Numer. Math. (2017) 135:833–873
DOI 10.1007/s00211-016-0818-x

Numerische Mathematik

A uniformly accurate (UA) multiscale time integrator Fourier pseudospectral method for the Klein–Gordon–Schrödinger equations in the nonrelativistic limit regime

A UA method for Klein–Gordon–Schrodinger equation

Weizhu Bao[1] · **Xiaofei Zhao**[1]

Received: 1 May 2015 / Revised: 26 April 2016 / Published online: 28 June 2016

Abstract A multiscale time integrator Fourier pseudospectral (MTI-FP) method is proposed and analyzed for solving the Klein–Gordon–Schrödinger (KGS) equations in the nonrelativistic limit regime with a dimensionless parameter $0 < \varepsilon \leq 1$ which is inversely proportional to the speed of light. In fact, the solution of the KGS equations propagates waves with wavelength at $O(\varepsilon^2)$ and $O(1)$ in time and space, respectively, when $0 < \varepsilon \ll 1$, which brings significantly numerical burden in practical computation. The MTI-FP method is designed by adapting a multiscale decomposition by frequency of the solution at each time step and applying the Fourier pseudospectral discretization and exponential wave integrators for spatial and temporal derivatives, respectively. We rigorously establish two independent error bounds for the MTI-FP at $O(\tau^2/\varepsilon^2 + h^{m_0})$ and $O(\varepsilon^2 + h^{m_0})$ for $\varepsilon \in (0, 1]$ with τ time step size, h mesh size and $m_0 \geq 4$ an integer depending on the regularity of the solution, which imply that the MTI-FP converges uniformly and optimally in space with exponential convergence rate if the solution is smooth, and uniformly in time with linear convergence rate at $O(\tau)$ for $\varepsilon \in (0, 1]$. In addition, the MTI-FP method converges optimally with quadratic convergence rate at $O(\tau^2)$ in the regime when $0 < \tau \lesssim \varepsilon^2$ and the error is at $O(\varepsilon^2)$ independent of τ in the regime when $0 < \varepsilon \lesssim \tau^{1/2}$. Thus the meshing strategy requirement (or ε-scalability) of the MTI-FP is $\tau = O(1)$ and $h = O(1)$ for $0 < \varepsilon \ll 1$, which is significantly better than that of classical methods. Numerical results demonstrate that our error bounds are optimal and sharp. Finally, the MTI-FP

✉ Weizhu Bao
matbaowz@nus.edu.sg
http://www.math.nus.edu.sg/~bao/

Xiaofei Zhao
zhxfnus@gmail.com

[1] Department of Mathematics, National University of Singapore, Singapore 119076, Singapore

method is applied to study numerically convergence rates of the KGS equations to its limiting models in the nonrelativistic limit regime.

Mathematics Subject Classification 65L05 · 65L20 · 65L70

1 Introduction

Consider the Klein–Gordon–Schrödinger (KGS) equations in d-dimensions ($d = 3, 2, 1$) [2,23,41]:

$$i\hbar\partial_t\psi(\mathbf{x},t) + \frac{\hbar^2}{2m_1}\Delta\psi(\mathbf{x},t) + g\phi(\mathbf{x},t)\psi(\mathbf{x},t) = 0, \quad \mathbf{x}\in\mathbb{R}^d, \tag{1.1a}$$

$$\frac{1}{c^2}\partial_{tt}\phi(\mathbf{x},t) - \Delta\phi(\mathbf{x},t) + \frac{m_2^2c^2}{\hbar^2}\phi(\mathbf{x},t) - g|\psi(\mathbf{x},t)|^2 = 0, \tag{1.1b}$$

which represent a classical model for describing the dynamics of a complex-valued scalar nucleon field $\psi := \psi(\mathbf{x},t)$ interacting with a neutral real-valued scalar meson field $\phi := \phi(\mathbf{x},t)$ through the Yukawa coupling with $0 \neq g \in \mathbb{R}$ the coupling constant. Here t is time, $\mathbf{x}\in\mathbb{R}^d$ is the spatial coordinate, $\hbar$ is the Planck constant, c is the speed of light, $m_1 > 0$ is the mass of a nucleon and $m_2 > 0$ is the mass of a meson.

In order to scale the KGS (1.1), we introduce

$$\tilde{t} = \frac{t}{t_s}, \quad \tilde{\mathbf{x}} = \frac{\mathbf{x}}{x_s}, \quad \tilde{\psi}(\tilde{\mathbf{x}},\tilde{t}) = x_s^{d/2}\,\psi(\mathbf{x},t), \quad \tilde{\phi}(\tilde{\mathbf{x}},\tilde{t}) = \frac{\phi(\mathbf{x},t)}{\phi_s}, \tag{1.2}$$

where x_s, t_s and ϕ_s are the dimensionless length unit, time unit and meson field unit, respectively, satisfying $t_s = \frac{2m_1x_s^2}{\hbar}$ and $\phi_s = \frac{\hbar x_s^{-d/2}}{\sqrt{2m_1}}$ with $v = \frac{x_s}{t_s} = \frac{\hbar}{2m_1x_s}$ being the wave speed. Plugging (1.2) into (1.1), after a simple computation and then removing all $\tilde{}$, we obtain the following dimensionless KGS equations in d-dimensions ($d = 3, 2, 1$):

$$i\,\partial_t\psi(\mathbf{x},t) + \Delta\psi(\mathbf{x},t) + \lambda\phi(\mathbf{x},t)\psi(\mathbf{x},t) = 0, \quad \mathbf{x}\in\mathbb{R}^d, \tag{1.3a}$$

$$\varepsilon^2\partial_{tt}\phi(\mathbf{x},t) - \Delta\phi(\mathbf{x},t) + \frac{\mu^2}{\varepsilon^2}\phi(\mathbf{x},t) - \lambda\,|\psi(\mathbf{x},t)|^2 = 0, \tag{1.3b}$$

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

$$0 < \varepsilon := \frac{v}{c} = \frac{x_s}{t_s\,c} = \frac{\hbar}{2cm_1x_s} \leq 1, \tag{1.4}$$

and $\mu = \frac{m_2}{2m_1} > 0$ and $\lambda = \frac{g\sqrt{2m_1}x_s^{2-d/2}}{\hbar} \in \mathbb{R}$ are two dimensionless constants which are independent of ε.

