ sufficiently small and independent of ε, such that, for any $0<\varepsilon\le 1$, when $0<\tau\le\tau_0\varepsilon^3$ and $0<h\le h_0\varepsilon^{1/2}$, the error bounds for* (3.7)-(3.8) *at $n=1$ satisfy*

$$\|\widehat{\eta}^1\|+\|\delta_x^+\widehat{\eta}^1\|\lesssim\frac{\tau^3}{\varepsilon^6}, \|\widehat{\mathbf{e}}^1\|+\|\delta_x^+\widehat{\mathbf{e}}^1\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}, \|\widehat{\phi}^1\|_\infty\le 1+N_\phi, \|\widehat{\Psi}^1\|_\infty\le 1+N_\Psi. \tag{3.15}$$

Proof. Under the Assumption (A) and $0<\tau\lesssim\varepsilon^3$, in view of (3.9) for $n=1$, (2.13) implies

$$\begin{aligned}|\widehat{\eta}_j^1|=&\bigg|\frac{\tau^3}{2}\int_0^1(1-s)^2\partial_{ttt}\phi(s\tau,x_j)ds+\Big[\frac{\tau}{\varepsilon^2}-\sin(\frac{\tau}{\varepsilon^2})\Big]\gamma(x_j)+\Big[2\sin^2(\frac{\tau}{2\varepsilon^2})-\frac{\tau^2}{2\varepsilon^4}\Big]\phi^0(x_j)\\&+\Big[\frac{\tau^2}{2\varepsilon^2}-2\sin^2(\frac{\tau}{2\varepsilon})\Big]\cdot\big[(\phi^0)''(x_j)+g(\Psi_j^0)^*\sigma_3\Psi_j^0\big]\bigg|\\ \le&\frac{\tau^3}{6}\|\partial_{ttt}\phi\|_{L^\infty}+\frac{\tau^3}{6\varepsilon^6}\|\gamma(x)\|_{L^\infty(\Omega)}+\frac{\tau^6}{24\varepsilon^{12}}N_\phi+\frac{\tau^6}{24\varepsilon^6}(\|(\phi^0)''(x)\|_{L^\infty(\Omega)}+gN_\Psi^2)\lesssim\frac{\tau^3}{\varepsilon^6},\end{aligned}$$

which also implies that $|\delta_x^+\widehat{\eta}_j^1|\lesssim\frac{\tau^3}{\varepsilon^6}$ and $|\delta_x^2\widehat{\eta}_j^1|\lesssim\frac{\tau^3}{\varepsilon^6}$, $j\in\mathscr{T}_M^0$. The estimates on $\widehat{\eta}^1$ and $\widehat{\phi}^1$ are obvious for sufficiently small τ.

Noticing $\widehat{\mathbf{e}}^0=\mathbf{0}\in X_M$, subtracting (3.8) from (3.13) leads to

$$\frac{i}{\tau}\widehat{\mathbf{e}}_j^1+\frac{i}{2\varepsilon}\sigma_1\delta_x\widehat{\mathbf{e}}_j^1-\frac{\omega}{2\varepsilon^2}\sigma_3\widehat{\mathbf{e}}_j^1=\widehat{\theta}_j^0+\widehat{\chi}_j^0,\quad j\in\mathscr{T}_M^0,\tag{3.16}$$

where

$$\begin{aligned}\widehat{\chi}_j^0=\frac{g}{4}\Big[&\Big(\phi(\tau,x_j)-\widetilde{F}_{N_2}(\widehat{\phi}_j^1)\Big)\sigma_3\Big(\Psi^0(x_j)+\mathbf{F}_{N_1}(\widehat{\Psi}_j^1)\Big)\\&+\big(\phi(\tau,x_j)+\phi^0(x_j)\big)\sigma_3\Big(\Psi(\tau,x_j)-\mathbf{F}_{N_1}(\widehat{\Psi}_j^1)\Big)\Big].\end{aligned}$$

In view of (3.6), we get

$$|\widehat{\chi}_j^0|\le C\Big[\Big(\|\Psi(t,x)\|_{L^\infty}+\Big|\mathbf{F}_{N_1}(\widehat{\Psi}_j^1)\Big|\Big)|\widehat{\eta}_j^1|+\|\phi(t,x)\|_{L^\infty}|\widehat{\mathbf{e}}_j^1|\Big],\quad j\in\mathscr{T}_M^0,\tag{3.17}$$

$$\begin{aligned}|\delta_x^+\widehat{\chi}_j^0|\le C\Big[&\Big(\|\Psi(t,x)\|_{L^\infty}+\Big|\mathbf{F}_{N_1}(\widehat{\Psi}_j^1)\Big|\Big)|\delta_x^+\widehat{\eta}_j^1|+\|\partial_x\Psi(t,x)\|_{L^\infty}|\widehat{\eta}_j^1|+\|\partial_x\phi(t,x)\|_{L^\infty}|\widehat{\mathbf{e}}_j^1|\\&+(\|\phi(t,x)\|_{L^\infty}+\|\widehat{\eta}^1\|_\infty)|\delta_x^+\widehat{\mathbf{e}}_j^1|\Big],\quad j\in\mathscr{T}_M^0,\end{aligned}\tag{3.18}$$

where the constant C is independent of h, τ and ε.

Multiplying $h\tau(\widehat{\mathbf{e}}_j^1)^*$ on both sides of (3.16) from left and summing up over $j\in\mathscr{T}_{M-1}^0$ yields

$$i\|\widehat{\mathbf{e}}^1\|^2+\frac{ih\tau}{2\varepsilon}\sum_{j\in\mathscr{T}_{M-1}^0}(\widehat{\mathbf{e}}_j^1)^*\sigma_1\delta_x\widehat{\mathbf{e}}_j^1-\frac{\omega h\tau}{2\varepsilon^2}\sum_{j\in\mathscr{T}_{M-1}^0}(\widehat{\mathbf{e}}_j^1)^*\sigma_3\widehat{\mathbf{e}}_j^1=h\tau\sum_{j\in\mathscr{T}_{M-1}^0}(\widehat{\mathbf{e}}_j^1)^*(\widehat{\theta}_j^0+\widehat{\chi}_j^0).\tag{3.19}$$

Taking the imaginary parts, we can derive the estimate for $\|\widehat{\mathbf{e}}^1\|$ by the Young's inequality and the triangle inequality, with the help of the property of $\mathbf{F}_{N_1}$,

$$\|\widehat{\mathbf{e}}^1\|^2=Im\Bigg[h\tau\sum_{j\in\mathscr{T}_{M-1}^0}(\widehat{\mathbf{e}}_j^1)^*\Big(\widehat{\theta}_j^0+\widehat{\chi}_j^0\Big)\Bigg]\lesssim\tau\Big(\|\widehat{\mathbf{e}}^1\|^2+\|\widehat{\theta}^0\|^2+\|\widehat{\eta}^1\|^2\Big),$$

where $Im(f)$ denotes the imaginary part of f. Thus, together with Lemma 3.1 and the estimates on $\widehat{\eta}^1$, for sufficiently small τ, the above inequality suggests

$$\|\widehat{\mathbf{e}}^1\|^2\lesssim\tau(\|\widehat{\theta}^0\|^2+\|\widehat{\eta}^1\|^2)\lesssim\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2.\tag{3.20}$$