We remark here that if one chooses the dimensionless length unit $x_s = \frac{\hbar}{2cm_1}$, $t_s = \frac{x_s}{c} = \frac{\hbar}{2c^2m_1}$ and $\phi_s = \frac{c^{d/2}\hbar^{1-d/2}}{(2m_1)^{(1-d)/2}}$ in (1.2), then $\varepsilon = 1$ in (1.4) and Eqs. (1.3) with $\varepsilon = 1$ take the form often appearing in the literature [2,23,41]. This choice of x_s is appropriate when the wave speed is at the same order of the speed of light. However,

when the wave speed is much smaller than the speed of light, a different choice of x_s is more appropriate. Note that the choice of x_s determines the observation scale of the time evolution of the particles and decides: (1) which phenomena are 'visible' by asymptotic analysis, and (2) which phenomena can be resolved in a discretization by specified spatial/temporal grids. In fact, there are two important parameter regimes: one is when $\varepsilon = 1$ ($\Longleftrightarrow x_s = \frac{\hbar}{2cm_1}$, $t_s = \frac{\hbar}{2c^2m_1}$ and $\phi_s = \frac{c^{d/2}\hbar^{1-d/2}}{(2m_1)^{(1-d)/2}}$), then Eqs. (1.3) describe the case that wave speed is at the same order of the speed of light; the other one is when $0 < \varepsilon \ll 1$, then Eq. (1.3) are in the nonrelativistic limit regime.

To study the dynamics of the KGS (1.3), the initial data is usually given as

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \quad \partial_t\phi(\mathbf{x}, 0) = \frac{1}{\varepsilon^2}\phi_1(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \tag{1.5}$$

where the complex-valued function ψ_0 and the real-valued functions ϕ_0 and ϕ_1 are independent of ε. The KGS equations (1.3) are dispersive and time symmetric. They conserve the *mass* of the nucleon field

$$\|\psi(\cdot, t)\|_{L^2}^2 := \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} \equiv \int_{\mathbb{R}^d} |\psi(\mathbf{x}, 0)|^2 \, d\mathbf{x} = \int_{\mathbb{R}^d} |\psi_0(\mathbf{x})|^2 \, d\mathbf{x}, \quad t \geq 0, \tag{1.6}$$

and the *Hamiltonian* or total *energy*

$$\begin{aligned} E(t) &:= \int_{\mathbb{R}^d} \left[\frac{1}{2} \left(\varepsilon^2 |\partial_t\phi|^2 + |\nabla\phi|^2 + \frac{\mu^2}{\varepsilon^2} |\phi|^2 \right) + |\nabla\psi|^2 - \lambda|\psi|^2\phi \right] d\mathbf{x} \\ &\equiv \int_{\mathbb{R}^d} \left[\frac{1}{2} \left(\frac{1}{\varepsilon^2} |\phi_1|^2 + |\nabla\phi_0|^2 + \frac{\mu^2}{\varepsilon^2} |\phi_0|^2 \right) + |\nabla\psi_0|^2 - \lambda|\psi_0|^2\phi_0 \right] d\mathbf{x} \\ &= E(0), \quad t \geq 0. \end{aligned} \tag{1.7}$$

For the KGS equations (1.3) with $\varepsilon = 1$, i.e. O(1)-speed of light regime, there are extensive analytical and numerical results in the literatures [3,37,44,45,47,48]. For the existence and uniqueness as well as regularity, we refer to [14,23–25,31–33,41,49] and references therein. For the numerical methods and comparison such as the finite difference time domain (FDTD) methods and Crank–Nicolson Fourier pseudospectral method, we refer to [13,50,52,53] and references therein. However, for the KGS equations (1.3) with $0 < \varepsilon \ll 1$, i.e. nonrelativistic limit regime (or the scaled speed of light goes to infinity), the analysis and efficient computation of the KGS equations (1.3) are mathematically and numerically rather complicated issues. The main difficulty is due to that the solution is highly oscillatory in time and the corresponding energy functional $E(t) = O(\varepsilon^{-2})$ in (1.7) becomes unbounded when $\varepsilon \to 0$.

Formally, in the nonrelativistic limit regime, i.e. $0 < \varepsilon \ll 1$, similar to the analysis of the nonrelativistic limit of the Klein–Gordon (KG) equation [39,40,42,43], taking the ansatz

$$\phi(\mathbf{x}, t) = \mathrm{e}^{i\mu t/\varepsilon^2} z(\mathbf{x}, t) + \mathrm{e}^{-i\mu t/\varepsilon^2} \bar{z}(\mathbf{x}, t) + o(\varepsilon), \qquad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0, \tag{1.8}$$

where $\bar{z}$ denotes the complex conjugate of a complex-valued function z, and plugging it into (1.3) and (1.5), we obtain a *semi-limiting model*—the Schrödinger equations with wave operator—as

$$i\partial_t \psi(\mathbf{x}, t) + \Delta\psi(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \tag{1.9a}$$

$$2i\mu\partial_t z(\mathbf{x}, t) + \varepsilon^2 \partial_{tt} z(\mathbf{x}, t) - \Delta z(\mathbf{x}, t) = 0, \tag{1.9b}$$

with the well-prepared initial data [6,7]

$$z(\mathbf{x}, 0) = \frac{1}{2}\left[\phi_0(\mathbf{x}) - \frac{i}{\mu}\phi_1(\mathbf{x})\right], \ \partial_t z(\mathbf{x}, 0) = -\frac{i}{2\mu}\Delta z(\mathbf{x}, 0), \ \psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}). \tag{1.10}$$

In addition, after dropping the second term in (1.9b), formally we get a *limiting model*—the Schrödinger equations—as

$$i\partial_t \psi(\mathbf{x}, t) + \Delta\psi(\mathbf{x}, t) = 0, \tag{1.11a}$$

$$2i\mu\partial_t z(\mathbf{x}, t) - \Delta z(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \tag{1.11b}$$

with the initial data

$$z(\mathbf{x}, 0) = \frac{1}{2}\left[\phi_0(\mathbf{x}) - \frac{i}{\mu}\phi_1(\mathbf{x})\right], \qquad \psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d. \tag{1.12}$$

This formally suggests that the solution of (1.3) propagates highly oscillatory waves with amplitude at $O(1)$ and wavelength at $O(\varepsilon^2)$ and $O(1)$ in time and space, respectively, when $0 < \varepsilon \ll 1$. To illustrate this, Fig. 1 shows the solution of the KGS equations (1.3)–(1.5) with $d = 1$, $\mu = \lambda = 1$, $\psi_0(x) = \frac{1+i}{2}\mathrm{sech}(x^2)$, $\phi_0(x) = \frac{1}{2}\mathrm{e}^{-x^2}$ and $\phi_1(x) = \frac{1}{\sqrt{2}}\mathrm{e}^{-x^2}$ for different $0 < \varepsilon \leq 1$.

The highly temporal oscillatory nature of the solution of the KGS equations (1.3) causes severe burden in practical computation, making the numerical approximation extremely challenging and costly in the regime $0 < \varepsilon \ll 1$. Recently, different numerical methods have been proposed and/or analyzed for the nonlinear KG equation in the nonrelativistic limit regime in which the solution shares similar oscillatory behavior as that of the KGS equations (1.3), including the FDTD methods [9], exponential wave integrator Fourier pseudospectral (EWI-FP) method [9,11], asymptotic preserving (AP) method [22], stroboscopic average method (SAM) [16], two-scale formulation (TSF) method [15] and multiscale time integrator Fourier pseudospectral (MTI-FP) method [8], etc. Among them, TSF and MTI-FP methods are uniformly accurate (UA) for $\varepsilon \in (0, 1]$, while FDTD, EWI-FP, AP and SAM methods are not. TSF method introduces an extra dimension to the original problem by separating the fast time scale out, which would require more computational and/or memory costs. From the practical computation point of view, the MTI-FP is simpler and thus more efficient than the TSF method. The main aim of this paper is to propose and analyze a MTI-FP method for the KGS equations (1.3) in the nonrelativistic limit regime by adapting a multiscale decomposition by frequency of the solution at each time step and applying the