Similarly as above, multiplying $h\tau(\delta_x^2\widehat{\mathbf{e}}_j^1)^*$ on both sides of (3.16) from left, summing up over $j\in\mathscr{T}_{M-1}^0$ and taking the imaginary parts, we obtain

$$\begin{aligned}\|\delta_x^+\widehat{\mathbf{e}}^1\|^2 &= Im\left[h\tau\sum_{j\in\mathscr{T}_{M-1}^0}(\delta_x^+\widehat{\mathbf{e}}_j^1)^*\delta_x^+(\widehat{\theta}_j^0+\widehat{\chi}_j^0)\right]\\ &\lesssim \tau\left(\|\delta_x^+\widehat{\mathbf{e}}^1\|^2+\|\widehat{\mathbf{e}}^1\|^2+\|\delta_x^+\widehat{\theta}^0\|^2+\|\delta_x^+\widehat{\eta}^1\|^2+\|\widehat{\eta}^1\|^2\right).\end{aligned}$$

For sufficiently small τ, Lemma 3.1, (3.20) and the estimates on $\widehat{\eta}^1$ imply

$$\|\delta_x^+\widehat{\mathbf{e}}^1\|^2 \lesssim \tau\left(\|\widehat{\mathbf{e}}^1\|^2+\|\delta_x^+\widehat{\theta}^0\|^2+\|\delta_x^+\widehat{\eta}^1\|^2+\|\widehat{\eta}^1\|^2\right) \lesssim \left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2. \tag{3.21}$$

Thus, the error estimates on $\widehat{\mathbf{e}}^1$ are proved. It remains to estimate $\|\widehat{\Psi}^1\|_\infty$. Using the discrete Sobolev inequality, for sufficiently small $0<\tau\lesssim\varepsilon^3/\sqrt{C_d(h)}$ and $0<h\lesssim\varepsilon^{1/2}/\sqrt{C_d(h)}$, we have

$$\|\widehat{\mathbf{e}}^1\|_\infty \le C_d(h)(\|\widehat{\mathbf{e}}^1\|+\|\delta_x^+\widehat{\mathbf{e}}^1\|) \le C\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right) \le 1,$$

and $\|\widehat{\Psi}^1\|_\infty \le \|\Psi(t,x)\|_{L^\infty}+\|\widehat{\mathbf{e}}^1\|_\infty \le N_\Psi+1$. ∎

Next, we study the growth of the errors. Subtracting (3.7)-(3.8) from (3.12)-(3.13), respectively, we have the error equations as

$$\varepsilon^2\delta_t^2\widehat{\eta}_j^n-\frac{1}{2}(\delta_x^2\widehat{\eta}_j^{n+1}+\delta_x^2\widehat{\eta}_j^{n-1})+\frac{1}{2\varepsilon^2}(\widehat{\eta}_j^{n+1}+\widehat{\eta}_j^{n-1})=\widehat{\zeta}_j^n+\widehat{\lambda}_j^n,\quad 1\le n\le\frac{T}{\tau}-1, \tag{3.22}$$

$$i\delta_t^+\widehat{\mathbf{e}}_j^n+\frac{i}{2\varepsilon}\sigma_1(\delta_x\widehat{\mathbf{e}}_j^{n+1}+\delta_x\widehat{\mathbf{e}}_j^n)-\frac{\omega}{2\varepsilon^2}\sigma_3(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^n)=\widehat{\theta}_j^n+\widehat{\chi}_j^n,\quad 0\le n\le\frac{T}{\tau}-1, \tag{3.23}$$

$$\widehat{\eta}_0^n=\widehat{\eta}_M^n,\quad \widehat{\eta}_{-1}^n=\widehat{\eta}_{M-1}^n,\quad \widehat{\eta}_j^0=0,\quad \widehat{\mathbf{e}}_0^n=\widehat{\mathbf{e}}_M^n,\quad \widehat{\mathbf{e}}_{-1}^n=\widehat{\mathbf{e}}_{M-1}^n,\ \widehat{\mathbf{e}}_j^0=0,\ j\in\mathscr{T}_M^0, \tag{3.24}$$

where $\widehat{\lambda}^n=(\widehat{\lambda}_0^n,\widehat{\lambda}_1^n,\cdots,\widehat{\lambda}_M^n)^T\in\widetilde{X}_M$ and $\widehat{\chi}^n=(\widehat{\chi}_0^n,\widehat{\chi}_1^n,\cdots,\widehat{\chi}_M^n)^T\in X_M$ are the errors of the nonlinear terms as

$$\widehat{\lambda}_j^n := g\left[\Psi^*(t_n,x_j)\sigma_3\Psi(t_n,x_j)-(\widehat{\Psi}_j^n)^*\sigma_3\mathbf{F}_{N_1}(\widehat{\Psi}_j^n)\right], \tag{3.25}$$

$$\widehat{\chi}_j^n := g\left[\phi^{n+1/2}(x_j)\sigma_3\Psi^{n+1/2}(x_j)-\widetilde{F}_{N_2,j}^{n+1/2}\sigma_3\mathbf{F}_{N_1,j}^{n+1/2}\right], \tag{3.26}$$

where $u^{n+1/2}(x_j)=(u(t_{n+1},x_j)+u(t_n,x_j))/2$ with $u=\Psi$ or $u=\phi$.

In order to prove Theorem 3.3, we control the nonlinear terms as follows.

LEMMA 3.3. *Under the Assumption (A), the nonlinear terms $\widehat{\lambda}^n$ and $\widehat{\chi}^n$ ($1\le n\le\frac{T}{\tau}-1$) satisfy*

$$\|\widehat{\lambda}^n\|\lesssim\|\widehat{\mathbf{e}}^n\|,\quad \|\delta_x^+\widehat{\lambda}^n\|\lesssim\|\delta_x^+\widehat{\mathbf{e}}^n\|+\|\widehat{\mathbf{e}}^n\|,\quad \|\widehat{\chi}^n\|\lesssim\|\widehat{\mathbf{e}}^{n+1/2}\|+\|\widehat{\eta}^{n+1/2}\|, \tag{3.27}$$

$$\|\delta_x^+\widehat{\chi}^n\|\lesssim\|\widehat{\mathbf{e}}^{n+1/2}\|+\|\delta_x^+\widehat{\mathbf{e}}^{n+1/2}\|+\|\widehat{\eta}^{n+1/2}\|+\|\delta_x^+\widehat{\eta}^{n+1/2}\|. \tag{3.28}$$

Proof. Noticing (3.6) and (3.25)-(3.26), by direct calculation for $j\in\mathscr{T}_M^0$ and $1\le n\le\frac{T}{\tau}-1$, we get

$$|\widehat{\lambda}_j^n|\le C\left(N_\Psi+\left|\mathbf{F}_{N_1}(\widehat{\Psi}_j^n)\right|\right)|\widehat{\mathbf{e}}_j^n|,\qquad |\widehat{\chi}_j^n|\le C\left(N_\Psi\left|\widehat{\eta}_j^{n+1/2}\right|+\left|\widetilde{F}_{N_2,j}^{n+1/2}\right|\cdot\left|\widehat{\mathbf{e}}_j^{n+1/2}\right|\right),$$

$$
\begin{aligned}
|\delta_x^+\widehat{\lambda}_j^n| \le & C\left[\left(\|\partial_x\Psi\|_{L^\infty}+\left|\delta_x^+\mathbf{F}_{N_1}(\widehat{\Psi}_j^n)\right|\right)|\widehat{\mathbf{e}}_j^n|+\left(N_\Psi+\left|\mathbf{F}_{N_1}(\widehat{\Psi}_j^n)\right|\right)|\delta_x^+\widehat{\mathbf{e}}_j^n|\right],\\
|\delta_x^+\widehat{\chi}_j^n| \le & C\Big[\|\partial_x\Psi\|_{L^\infty}\left|\widehat{\eta}_j^{n+1/2}\right|+N_\Psi\left|\delta_x^+\widehat{\eta}_j^{n+1/2}\right|+\left|\delta_x^+\widetilde{F}_{N_2,j}^{n+1/2}\right|\cdot\left|\widehat{\mathbf{e}}_j^{n+1/2}\right|\\
&+\left|\widetilde{F}_{N_2,j}^{n+1/2}\right|\cdot\left|\delta_x^+\widehat{\mathbf{e}}_j^{n+1/2}\right|\Big],
\end{aligned}
$$

where the constant C is independent of h, τ and ε. Under the Assumption (A), combining the above inequalities with the properties of $\mathbf{F}_{N_1}$ and $\widetilde{F}_{N_2}$ will complete the proof.

∎

Proof. **(Proof of Theorem 3.3.)** When $n=0$, the estimates in (3.10)-(3.11) are obvious and the $n=1$ case is already verified in Lemma 3.2 for sufficiently small $0<\tau<\tau_1$ and $0<h<h_1$. Thus we only need to prove (3.10)-(3.11) for $2\le n\le\frac{T}{\tau}$. The proof is divided into two parts.

Part 1. (estimate $\|\widehat{\eta}^{n+1}\|+\|\delta_x^+\widehat{\eta}^{n+1}\|+\|\widehat{\mathbf{e}}^{n+1}\|+\|\delta_x^+\widehat{\mathbf{e}}^{n+1}\|$ for $1\le n\le\frac{T}{\tau}-1$): computing $h(\widehat{\eta}_j^{n+1}-\widehat{\eta}_j^{n-1})^*(3.22)$ $-h(\delta_x^2\widehat{\eta}_j^{n+1}-\delta_x^2\widehat{\eta}_j^{n-1})^*(3.22)$, summing up over $j\in\mathscr{T}_{M-1}^0$ and applying the Cauchy inequality, Lemmas 3.1 & 3.3 imply

$$
\begin{aligned}
&\varepsilon^2(\|\delta_t^+\widehat{\eta}^n\|^2-\|\delta_t^+\widehat{\eta}^{n-1}\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^n\|^2-\|\delta_x^+\delta_t^+\widehat{\eta}^{n-1}\|^2)+\frac{1}{2}(\|\delta_x^+\widehat{\eta}^{n+1}\|^2-\|\delta_x^+\widehat{\eta}^{n-1}\|^2\\
&\quad+\|\delta_x^2\widehat{\eta}^{n+1}\|^2-\|\delta_x^2\widehat{\eta}^{n-1}\|^2)+\frac{1}{2\varepsilon^2}(\|\widehat{\eta}^{n+1}\|^2-\|\widehat{\eta}^{n-1}\|^2+\|\delta_x^+\widehat{\eta}^{n+1}\|^2-\|\delta_x^+\widehat{\eta}^{n-1}\|^2)\\
=&h\sum_{j\in\mathscr{T}_{M-1}^0}\left[(\widehat{\eta}_j^{n+1}-\widehat{\eta}_j^{n-1})(\widehat{\zeta}_j^n+\widehat{\lambda}_j^n)+\delta_x^+(\widehat{\eta}_j^{n+1}-\widehat{\eta}_j^{n-1})\delta_x^+(\widehat{\zeta}_j^n+\widehat{\lambda}_j^n)\right]\\
\le&\tau\varepsilon^2(\|\delta_t^+\widehat{\eta}^n\|^2+\|\delta_t^+\widehat{\eta}^{n-1}\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^n\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^{n-1}\|^2)\\
&+\frac{\tau}{\varepsilon^2}(\|\widehat{\zeta}^n\|^2+\|\widehat{\lambda}^n\|^2+\|\delta_x^+\widehat{\zeta}^n\|^2+\|\delta_x^+\widehat{\lambda}^n\|^2)\\
\lesssim&\tau\varepsilon^2(\|\delta_t^+\widehat{\eta}^n\|^2+\|\delta_t^+\widehat{\eta}^{n-1}\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^n\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^{n-1}\|^2)\\
&+\frac{\tau}{\varepsilon^2}\left[\|\widehat{\mathbf{e}}^n\|^2+\|\delta_x^+\widehat{\mathbf{e}}^n\|^2+\left(h^2+\frac{\tau^2}{\varepsilon^6}\right)^2\right],\quad 1\le n\le\frac{T}{\tau}-1.
\end{aligned}\tag{3.29}
$$

Then, computing $h\tau(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^n)^*(3.23)$ $-h\tau\delta_x^2(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^n)^*(3.23)$, taking the imaginary parts, summing up over $j\in\mathscr{T}_{M-1}^0$ and making use of the triangle inequality, the Cauchy inequality and Lemmas 3.1 & 3.3, we derive

$$
\begin{aligned}
&\|\widehat{\mathbf{e}}^{n+1}\|^2-\|\widehat{\mathbf{e}}^n\|^2+\|\delta_x^+\widehat{\mathbf{e}}^{n+1}\|^2-\|\delta_x^+\widehat{\mathbf{e}}^n\|^2\\
=&2h\tau\sum_{j\in\mathscr{T}_{M-1}^0}Im\left[(\widehat{\mathbf{e}}_j^{n+1/2})^*(\widehat{\theta}_j^n+\widehat{\chi}_j^n)+\delta_x^+(\widehat{\mathbf{e}}_j^{n+1/2})^*\delta_x^+(\widehat{\theta}_j^n+\widehat{\chi}_j^n)\right]\\
\le&\tau(\|\widehat{\mathbf{e}}^{n+1}\|^2+\|\widehat{\mathbf{e}}^n\|^2+\|\delta_x^+\widehat{\mathbf{e}}^{n+1}\|^2+\|\delta_x^+\widehat{\mathbf{e}}^n\|^2+\|\widehat{\theta}^n\|^2+\|\widehat{\chi}^n\|^2+\|\delta_x^+\widehat{\theta}^n\|^2+\|\delta_x^+\widehat{\chi}^n\|^2)\\
\lesssim&\tau\sum_{k=n}^{n+1}(\|\widehat{\mathbf{e}}^k\|^2+\|\delta_x^+\widehat{\mathbf{e}}^k\|^2+\|\widehat{\eta}^k\|^2+\|\delta_x^+\widehat{\eta}^k\|^2)+\tau\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\ 1\le n\le\frac{T}{\tau}-1.
\end{aligned}\tag{3.30}
$$

Define

$$
\mathcal{S}^n=\varepsilon^2(\|\delta_t^+\widehat{\eta}^n\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^n\|^2)+\frac{1}{2\varepsilon^2}\sum_{k=n}^{n+1}\left[\varepsilon^2(\|\delta_x^+\widehat{\eta}^k\|^2+\|\delta_x^2\widehat{\eta}^k\|^2)+\|\widehat{\eta}^k\|^2+\|\delta_x^+\widehat{\eta}^k\|^2\right]
$$

$$+\frac{1}{\varepsilon^2}(\|\widehat{\mathbf{e}}^{n+1}\|^2+\|\delta_x^+\widehat{\mathbf{e}}^{n+1}\|^2),\quad n\geq 0. \tag{3.31}$$