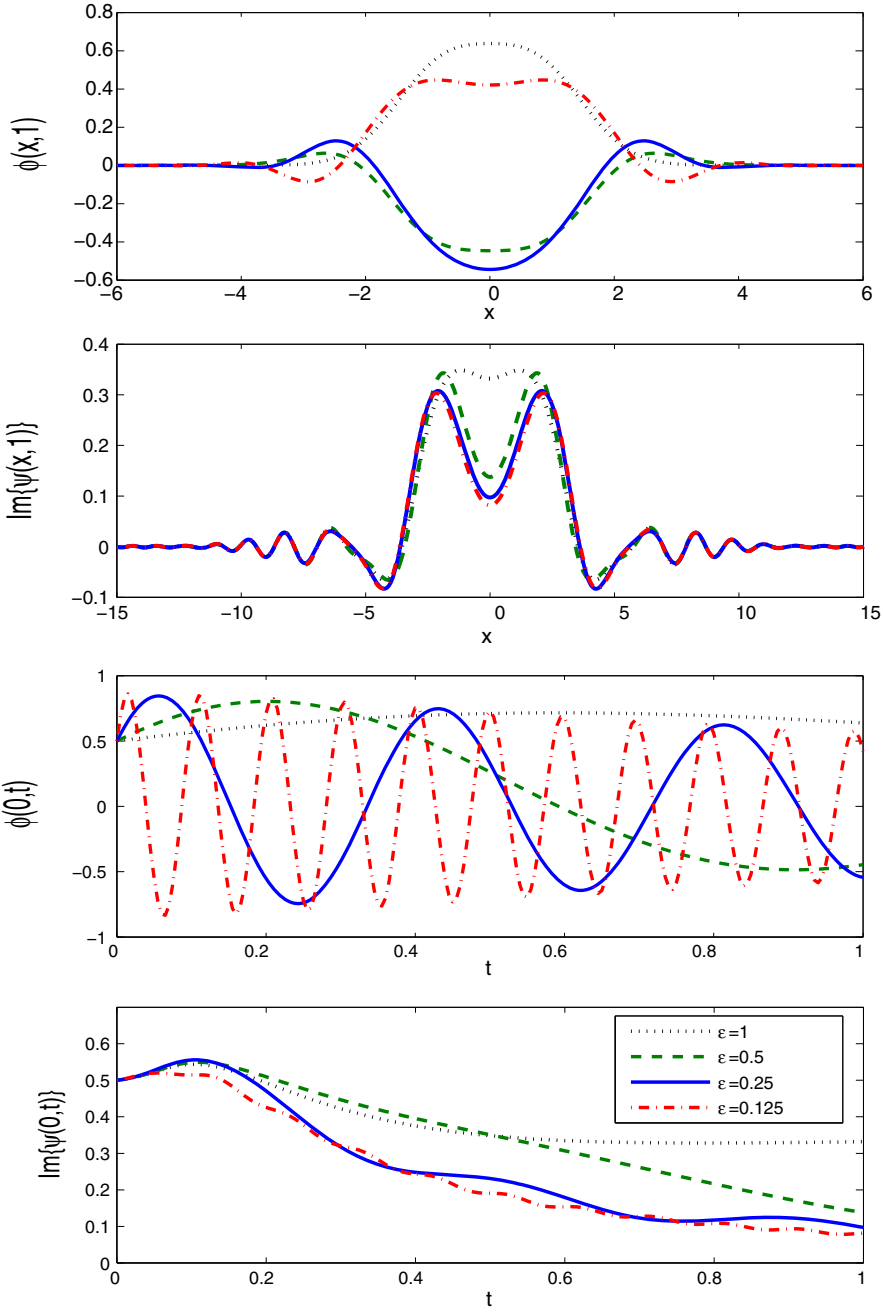

Fig. 1 Plots of the solution of the KGS (1.3)–(1.5) with $d = 1$ for different ε, where $\mathrm{Im}\{\psi\}$ denotes the imaginary part of ψ

Fourier pseudospectral discretization and exponential wave integrators for spatial and temporal derivatives, respectively. Two independent error bounds will be established for the MTI-FP, which imply that the MTI-FP converges uniformly and/or optimally for $0 < \varepsilon \leq 1$. The MTI-FP method is also applied to study numerically convergence rates of the KGS equations (1.3) to its limiting models (1.9)–(1.10) and (1.11)–(1.12).

The paper is organized as follows. In Sect. 2, we introduce a multiscale decomposition for the KGS equations (1.3) based on frequency. A MTI-FP method is proposed in Sect. 3, and its rigorous error bounds in energy space are established in Sect. 4. Numerical results are reported in Sect. 5. Finally, some conclusions are drawn in Sect. 6. Throughout this paper, we adopt the standard Sobolev spaces [1] and use the notation $A \lesssim B$ to represent that there exists a generic constant $C > 0$, which is independent of time step τ (or n), mesh size h and ε, such that $|A| \leq CB$.

2 Multiscale decomposition

Let $\tau = \Delta t > 0$ be the time step size, and denote time steps by $t_n = n\tau$ for $n = 0, 1, \ldots$. In this section, we present a multiscale decomposition of the solution of (1.3) on the time interval $[t_n, t_{n+1}]$ with given initial data at $t = t_n$ as

$$\phi(\mathbf{x}, t_n) = \phi_0^n(\mathbf{x}) = O(1), \quad \partial_t \phi(\mathbf{x}, t_n) = \frac{1}{\varepsilon^2}\phi_1^n(\mathbf{x}) = O\left(\frac{1}{\varepsilon^2}\right), \tag{2.1a}$$

$$\psi(\mathbf{x}, t_n) = \psi_0^n(\mathbf{x}) = O(1). \tag{2.1b}$$

Similar to the analytical study of the nonlinear KG equation in the nonrelativistic limit regime in [8,42], we take an ansatz for the function $\phi(\mathbf{x}, t) := \phi(\mathbf{x}, t_n + s)$ of (1.3b) on the time interval $[t_n, t_{n+1}]$ with (2.1) as [8,12]

$$\phi(\mathbf{x}, t_n + s) = \mathrm{e}^{i\mu s/\varepsilon^2} z^n(\mathbf{x}, s) + \mathrm{e}^{-i\mu s/\varepsilon^2} \overline{z^n}(\mathbf{x}, s) + r^n(\mathbf{x}, s), \quad \mathbf{x} \in \mathbb{R}^d, \ \ 0 \leq s \leq \tau. \tag{2.2}$$

Differentiating (2.2) with respect to s, we have

$$\begin{aligned} \partial_s \phi(\mathbf{x}, t_n + s) = {} & \mathrm{e}^{i\mu s/\varepsilon^2} \left[\partial_s z^n(\mathbf{x}, s) + \frac{i\mu}{\varepsilon^2} z^n(\mathbf{x}, s) \right] + \partial_s r^n(\mathbf{x}, s) \\ & + \mathrm{e}^{-i\mu s/\varepsilon^2} \left[\partial_s \overline{z^n}(\mathbf{x}, s) - \frac{i\mu}{\varepsilon^2} \overline{z^n}(\mathbf{x}, s) \right], \quad \mathbf{x} \in \mathbb{R}^d, \ \ 0 \leq s \leq \tau. \end{aligned} \tag{2.3}$$

Plugging (2.2) into (1.3), we get for $\mathbf{x} \in \mathbb{R}^d$, $0 \leq s \leq \tau$ and $\psi(\mathbf{x}, t_n + s) =: \psi^n(\mathbf{x}, s)$

$$\begin{aligned} & \mathrm{e}^{i\mu s/\varepsilon^2} \left[\varepsilon^2 \partial_{ss} z^n(\mathbf{x}, s) + 2i\mu \partial_s z^n(\mathbf{x}, s) - \Delta z^n(\mathbf{x}, s) \right] \\ & + \mathrm{e}^{-i\mu s/\varepsilon^2} \left[\varepsilon^2 \partial_{ss} \overline{z^n}(\mathbf{x}, s) - 2i\mu \partial_s \overline{z^n}(\mathbf{x}, s) - \Delta \overline{z^n}(\mathbf{x}, s) \right] \\ & + \varepsilon^2 \partial_{ss} r^n(\mathbf{x}, s) - \Delta r^n(\mathbf{x}, s) + \frac{\mu^2}{\varepsilon^2} r^n(\mathbf{x}, s) = \lambda \left| \psi^n(\mathbf{x}, s) \right|^2. \end{aligned}$$