Under the condition $0<\tau\leq\tau_2\varepsilon^3$ for some $\tau_2>0$, in view of the initial data (3.24) and Lemma 3.2, we get

$$\begin{aligned}\mathcal{S}^0=&\varepsilon^2(\|\delta_t^+\widehat{\eta}^0\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^0\|^2)+\frac{1}{2\varepsilon^2}\left[\varepsilon^2(\|\delta_x^+\widehat{\eta}^1\|^2+\|\delta_x^2\widehat{\eta}^1\|^2)+\|\widehat{\eta}^1\|^2+\|\delta_x^+\widehat{\eta}^1\|^2\right]\\&+\frac{1}{\varepsilon^2}(\|\widehat{\mathbf{e}}^1\|^2+\|\delta_x^+\widehat{\mathbf{e}}^1\|^2)\lesssim\frac{1}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2.\end{aligned}$$

The inequalities (3.29) and (3.30) imply

$$\mathcal{S}^n-\mathcal{S}^{n-1}\lesssim\tau(\mathcal{S}^n+\mathcal{S}^{n-1})+\frac{\tau}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\quad 1\leq n\leq\frac{T}{\tau}-1.$$

Summing the above inequalities for time steps from 1 to n, we have

$$\mathcal{S}^n-\mathcal{S}^0\lesssim\tau\sum_{k=0}^{n}\mathcal{S}^k+\frac{T}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\quad 1\leq n\leq\frac{T}{\tau}-1.$$

Hence, the discrete Gronwall's inequality [26, 30] would suggest that there exists a constant $\tau_3>0$, sufficiently small; such that, when $0<\tau\leq\tau_3$, the following holds

$$\mathcal{S}^n\lesssim\mathcal{S}^0+\frac{T}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\quad 1\leq n\leq\frac{T}{\tau}-1. \tag{3.32}$$

Recalling (3.31), we obtain

$$\|\widehat{\eta}^{n+1}\|+\|\delta_x^+\widehat{\eta}^{n+1}\|+\|\widehat{\mathbf{e}}^{n+1}\|^2+\|\delta_x^+\widehat{\mathbf{e}}^{n+1}\|^2\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6},\quad 1\leq n\leq\frac{T}{\tau}-1. \tag{3.33}$$

Part 2. (estimate $\|\widehat{\phi}^{n+1}\|_\infty$ and $\|\widehat{\Psi}^{n+1}\|_\infty$ for $1\leq n\leq\frac{T}{\tau}-1$): the discrete Sobolev inequality will imply

$$\|\widehat{\eta}^{n+1}\|_\infty\leq C_d(h)(\|\widehat{\eta}^{n+1}\|+\|\delta_x^+\widehat{\eta}^{n+1}\|)\leq C\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right),\quad \|\widehat{\mathbf{e}}^{n+1}\|_\infty\leq C\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right).$$

Thus, there exist $h_2>0$ and $\tau_4>0$, sufficiently small; when $0<h\leq h_2\varepsilon^{1/2}/\sqrt{C_d(h)}$ and $0<\tau\leq\tau_4\varepsilon^3/\sqrt{C_d(h)}$, we get

$$\begin{aligned}&\|\widehat{\phi}^{n+1}\|_\infty\leq\|\phi(t_{n+1},x)\|_{L^\infty}+\|\widehat{\eta}^{n+1}\|_\infty\leq N_\phi+1,\\&\|\widehat{\Psi}^{n+1}\|_\infty\leq\|\Psi(t_{n+1},x)\|_{L^\infty}+\|\widehat{\mathbf{e}}^{n+1}\|_\infty\leq N_\Psi+1.\end{aligned}$$

The proof of Theorem 3.3 is then complete by choosing $\tau_0=\min\{\tau_1,\tau_2,\tau_3,\tau_4\}$ and $h_0=\min\{h_1,h_2\}$. ∎

Proof. **(Proof of Theorem 3.1.)** In view of the definition of ρ, Theorem 3.3 implies that (3.7)-(3.8) collapse to (2.3)-(2.4). By the unique solvability of the CNFD (c.f. Remark 2.1), $(\widehat{\phi}^n,\widehat{\Psi}^n)$ is identical to (ϕ^n,Ψ^n). Thus Theorem 3.1 is a direct consequence of Theorem 3.3. ∎

3.3. The proof of Theorem 3.2. For the SIFD1 (2.5)-(2.6), we establish the estimates in Theorem 3.2. Throughout this section, the stability condition $\tau \le \alpha\varepsilon^2 h/\sqrt{h^2+\varepsilon^2}$ $(0<\alpha<1)$ is assumed. Here, we sketch the proof and omit those parts similar to the proof in Section 3.2.

Determine another approximation to $(\phi(t_n,x_j),\Psi(t_n,x_j))$ from

$$\varepsilon^2\delta_t^2\widehat{\phi}_j^n-\delta_x^2\widehat{\phi}_j^n+\frac{1}{\varepsilon^2}\mathcal{A}\widehat{\phi}_j^n=g(\widehat{\Psi}_j^n)^*\sigma_3\mathbf{F}_{N_1}(\widehat{\Psi}_j^n),\ \widehat{\phi}^0=\phi^0,\ \widehat{\phi}^1=\phi^1,\ j\in\mathcal{T}_M^0,\ n\ge 1, \tag{3.34}$$

$$i\delta_t\widehat{\Psi}_j^n=\left[-\frac{i}{\varepsilon}\sigma_1\delta_x+\frac{\omega}{\varepsilon^2}\sigma_3\right]\mathcal{A}\widehat{\Psi}_j^n+g\widetilde{F}_{N_2}(\widehat{\phi}_j^n)\sigma_3\mathcal{A}\mathbf{F}_{N_1,j}^n,\widehat{\Psi}^0=\Psi^0,\widehat{\Psi}^1=\Psi^1,j\in\mathcal{T}_M^0,n\ge 1, \tag{3.35}$$

where $\mathcal{A}\mathbf{F}_{N_1,j}^n=[\mathbf{F}_{N_1}(\widehat{\Psi}_j^{n+1})+\mathbf{F}_{N_1}(\widehat{\Psi}_j^{n-1})]/2$. For sufficiently small τ, the unique solvability of (3.34)-(3.35) holds true in view of the Lipschitz property of $\mathbf{F}_{N_1}$ and $\widetilde{F}_{N_2}$. Introduce the error functions as

$$\widehat{\mathbf{e}}_j^n=\Psi(t_n,x_j)-\widehat{\Psi}_j^n,\quad \widehat{\eta}_j^n=\phi(t_n,x_j)-\widehat{\phi}_j^n,\quad j\in\mathcal{T}_M^0,\quad 0\le n\le\frac{T}{\tau}, \tag{3.36}$$

then the following error estimates hold.

THEOREM 3.4. *Under the Assumption (A), there exist constants $h_0>0$ and $\tau_0>0$ sufficiently small and independent of ε, such that, for any $0<\varepsilon\le 1$, when $0<h\le h_0\varepsilon^{1/2}$ and $0<\tau\le\tau_0\varepsilon^3$,* (3.34)-(3.35) *have the error bounds as*

$$\|\widehat{\eta}^n\|+\|\delta_x^+\widehat{\eta}^n\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6},\quad \|\widehat{\mathbf{e}}^n\|+\|\delta_x^+\widehat{\mathbf{e}}^n\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}, \tag{3.37}$$

$$\|\widehat{\phi}^n\|_\infty\le 1+N_\phi,\qquad \|\widehat{\Psi}^n\|_\infty\le 1+N_\Psi,\qquad 0\le n\le\frac{T}{\tau}. \tag{3.38}$$

Similar to the proof of Theorem 3.1, if Theorem 3.4 holds, $(\widehat{\phi}^n,\widehat{\Psi}^n)$ is then identical to (ϕ^n,Ψ^n), and Theorem 3.2 holds ture. Thus, we only need to show the proof of Theorem 3.4. We use similar notations as those in Section 3.2 and denote the local truncation errors $\widehat{\theta}^n=(\widehat{\theta}_0^n,\widehat{\theta}_1^n,\cdots,\widehat{\theta}_M^n)^T\in X_M$ and $\widehat{\zeta}^n=(\widehat{\zeta}_0^n,\widehat{\zeta}_1^n,\cdots,\widehat{\zeta}_M^n)^T\in\widetilde{X}_M$ of (3.34)-(3.35) as

$$\widehat{\zeta}_j^n:=\varepsilon^2\delta_t^2\phi(t_n,x_j)-\delta_x^2\phi(t_n,x_j)+\frac{1}{2\varepsilon^2}(\phi(t_{n+1},x_j)+\phi(t_{n-1},x_j))-g\Psi^*(t_n,x_j)\sigma_3\Psi(t_n,x_j), \tag{3.39}$$

$$\begin{aligned}\widehat{\theta}_j^n:=&i\delta_t\Psi(t_n,x_j)+\frac{i}{2\varepsilon}\sigma_1\delta_x(\Psi(t_{n+1},x_j)+\Psi(t_{n-1},x_j))-\frac{\omega}{2\varepsilon^2}\sigma_3(\Psi(t_{n+1},x_j)+\Psi(t_{n-1},x_j))\\&-\frac{g}{2}\phi(t_n,x_j)\sigma_3(\Psi(t_{n+1},x_j)+\Psi(t_{n-1},x_j)),\quad j\in\mathcal{T}_M^0,\quad 1\le n\le\frac{T}{\tau}-1.\end{aligned} \tag{3.40}$$

Similarly as Lemma 3.1, under the Assumption (A), we have the estimates on $(\widehat{\zeta}^n,\widehat{\theta}^n)$ as

$$\|\widehat{\zeta}^n\|+\|\delta_x^+\widehat{\zeta}^n\|\lesssim h^2+\frac{\tau^2}{\varepsilon^6},\quad \|\widehat{\theta}^n\|+\|\delta_x^+\widehat{\theta}^n\|\lesssim\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6},\quad 1\le n\le\frac{T}{\tau}-1. \tag{3.41}$$

The error equations for (3.34)-(3.35) can be derived as

$$\varepsilon^2\delta_t^2\widehat{\eta}_j^n-\frac{1}{2}\delta_x^2\widehat{\eta}_j^n+\frac{1}{2\varepsilon^2}(\widehat{\eta}_j^{n+1}+\widehat{\eta}_j^{n-1})=\widehat{\zeta}_j^n+\widehat{\lambda}_j^n,\quad 1\le n\le\frac{T}{\tau}-1, \tag{3.42}$$

$$i\delta_t\widehat{\mathbf{e}}_j^n+\frac{i}{2\varepsilon}\sigma_1\delta_x(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^{n-1})-\frac{\omega}{2\varepsilon^2}\sigma_3(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^{n-1})=\widehat{\theta}_j^n+\widehat{\chi}_j^n,\ 1\le n\le\frac{T}{\tau}-1,\quad(3.43)$$

$$\widehat{\eta}_0^n=\widehat{\eta}_M^n,\quad \widehat{\eta}_{-1}^n=\widehat{\eta}_{M-1}^n,\quad \widehat{\eta}_j^0=0,\quad \widehat{\mathbf{e}}_0^n=\widehat{\mathbf{e}}_M^n,\quad \widehat{\mathbf{e}}_{-1}^n=\widehat{\mathbf{e}}_{M-1}^n,\ \widehat{\mathbf{e}}_j^0=0,\ j\in\mathscr{T}_M^0,\quad(3.44)$$

where $\lambda^n=(\lambda_0^n,\lambda_1^n,\cdots,\lambda_M^n)^T\in\widetilde{X}_M$ and $\chi^n=(\chi_0^n,\chi_1^n,\cdots,\ \chi_M^n)^T\in X_M$ $(1\le n\le T/\tau-1)$ are given below

$$\widehat{\lambda}_j^n:=g\left[\Psi^*(t_n,x_j)\sigma_3\Psi(t_n,x_j)-(\widehat{\Psi}_j^n)^*\sigma_3\mathbf{F}_{N_1}(\widehat{\Psi}_j^n)\right],\quad j\in\mathscr{T}_M^0,\tag{3.45}$$

$$\widehat{\chi}_j^n:=g\left[\frac{1}{2}\phi(t_n,x_j)\sigma_3(\Psi(t_{n+1},x_j)+\Psi(t_{n-1},x_j))-\widetilde{F}_{N_2}(\widehat{\phi}_j^n)\sigma_3\mathcal{A}\mathbf{F}_{N_1,j}^n\right],\tag{3.46}$$

and can be controlled as

$$\|\widehat{\lambda}^n\|\lesssim\|\widehat{\mathbf{e}}^n\|,\quad \|\delta_x^+\widehat{\lambda}_j^n\|\lesssim\|\delta_x^+\widehat{\mathbf{e}}^n\|+\|\widehat{\mathbf{e}}^n\|,\quad \|\widehat{\chi}^n\|\lesssim\|\widehat{\mathbf{e}}^{n+1}\|+\|\widehat{\mathbf{e}}^{n-1}\|+\|\widehat{\eta}^n\|,\tag{3.47}$$

$$\|\delta_x^+\widehat{\chi}^n\|\lesssim\|\delta_x^+\widehat{\mathbf{e}}^{n+1}\|+\|\delta_x^+\widehat{\mathbf{e}}^{n-1}\|+\|\delta_x^+\widehat{\eta}^n\|+\|\widehat{\mathbf{e}}^{n+1}\|+\|\widehat{\mathbf{e}}^{n-1}\|+\|\widehat{\eta}^n\|.\tag{3.48}$$

Now we proceed to prove Theorem 3.4.

Proof. **(Proof of Theorem 3.4.)** Since the conclusions in (3.37)-(3.38) for $n=0$ are obvious, thus we only need to prove (3.37)-(3.38) for $1\le n\le\frac{T}{\tau}$. For $n=1$, similar as Lemma 3.2, under the Assumption (A) and the stability condition $\tau\le\alpha\varepsilon^2h/\sqrt{h^2+\varepsilon^2}$ $(0<\alpha<1)$, we can derive

$$\begin{aligned}|\widehat{\mathbf{e}}_j^1|&=\left|\tau^2\int_0^1(1-s)\partial_{tt}\Psi(s\tau,x_j)ds+i\omega\left[\sin\left(\frac{\tau}{\varepsilon^2}\right)-\frac{\tau}{\varepsilon^2}\right]\sigma_3\Psi_j^0+\left[\sin\left(\frac{\tau}{\varepsilon}\right)-\frac{\tau}{\varepsilon}\right]\cdot\sigma_1(\Psi^0)'(x_j)\right|\\&\le\frac{\tau^2}{2}\|\partial_{tt}\Psi\|_{L^\infty}+\frac{\omega\tau^3}{6\varepsilon^6}\|\Psi^0(x)\|_{L^\infty(\Omega)}+\frac{\tau^3}{2\varepsilon^3}\|(\Psi^0)'(x)\|_{L^\infty(\Omega)}\le C\frac{\tau^2}{\varepsilon^4}\le1,\end{aligned}$$

and $|\widehat{\eta}^1|+|\delta_x^+\widehat{\eta}^1|\le C\dfrac{\tau^3}{\varepsilon^6}\le1$. The conclusions of Theorem 3.4 at $n=1$ follow by the triangle inequality with sufficiently small $0<\tau\le\tau_1\varepsilon^3$ $(\tau_1>0)$.