Substituting (2.2) into (1.3a) and multiplying the above equation by $\mathrm{e}^{-i\mu s/\varepsilon^2}$ and $\mathrm{e}^{i\mu s/\varepsilon^2}$, respectively, we can re-formulate the KGS equations (1.3) for $\psi^n := \psi^n(\mathbf{x}, s)$, $z^n := z^n(\mathbf{x}, s)$ and $r^n := r^n(\mathbf{x}, s)$ as

$$\begin{cases} i\partial_s\psi^n + \Delta\psi^n + \lambda\left(\mathrm{e}^{\frac{i\mu s}{\varepsilon^2}} z^n\psi^n + \mathrm{e}^{-\frac{i\mu s}{\varepsilon^2}}\overline{z^n}\psi^n + r^n\psi^n\right) = 0, \\ 2i\mu\partial_s z^n + \varepsilon^2\partial_{ss} z^n - \Delta z^n = 0, \quad \mathbf{x}\in\mathbb{R}^d, \quad 0\le s\le\tau, \\ \varepsilon^2\partial_{ss} r^n - \Delta r^n + \frac{\mu^2}{\varepsilon^2} r^n = \lambda|\psi^n|^2. \end{cases} \tag{2.4}$$

In order to find proper initial conditions for the system (2.4), setting $s = 0$ in (2.2) and (2.3), noticing (2.1a), we obtain

$$\begin{cases} z^n(\mathbf{x}, 0) + \overline{z^n}(\mathbf{x}, 0) + r^n(\mathbf{x}, 0) = \phi_0^n(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^d, \\ \frac{i\mu}{\varepsilon^2}\left[z^n(\mathbf{x}, 0) - \overline{z^n}(\mathbf{x}, 0)\right] + \partial_s z^n(\mathbf{x}, 0) + \partial_s\overline{z^n}(\mathbf{x}, 0) + \partial_s r^n(\mathbf{x}, 0) = \frac{\phi_1^n(\mathbf{x})}{\varepsilon^2}. \end{cases} \tag{2.5}$$

Now we decompose the above initial data so as to: (1) equate $O\left(\frac{1}{\varepsilon^2}\right)$ and $O(1)$ terms in the second equation of (2.5), respectively, and (2) be well-prepared for the second equation in (2.4) when $0 < \varepsilon \ll 1$, i.e. $\partial_s z^n(\mathbf{x}, 0)$ is determined from the second equation in (2.4) by setting $\varepsilon = 0$ and $s = 0$ [6–8]:

$$\begin{cases} z^n(\mathbf{x}, 0) + \overline{z^n}(\mathbf{x}, 0) = \phi_0^n(\mathbf{x}), \quad i\mu\left[z^n(\mathbf{x}, 0) - \overline{z^n}(\mathbf{x}, 0)\right] = \phi_1^n(\mathbf{x}), \\ 2i\mu\partial_s z^n(\mathbf{x}, 0) - \Delta z^n(\mathbf{x}, 0) = 0, \quad \mathbf{x}\in\mathbb{R}^d, \\ r^n(\mathbf{x}, 0) = 0, \quad \partial_s r^n(\mathbf{x}, 0) + \partial_s z^n(\mathbf{x}, 0) + \partial_s\overline{z^n}(\mathbf{x}, 0) = 0. \end{cases} \tag{2.6}$$

Solving (2.6) and noticing (2.1b), we get the initial data for (2.4) as

$$\begin{cases} z^n(\mathbf{x}, 0) = \frac{1}{2}\left[\phi_0^n(\mathbf{x}) - \frac{i}{\mu}\phi_1^n(\mathbf{x})\right], \quad \partial_s z^n(\mathbf{x}, 0) = -\frac{i}{2\mu}\Delta z^n(\mathbf{x}, 0), \quad \mathbf{x}\in\mathbb{R}^d, \\ \psi^n(\mathbf{x}, 0) = \psi_0^n(\mathbf{x}), \quad r^n(\mathbf{x}, 0) = 0, \quad \partial_s r^n(\mathbf{x}, 0) = -\partial_s z^n(\mathbf{x}, 0) - \partial_s\overline{z^n}(\mathbf{x}, 0). \end{cases} \tag{2.7}$$

The above decomposition can be called as multiscale decomposition by frequency (MDF). In fact, it can also be regarded as to decompose slow waves at ε^2-wavelength and fast waves at other wavelengths, thus it can also be called as fast-slow wave decomposition. After solving the decomposed system (2.4) with the initial data (2.7), we get $\psi^n(\mathbf{x}, \tau)$, $z^n(\mathbf{x}, \tau)$, $\partial_s z^n(\mathbf{x}, \tau)$, $r^n(\mathbf{x}, \tau)$ and $\partial_s r^n(\mathbf{x}, \tau)$. Then we can reconstruct the solution of the KGS (1.3) at $t = t_{n+1}$ by setting $s = \tau$ in (2.2) and (2.3), i.e.