Next, we estimate $\|\eta^{n+1}\|+\|\delta_x^+\eta^{n+1}\|+\|\mathbf{e}^{n+1}\|+\|\delta_x^+\mathbf{e}^{n+1}\|$ for $1\le n\le\frac{T}{\tau}-1$. Define

$$\begin{aligned}\mathcal{S}^n=&\left(\varepsilon^2-\frac{\tau^2}{h^2}\right)(\|\delta_t^+\widehat{\eta}^n\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^n\|^2)+\frac{1}{2\varepsilon^2}\sum_{k=n}^{n+1}\left(\|\widehat{\eta}^k\|^2+\|\widehat{\mathbf{e}}^k\|^2+\|\delta_x^+\widehat{\eta}^k\|^2+\|\delta_x^+\widehat{\mathbf{e}}^k\|^2\right)\\&+\frac{1}{2h}\sum_{j\in\mathscr{T}_{M-1}^0}\left[(\widehat{\eta}_{j+1}^{n+1}-\widehat{\eta}_j^n)^2+(\widehat{\eta}_{j+1}^n-\widehat{\eta}_j^{n+1})^2+(\delta_x^+\widehat{\eta}_{j+1}^{n+1}-\delta_x^+\widehat{\eta}_j^n)^2\right.\\&\qquad\left.+(\delta_x^+\widehat{\eta}_{j+1}^n-\delta_x^+\widehat{\eta}_j^{n+1})^2\right].\end{aligned}\tag{3.49}$$

Under the stability condition $\tau\le\alpha\varepsilon^2h/\sqrt{h^2+\varepsilon^2}$ $(0<\alpha<1)$, using the estimates for $\widehat{\eta}_j^1$ and $\widehat{\mathbf{e}}^1$, we can conclude that

$$\mathcal{S}^0=\varepsilon^2(\|\delta_t^+\widehat{\eta}^0\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^0\|^2)+\frac{1}{2\varepsilon^2}(\|\widehat{\eta}^1\|^2+\|\widehat{\mathbf{e}}^1\|^2+\|\delta_x^+\widehat{\eta}^1\|^2+\|\delta_x^+\widehat{\mathbf{e}}^1\|^2)\lesssim\frac{\tau^4}{\varepsilon^{10}},\tag{3.50}$$

and for $0<\varepsilon^2C_b=\varepsilon^2(1-\alpha^2)\le\varepsilon^2-\tau^2/h^2$ (using the stability assumption to get $\tau^2/h^2\le\varepsilon^2\alpha^2$), we have

$$\mathcal{S}^n\ge\frac{1}{2\varepsilon^2}\sum_{k=n}^{n+1}\left(\|\widehat{\eta}^k\|^2+\|\widehat{\mathbf{e}}^k\|^2+\|\delta_x^+\widehat{\eta}^k\|^2+\|\delta_x^+\widehat{\mathbf{e}}^k\|^2\right)+C_b\varepsilon^2(\|\delta_t^+\widehat{\eta}^n\|^2+\|\delta_x^+\delta_t^+\widehat{\eta}^n\|^2).\tag{3.51}$$

On the one hand, computing $h(\widehat{\eta}_j^{n+1}-\widehat{\eta}_j^{n-1})^*(3.42)-h\delta_x^2(\widehat{\eta}_j^{n+1}-\widehat{\eta}_j^{n-1})^*(3.42)$, summing up over $j\in\mathscr{T}_{M-1}^0$, using the summation by parts formula, (3.41) and (3.47), for $1\le n\le \frac{T}{\tau}-1$, we obtain

$$\begin{aligned}
&\left(\varepsilon^2-\frac{\tau^2}{h^2}\right)\left(\|\delta_t^+\eta^n\|^2-\|\delta_t^+\eta^{n-1}\|^2+\|\delta_x^+\delta_t^+\eta^n\|^2-\|\delta_x^+\delta_t^+\eta^{n-1}\|^2\right)\\
&\quad+\frac{1}{2\varepsilon^2}\left(\|\eta^{n+1}\|^2-\|\eta^{n-1}\|^2+\|\delta_x^+\eta^{n+1}\|^2-\|\delta_x^+\eta^{n-1}\|^2\right)\\
&\quad+\frac{1}{2h}\sum_{j\in\mathscr{T}_{M-1}^0}\left[(\eta_{j+1}^{n+1}-\eta_j^n)^2+(\eta_{j+1}^n-\eta_j^{n+1})^2-(\eta_{j+1}^n-\eta_j^{n-1})^2-(\eta_{j+1}^{n-1}-\eta_j^n)^2\right]\\
&\quad+\frac{1}{2h}\sum_{j\in\mathscr{T}_{M-1}^0}\Big[(\delta_t^+\eta_{j+1}^{n+1}-\delta_t^+\eta_j^n)^2+(\delta_t^+\eta_{j+1}^n-\delta_t^+\eta_j^{n+1})^2-(\delta_t^+\eta_{j+1}^n-\delta_t^+\eta_j^{n-1})^2\\
&\qquad\qquad\qquad-(\delta_t^+\eta_{j+1}^{n-1}-\delta_t^+\eta_j^n)^2\Big]\\
&=h\sum_{j\in\mathscr{T}_{M-1}^0}\left[(\zeta_j^n+\lambda_j^n)(\eta_j^{n+1}-\eta_j^{n-1})+\delta_x^+(\zeta_j^n+\lambda_j^n)\delta_x^+(\eta_j^{n+1}-\eta_j^{n-1})\right]\\
&\lesssim\varepsilon^2\tau\sum_{k=n-1}^{n}\left(\|\delta_t^+\eta^k\|^2+\|\delta_x^+\delta_t^+\eta^k\|^2\right)+\frac{\tau}{\varepsilon^2}\left(\|\delta_x^+\mathbf{e}^n\|^2+\|\mathbf{e}^n\|^2\right)+\frac{\tau}{\varepsilon^2}\left(h^2+\frac{\tau^2}{\varepsilon^6}\right)^2.
\end{aligned}\tag{3.52}$$

On the other hand, computing $2h\tau(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^{n-1})^*(3.43)-2h\tau\delta_x^2(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^{n-1})^*$ (3.43), taking the imaginary parts, summing up over $j\in\mathscr{T}_{M-1}^0$, in view of (3.41), (3.47) and (3.48), for $1\le n\le\frac{T}{\tau}-1$, we could get

$$\begin{aligned}
&\|\mathbf{e}^{n+1}\|^2-\|\mathbf{e}^{n-1}\|^2+\|\delta_x^+\mathbf{e}^{n+1}\|^2-\|\delta_x^+\mathbf{e}^{n-1}\|^2\\
&=h\tau\sum_{j\in\mathscr{T}_{M-1}^0}Im\left[\left(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^{n-1}\right)^*(\widehat{\theta}_j^n+\widehat{\chi}_j^n)+\delta_x^+\left(\widehat{\mathbf{e}}_j^{n+1}+\widehat{\mathbf{e}}_j^{n-1}\right)^*\delta_x^+(\widehat{\theta}_j^n+\widehat{\chi}_j^n)\right]\\
&\lesssim\tau\left(\sum_{k=n+1,n-1}\left(\|\mathbf{e}^k\|^2+\|\delta_x^+\mathbf{e}^k\|^2\right)+\|\widehat{\eta}^n\|^2+\|\delta_x^+\widehat{\eta}^n\|^2\right)+\tau\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2.
\end{aligned}\tag{3.53}$$

Combining (3.49), (3.52) and (3.53), we have

$$\mathcal{S}^n-\mathcal{S}^{n-1}\lesssim C_\alpha\tau(\mathcal{S}^n+\mathcal{S}^{n-1})+\frac{\tau}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\quad 1\le n\le\frac{T}{\tau}-1,\tag{3.54}$$

where $C_\alpha=\max\{1/(1-\alpha^2),2\}$. Summing up the above inequality for time steps from 1 to n, we arrive at

$$\mathcal{S}^n\lesssim 2C_\alpha\tau\sum_{k=0}^{n}\mathcal{S}^n+\mathcal{S}^0+\frac{T}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\quad 1\le n\le\frac{T}{\tau}-1.\tag{3.55}$$

By the discrete Gronwall's inequality [26, 30], there exists a constant $\tau_2>0$, such that, when $0<\tau\le\tau_2$, sufficiently small; depending on the parameter $\alpha\in(0,1)$ in the stability assumption,

$$\mathcal{S}^n\le\frac{C}{\varepsilon^2}\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2,\quad 1\le n\le\frac{T}{\tau}-1,\tag{3.56}$$

where C depends on T, g, ω, the exact solution $(\phi(t,x),\Psi(t,x))$ and the parameter $\alpha\in(0,1)$ in the stability assumption. Together with (3.51), the above inequality results in

$$\|\delta_x^+\eta^{n+1}\|^2+\|\eta^{n+1}\|^2+\|\delta_x^+\mathbf{e}^{n+1}\|^2+\|\mathbf{e}^{n+1}\|^2\le C\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right)^2, \tag{3.57}$$

with C independent of h, τ and ε. Thus, the estimates on η^{n+1} and $\mathbf{e}^{n+1}$ are complete.

Lastly, we prove the estimates of $\|\Psi^{n+1}\|_\infty$ and $\|\phi^{n+1}\|_\infty$ for $1\le n\le\frac{T}{\tau}-1$. In fact, the discrete Sobolev inequality will imply

$$\|\widehat{\eta}^{n+1}\|_\infty\le C_d(h)(\|\delta_x^+\widehat{\eta}^{n+1}\|+\|\widehat{\eta}^{n+1}\|)\le C\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right),\quad \|\widehat{\mathbf{e}}^{n+1}\|_\infty\le C\left(\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon^6}\right).$$

There exist $h_1>0$ and $\tau_3>0$ sufficiently small, when $\tau\le\tau_3\varepsilon^3/\sqrt{C_d(h)}$ and $h\le h_1\varepsilon^{1/2}/\sqrt{C_d(h)}$, the triangle inequality gives

$$\begin{aligned}\|\phi^{n+1}\|_\infty&\le\|\phi(t_{n+1},x)\|_{L^\infty}+\|\eta^{n+1}\|_\infty\le N_\Phi+1,\\ \|\Psi^{n+1}\|_\infty&\le\|\Psi(t_{n+1},x)\|_{L^\infty}+\|\mathbf{e}^{n+1}\|_\infty\le N_\Psi+1.\end{aligned}$$

Overall, the estimates in Theorem 3.4 are valid under the stability condition $\tau\le\alpha\varepsilon^2h/\sqrt{h^2+\varepsilon^2}$ $(0<\alpha<1)$ and the choices of $\tau_0=\min\{\tau_1,\tau_2,\tau_3\}$ and $h_0=h_1$. Hence, the proofs of Theorem 3.4 and Theorem 3.2 are complete. ∎

4. Numerical examples

In this section, we apply the FDTD methods presented in Section 2 for the KGD (2.1) and report numerical results to verify our error analysis. In the computation, the problem is solved numerically with the 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 using the TSFP method [6, 20] with a very small time step and a very fine mesh size, e.g. $\tau_e=5\times10^{-6}$ and $h_e=1/1024$. Denote $(\phi_{\tau,h}^n,\Psi_{\tau,h}^n)$ as the numerical solution obtained by a numerical method with time step τ and mesh size h. In order to quantify the numerical results, we define the discrete H^1-error as follows:

$$e_u(t_n)=\sqrt{\|u(t_n,\cdot)-u_{\tau,h}^n\|^2+\|\delta_x^+(u(t_n,\cdot)-u_{\tau,h}^n)\|^2},\quad u=\phi \text{ or } \Psi.$$

The initial data is given as

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

Firstly, we test the spatial errors. In order to do this, we choose a very small time step. e.g. $\tau=\tau_e$, such that the errors from the time discretization are negligible, and solve the KGD (2.1) with the FDTD methods under different mesh sizes h. Table 4.1 lists the numerical errors e_Ψ and e_ϕ at $t=2$ with different mesh sizes h for the CNFD (2.3)-(2.4). Table 4.2 shows the similar results about the spatial discretization errors for the SIFD1 (2.5)-(2.6).

Secondly, we check the temporal errors at $t=2$, listed in Tables 4.3-4.4. Due to the stability constraints for the SIFD1 (2.5)-(2.6), we set

$$\tau<\varepsilon^2h/\sqrt{h^2+\varepsilon^2}$$

ε-Scalability	$h_0=1/2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0=1/2$	6.36E-1	1.90E-1	4.94E-2	1.24E-2	3.11E-3
order	-	1.74	1.95	1.99	2.00
$\varepsilon_0=1/4$	6.16E-1	1.97E-1	5.18E-2	1.31E-2	3.28E-3
order	-	1.65	1.92	1.99	2.00
$\varepsilon_0=1/8$	6.36E-1	2.10E-1	5.59E-2	1.41E-2	3.54E-3
order	-	1.60	1.91	1.98	2.00
$\varepsilon_0=1/16$	6.42E-1	2.15E-1	5.75E-2	1.46E-2	3.70E-3
order	-	1.58	1.91	1.98	1.98
$\varepsilon_0=1/2$	1.13E-1	2.99E-2	7.49E-3	1.87E-3	4.68E-4
order	-	1.91	2.00	2.00	2.00
$\varepsilon_0=1/4$	1.52E-1	3.99E-2	1.00E-2	2.51E-3	6.29E-4
order	-	1.93	1.99	2.00	2.00
$\varepsilon_0=1/8$	1.77E-1	4.80E-2	1.22E-2	3.06E-3	7.68E-4
order	-	1.88	1.98	1.99	2.00
$\varepsilon_0=1/16$	1.87E-1	5.11E-2	1.31E-2	3.40E-3	9.98E-4
order	-	1.87	1.96	1.95	1.77

TABLE 4.1. *Spatial errors of CNFD with $\tau=5E-6$, e_Ψ (upper rows) and e_ϕ (lower rows).*