$$\begin{cases} \psi(\mathbf{x}, t_{n+1}) = \psi^n(\mathbf{x}, \tau) =: \psi_0^{n+1}(\mathbf{x}), \quad \partial_t\phi(\mathbf{x}, t_{n+1}) = \frac{1}{\varepsilon^2}\phi_1^{n+1}(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^d, \ n\ge 0, \\ \phi(\mathbf{x}, t_{n+1}) = \mathrm{e}^{i\mu\tau/\varepsilon^2} z^n(\mathbf{x}, \tau) + \mathrm{e}^{-i\mu\tau/\varepsilon^2}\overline{z^n}(\mathbf{x}, \tau) + r^n(\mathbf{x}, \tau) =: \phi_0^{n+1}(\mathbf{x}), \end{cases} \tag{2.8}$$

with

$$\begin{aligned}\phi_1^{n+1}(\mathbf{x}) := & \, \mathrm{e}^{i\mu\tau/\varepsilon^2}\left[\varepsilon^2\partial_s z^n(\mathbf{x},\tau)+i\mu z^n(\mathbf{x},\tau)\right]\\ & +\mathrm{e}^{-i\mu\tau/\varepsilon^2}\left[\varepsilon^2\partial_s \overline{z^n}(\mathbf{x},\tau)-i\mu\overline{z^n}(\mathbf{x},\tau)\right]\\ & +\varepsilon^2\partial_s r^n(\mathbf{x},\tau), \quad \mathbf{x}\in\mathbb{R}^d, \quad n\geq 0.\end{aligned}$$

In summary, the MDF proceeds as a decomposition-solution-reconstruction flow at each time interval, and this makes it essentially different from the classical modulated Fourier expansion [17–20,34–36] which only carries out the decomposition at the initial time $t = 0$. In addition, due to that $r^n(\mathbf{x}, 0) \equiv 0$ in (2.7) for $n \geq 0$, the numerical error for discretizing the highly oscillatory equation, i.e. the third equation in (2.4), will not accumlated. This enables us to design the uniformly accurate MTI-FP method for $0 < \varepsilon \leq 1$.

3 An MTI-FP method

For the simplicity of notations and without loss of generality, we take $\mu = \lambda = 1$ in (1.3) and present our numerical method in one space dimension (1D). Generalizations to higher dimensions are straightforward and the results remain valid. We truncate the whole space problem (1.3) into a finite interval $\Omega = (a, b)$ with periodic boundary conditions, where due to the fast decay of the solution at far field, the truncation error can be negligible by choosing a, b sufficiently large. In 1D, the problem (1.3) with $\mu = \lambda = 1$ collapses to

$$\begin{cases} i\partial_t\psi(x,t)+\partial_{xx}\psi(x,t)+\phi(x,t)\psi(x,t)=0, \quad x\in\Omega, \quad t>0,\\ \varepsilon^2\partial_{tt}\phi(x,t)-\partial_{xx}\phi(x,t)+\frac{1}{\varepsilon^2}\phi(x,t)=|\psi(x,t)|^2, \quad x\in\Omega, \quad t>0,\\ \phi(a,t)=\phi(b,t), \quad \partial_x\phi(a,t)=\partial_x\phi(b,t), \quad t\geq 0,\\ \psi(a,t)=\psi(b,t), \quad \partial_x\psi(a,t)=\partial_x\psi(b,t),\\ \phi(x,0)=\phi_0(x), \quad \partial_t\phi(x,0)=\frac{\phi_1(x)}{\varepsilon^2}, \quad \psi(x,0)=\psi_0(x), \quad x\in\overline{\Omega}=[a,b]. \end{cases} \tag{3.1}$$

We remark that the boundary conditions considered here are inspired by the inherent physical nature of the system and they have been widely used in the literatures for the simulation of the KGS equations [10,13,52,53].

Consequently, for $n \geq 0$, the decomposed system MDF (2.4) in 1D collapses to

$$\begin{cases} i\partial_s\psi^n+\partial_{xx}\psi^n+\mathrm{e}^{is/\varepsilon^2}z^n\psi^n+\mathrm{e}^{-is/\varepsilon^2}\overline{z^n}\psi^n+r^n\psi^n=0,\\ 2i\partial_s z^n+\varepsilon^2\partial_{ss}z^n-\partial_{xx}z^n=0, \quad a<x<b, \ 0<s\leq\tau,\\ \varepsilon^2\partial_{ss}r^n-\partial_{xx}r^n+\frac{1}{\varepsilon^2}r^n=|\psi^n|^2. \end{cases} \tag{3.2}$$

The initial and boundary conditions for the above system are

$$\begin{cases} z^n(a,s) = z^n(b,s), \quad \partial_x z^n(a,s) = \partial_x z^n(b,s), \\ r^n(a,s) = r^n(b,s), \quad \partial_x r^n(a,s) = \partial_x r^n(b,s), \\ \psi^n(a,s) = \psi^n(b,s), \quad \partial_x \psi^n(a,s) = \partial_x \psi^n(b,s), \quad 0 \le s \le \tau; \\ z^n(x,0) = \frac{1}{2}\left[\phi_0^n(x) - i\phi_1^n(x)\right], \quad \partial_s z^n(x,0) = -\frac{i}{2}\partial_{xx} z^n(x,0), \\ r^n(x,0) = 0, \quad \partial_s r^n(x,0) = -\partial_s z^n(x,0) - \partial_s \overline{z^n}(x,0), \\ \psi^n(x,0) = \psi_0^n(x), \quad a \le x \le b. \end{cases} \tag{3.3}$$

In what follows, we present a numerical integrator Fourier pseudospectral discretization for the MDF (3.2) with (3.3), in which we apply the Fourier pseudospectral discretization to spatial derivatives followed by using some proper exponential wave integrators (EWI) for temporal discretizations in phase (Fourier) space.