ε-Scalability	$h_0=1/2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0=1/2$	6.36E-1	1.90E-1	4.94E-2	1.24E-2	3.11E-3
order	-	1.74	1.95	1.99	2.00
$\varepsilon_0=1/4$	6.16E-1	1.97E-1	5.18E-2	1.31E-2	3.28E-3
order	-	1.65	1.92	1.99	2.00
$\varepsilon_0=1/8$	6.36E-1	2.10E-1	5.59E-2	1.41E-2	3.55E-3
order	-	1.60	1.91	1.98	2.00
$\varepsilon_0=1/16$	6.42E-1	2.15E-1	5.76E-2	1.48E-2	3.92E-3
order	-	1.58	1.90	1.96	1.91
$\varepsilon_0=1/2$	1.13E-1	2.99E-2	7.49E-3	1.87E-3	4.67E-4
order	-	1.91	2.00	2.00	2.00
$\varepsilon_0=1/4$	1.52E-1	3.99E-2	1.00E-2	2.51E-3	6.29E-4
order	-	1.93	1.99	2.00	2.00
$\varepsilon_0=1/8$	1.77E-1	4.80E-2	1.22E-2	3.06E-3	7.68E-4
order	-	1.88	1.98	1.99	2.00
$\varepsilon_0=1/16$	1.87E-1	5.11E-2	1.31E-2	3.40E-3	9.96E-4
order	-	1.87	1.96	1.95	1.77

TABLE 4.2. *Spatial errors of SIFD1 with $\tau=5E-6$, e_Ψ (upper rows) and e_ϕ (lower rows).*

in Table 4.4. The numerical results of the other two discretizations (SIFD2 and LFFD) are similar to those of CNFD and SIFD1, and are skipped here for brevity.

From Tables 4.1-4.4 and additional results not shown here, we can draw the following observations:

For any fixed $\varepsilon=\varepsilon_0>0$, the FDTD methods are second-order accurate in both temporal and spatial discretizations. In the nonrelativistic limit regime, i.e. $0<\varepsilon\ll 1$, each column in Tables 4.1-4.2 shows that the spatial errors are almost independent of ε.

ε-Scalability	$\tau_0=0.1$	$\tau_0/8$	$\tau_0/8^2$	$\tau_0/8^3$	$\tau_0/8^4$
$\varepsilon_0=1/2$	2.53E+0	<u>9.06E-3</u>	1.42E-4	2.93E-6	1.02E-6
order	-	2.71	2.00	1.87	-
$\varepsilon_0=1/4$	2.32E+0	2.99E-1	<u>4.74E-3</u>	7.45E-5	1.89E-6
order	-	0.99	1.99	2.00	1.77
$\varepsilon_0=1/8$	2.31E+0	4.78E-1	2.55E-1	<u>3.98E-3</u>	6.27E-5
order	-	0.76	0.30	2.00	2.00
$\varepsilon_0=1/16$	2.31E+0	2.52E+0	9.98E-1	2.47E-1	<u>3.86E-3</u>
order	-	-0.04	0.45	0.67	2.00
$\varepsilon_0=1/2$	1.65E+0	<u>1.30E-2</u>	2.04E-4	3.43E-6	1.49E-6
order	-	2.33	2.00	1.96	-
$\varepsilon_0=1/4$	2.52E+0	4.36E-1	<u>6.86E-3</u>	1.07E-4	1.80E-6
order	-	0.84	2.00	2.00	1.97
$\varepsilon_0=1/8$	1.48E+0	3.60E+0	6.83E-1	<u>1.06E-2</u>	1.66E-4
order	-	-0.43	0.80	2.00	2.00
$\varepsilon_0=1/16$	2.17E+0	4.60E+0	3.58E+0	5.66E-1	<u>8.30E-3</u>
order	-	-0.36	0.12	0.89	2.03

TABLE 4.3. *Temporal errors of CNFD under $O(\varepsilon^3)$ with $h=1/2048$, e_Ψ (upper rows) and e_ϕ (lower rows).*

ε-Scalability	$\tau_0=0.1$ $h_0=2$	$\tau_0/8$ $h_0/8$	$\tau_0/8^2$ $h_0/8^2$	$\tau_0/8^3$ $h_0/8^3$	$\tau_0/8^4$ $h_0/8^4$
$\varepsilon_0=1/2$	2.10E+0	<u>2.08E-1</u>	3.40E-3	5.32E-5	2.08E-6
order	-	1.11	1.98	2.00	-
$\varepsilon_0=1/4$	2.16E+0	1.16E+0	<u>1.90E-2</u>	2.97E-4	5.94E-6
order	-	0.30	1.98	2.00	1.88
$\varepsilon_0=1/8$	2.18E+0	3.20E+0	9.95E-1	<u>1.58E-2</u>	2.49E-4
order	-	-0.18	0.56	1.99	1.99
$\varepsilon_0=1/16$	2.17E+0	3.55E+0	3.53E-1	9.79E-1	<u>1.55E-2</u>
order	-	-0.24	1.11	-0.49	1.99
$\varepsilon_0=1/2$	1.69E+0	<u>3.69E-2</u>	5.78E-4	9.08E-6	1.48E-6
order	-	1.84	2.00	2.00	-
$\varepsilon_0=1/4$	2.39E+0	4.19E-1	<u>6.55E-3</u>	1.02E-4	1.60E-6
order	-	0.84	2.00	2.00	2.00
$\varepsilon_0=1/8$	1.24E+0	3.35E+0	6.77E-1	<u>1.06E-2</u>	1.65E-4
order	-	-0.48	0.77	2.00	2.00
$\varepsilon_0=1/16$	1.86E+0	4.52E+0	3.64E+0	5.64E-1	<u>8.27E-3</u>
order	-	-0.43	0.10	0.90	2.03

TABLE 4.4. *Temporal errors of SIFD1 under $O(\varepsilon^3)$, e_Ψ (upper rows) and e_ϕ (lower rows).*

We note that the h^2/ε spatial error comes from the 'free' Dirac operator $-\frac{i}{\varepsilon}\sigma_1\partial_x+\frac{\omega}{\varepsilon^2}\sigma_3$ in the Dirac component, which is mainly caused by the lowest frequencies of the solution in phase space [6, 7]. However, such dependence on ε is not visible in most numerical tests, as usually, only a very small fraction of the solution lies in the lowest frequencies. In fact, by using the example in [6], i.e. choosing $g=0$, $\Psi^0(x)=(e^{9\pi i(x+1)},e^{9\pi i(x+1)})^T$, $\phi^0(x)=0$ and $\gamma(x)=0$ $(-1\le x\le 1)$ in (2.1), we could observe numerically the spatial errors of order h^2/ε and the details are omitted here for brevity. In addition, Tables 4.3-4.4 suggest that the 'correct' ε-scalability of the time step is $\tau = O(\varepsilon^3)$ which verifies our theoretical results. In fact, for $0 < \varepsilon \ll 1$, we can obtain second-order convergence in time only when $\tau \lesssim \varepsilon^3$ (cf. upper triangles in the lower parts of Tables 4.3-4.4).

5. Conclusion

Four conservative/non-conservative implicit/semi-implicit/explicit FDTD methods were analyzed and compared based on their temporal/spatial resolution for numerically solving the KGD system in the nonrelativistic limit regime, i.e. $0 < \varepsilon \ll 1$. The main difficulty was that the KGD system admits rapid oscillations in time as $\varepsilon \to 0^+$, while the nonlinear Yukawa interaction and the indefinite Dirac operator bring another significant difficulty. Error estimates were rigorously established using energy methods and the cut-off technique, which are geared towards understanding the temporal resolution capacity of the FDTD methods for the KGD system in the nonrelativistic limit regime. The estimates suggest that the ε-scalability and meshing strategy of the FDTD methods should be $\tau = O(\varepsilon^3)$ and $h = O(\sqrt{\varepsilon})$ for $0 < \varepsilon \ll 1$.

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