Choose the mesh size $h := \Delta x = (b-a)/N$ with N a positive integer and denote grid points as $x_j := a + jh$ for $j = 0, 1, \ldots, N$. Define

$$X_N := \text{span}\left\{ \mathrm{e}^{i\mu_l(x-a)} \ : \ x \in \overline{\Omega}, \ \mu_l = \frac{2\pi l}{b-a}, \ l = -\frac{N}{2}, \ldots, \frac{N}{2} - 1 \right\},$$

$$Y_N := \left\{ \mathbf{v} = (v_0, v_1, \ldots, v_N) \in \mathbb{C}^{N+1} \ : \ v_0 = v_N \right\}, \ \|\mathbf{v}\|_{l^2} = h \sum_{j=0}^{N-1} |v_j|^2.$$

For a periodic function $v(x)$ on $\overline{\Omega}$ and a vector $\mathbf{v} \in Y_N$, let $P_N : L^2(\Omega) \to X_N$ be the standard L^2-projection operator, and $I_N : C(\Omega) \to X_N$ or $Y_N \to X_N$ be the trigonometric interpolation operator [30,46], i.e.

$$(P_N v)(x) = \sum_{l=-N/2}^{N/2-1} \widehat{v}_l \mathrm{e}^{i\mu_l(x-a)}, \quad (I_N \mathbf{v})(x) = \sum_{l=-N/2}^{N/2-1} \widetilde{\mathbf{v}}_l \mathrm{e}^{i\mu_l(x-a)}, \tag{3.4}$$

where $\widehat{v}_l$ and $\widetilde{\mathbf{v}}_l$ are the Fourier and discrete Fourier transform coefficients of the periodic function $v(x)$ and vector $\mathbf{v}$, respectively, defined as

$$\widehat{v}_l = \frac{1}{b-a}\int_a^b v(x)\mathrm{e}^{-i\mu_l(x-a)}dx, \quad \widetilde{\mathbf{v}}_l = \frac{1}{N}\sum_{j=0}^{N-1} v_j \mathrm{e}^{-i\mu_l(x_j-a)}. \tag{3.5}$$

Then a Fourier spectral method for discretizing (3.2) reads:
Find $z_N^n := z_N^n(x,s),\ r_N^n := r_N^n(x,s),\ \psi_N^n := \psi_N^n(x,s) \in X_N$ for $0 \le s \le \tau$, i.e.

$$\begin{cases} z_N^n(x,s) = \sum\limits_{l=-N/2}^{N/2-1} \widehat{(z_N^n)}_l(s) e^{i\mu_l(x-a)}, \quad r_N^n(x,s) = \sum\limits_{l=-N/2}^{N/2-1} \widehat{(r_N^n)}_l(s) e^{i\mu_l(x-a)}, \\ \psi_N^n(x,s) = \sum\limits_{l=-N/2}^{N/2-1} \widehat{(\psi_N^n)}_l(s) e^{i\mu_l(x-a)}, \end{cases} \tag{3.6}$$

such that

$$\begin{cases} i\partial_s \psi_N^n + \partial_{xx}\psi_N^n + e^{is/\varepsilon^2} P_N(z_N^n \psi_N^n) + e^{-is/\varepsilon^2} P_N(\overline{z_N^n}\psi_N^n) + P_N(r_N^n \psi_N^n) = 0, \\ 2i\partial_s z_N^n + \varepsilon^2 \partial_{ss} z_N^n - \partial_{xx} z_N^n = 0, \quad 0 < s \le \tau, \quad a < x < b, \\ \varepsilon^2 \partial_{ss} r_N^n - \partial_{xx} r_N^n + \frac{1}{\varepsilon^2} r_N^n = P_N\left(|\psi_N^n|^2\right). \end{cases} \tag{3.7}$$

Substituting (3.6) into (3.7) and noticing the orthogonality of the Fourier basis, we get

$$\begin{cases} i\widehat{(\psi_N^n)}_l'(s) - \mu_l^2 \widehat{(\phi_N^n)}_l(s) + e^{\frac{is}{\varepsilon^2}} \widehat{(z_N^n \psi_N^n)}_l(s) + e^{-\frac{is}{\varepsilon^2}} \widehat{(\overline{z_N^n}\psi_N^n)}_l(s) + \widehat{(r_N^n \psi_N^n)}_l(s) = 0, \\ 2i\widehat{(z_N^n)}_l'(s) + \varepsilon^2 \widehat{(z_N^n)}_l''(s) + \mu_l^2 \widehat{(z_N^n)}_l(s) = 0, \quad 0 < s \le \tau, \\ \varepsilon^2 \widehat{(r_N^n)}_l''(s) + \left(\mu_l^2 + \frac{1}{\varepsilon^2}\right) \widehat{(r_N^n)}_l(s) = \widehat{(|\psi_N^n|^2)}_l(s), \quad -\frac{N}{2} \le l \le \frac{N}{2} - 1. \end{cases} \tag{3.8}$$

For each $-N/2 \le l \le N/2-1$, we can rewrite (3.8) by using the variation-of-constant formula as

$$\widehat{(z_N^n)}_l(s) = a_l(s)\widehat{(z_N^n)}_l(0) + \varepsilon^2 b_l(s)\widehat{(z_N^n)}_l'(0), \qquad 0 \le s \le \tau, \tag{3.9a}$$

$$\widehat{(r_N^n)}_l(s) = \frac{\sin(\omega_l s)}{\omega_l}\widehat{(r_N^n)}_l'(0) + \int_0^s \frac{\sin\left(\omega_l(s-\theta)\right)}{\varepsilon^2 \omega_l} \widehat{(|\psi_N^n|^2)}_l(\theta)\, d\theta, \tag{3.9b}$$

$$\begin{aligned} \widehat{(\psi_N^n)}_l(s) = {} & e^{-i\mu_l^2 s}\widehat{(\psi_N^n)}_l(0) + i e^{-i\mu_l^2 s} \int_0^s e^{i\left(\mu_l^2 + \frac{1}{\varepsilon^2}\right)\theta} \widehat{(z_N^n \psi_N^n)}_l(\theta)\, d\theta \\ & + i e^{-i\mu_l^2 s} \int_0^s e^{i\left(\mu_l^2 - \frac{1}{\varepsilon^2}\right)\theta} \widehat{(\overline{z_N^n}\psi_N^n)}_l(\theta)\, d\theta + i \int_0^s e^{i\mu_l^2(\theta - s)} \widehat{(r_N^n \psi_N^n)}_l(\theta)\, d\theta, \end{aligned} \tag{3.9c}$$

where

$$\begin{cases} a_l(s) := \frac{\lambda_l^+ e^{is\lambda_l^-} - \lambda_l^- e^{is\lambda_l^+}}{\lambda_l^+ - \lambda_l^-}, \quad b_l(s) := i\frac{e^{is\lambda_l^+} - e^{is\lambda_l^-}}{\varepsilon^2(\lambda_l^- - \lambda_l^+)}, \quad 0 \le s \le \tau, \\ \lambda_l^{\pm} = -\frac{1}{\varepsilon^2}\left(1 \pm \sqrt{1 + \mu_l^2 \varepsilon^2}\right), \quad \omega_l = \frac{1}{\varepsilon^2}\sqrt{1 + \mu_l^2 \varepsilon^2} = O\left(\frac{1}{\varepsilon^2}\right). \end{cases} \tag{3.10}$$

Differentiating (3.9a) and (3.9b) with respect to s, we obtain

$$\widehat{(z_N^n)}_l'(s) = a_l'(s)\widehat{(z_N^n)}_l(0) + \varepsilon^2 b_l'(s)\widehat{(z_N^n)}_l'(0), \quad 0 \le s \le \tau, \tag{3.11a}$$

$$\widehat{(r_N^n)}_l'(s) = \cos(\omega_l s)\widehat{(r_N^n)}_l'(0) + \int_0^s \frac{\cos(\omega_l(s-\theta))}{\varepsilon^2}\widehat{(|\psi_N^n|^2)}_l(\theta)\,d\theta, \tag{3.11b}$$

where

$$a_l'(s) = i\lambda_l^+\lambda_l^- \frac{e^{is\lambda_l^-} - e^{is\lambda_l^+}}{\lambda_l^+ - \lambda_l^-}, \quad b_l'(s) = \frac{\lambda_l^+ e^{is\lambda_l^+} - \lambda_l^- e^{is\lambda_l^-}}{\varepsilon^2(\lambda_l^+ - \lambda_l^-)}, \quad 0 \le s \le \tau.$$

Taking $s = \tau$ in (3.9) and (3.11), we immediately get

$$\begin{aligned}
\widehat{(z_N^n)}_l(\tau) &= a_l(\tau)\widehat{(z_N^n)}_l(0) + \varepsilon^2 b_l(\tau)\widehat{(z_N^n)}_l'(0),\\
\widehat{(z_N^n)}_l'(\tau) &= a_l'(\tau)\widehat{(z_N^n)}_l(0) + \varepsilon^2 b_l'(\tau)\widehat{(z_N^n)}_l'(0).
\end{aligned} \tag{3.12}$$

In order to approximate the definite integrals in (3.9b), (3.9c) and (3.11b) with $s = \tau$, we adapt the Gautschi's type quadrature [8,12,26–29,38]

$$\begin{aligned}
\int_0^\tau e^{i\delta\theta} f(\theta)\,d\theta &\approx \int_0^\tau e^{i\delta\theta}\left[f(0) + \theta f'(0)\right] d\theta\\
&= \frac{i - ie^{i\delta\tau}}{\delta} f(0) + \frac{(1 - i\delta\tau)e^{i\delta\tau} - 1}{\delta^2} f'(0)
\end{aligned}$$

except the last term in (3.9c) which is approximated via a combination of the Gautschi's and Deuflhard's quadratures as [12,21,36]

$$\begin{aligned}
\int_0^\tau e^{i\mu_l^2(\theta-\tau)}\widehat{(r_N^n\psi_N^n)}_l(\theta)\,d\theta &\approx \int_0^\tau e^{i\mu_l^2(\theta-\tau)}\left[\widehat{(A_1)}_l(\theta) + \theta\,\widehat{(A_2)}_l(\theta)\right] d\theta\\
&\approx \frac{\tau}{2}\left[\widehat{(A_1)}_l(\tau) + \tau\,\widehat{(A_2)}_l(\tau)\right],
\end{aligned} \tag{3.13}$$

where $A_1(x,\theta) := r_N^n(x,\theta)\psi_N^n(x,0)$ and $A_2(x,\theta) := r_N^n(x,\theta)\partial_s\psi_N^n(x,0)$ for $0 \le \theta \le \tau$ and thus $A_1(x,0) = A_2(x,0) \equiv 0$ since $r_N^n(x,0) \equiv 0$. Thus (3.9b), (3.9c) and (3.11b) with $s = \tau$ can be approximated as

$$\begin{cases}
\widehat{(r_N^n)}_l(\tau) &\approx \frac{\sin(\omega_l\tau)}{\omega_l}\widehat{(r_N^n)}_l'(0) + p_l(\tau)\widehat{(|\psi_N^n|^2)}_l(0) + q_l(\tau)\widehat{(|\psi_N^n|^2)}_l'(0),\\
\widehat{(r_N^n)}_l'(\tau) &\approx \cos(\omega_l\tau)\widehat{(r_N^n)}_l'(0) + p_l'(\tau)\widehat{(|\psi_N^n|^2)}_l(0) + q_l'(\tau)\widehat{(|\psi_N^n|^2)}_l'(0),\\
\widehat{(\psi_N^n)}_l(\tau) &\approx e^{-i\mu_l^2\tau}\widehat{(\psi_N^n)}_l(0) + c_l^+(\tau)\widehat{(z_N^n\psi_N^n)}_l(0) + d_l^+(\tau)\widehat{(z_N^n\psi_N^n)}_l'(0)\\
&\quad + c_l^-(\tau)\widehat{(\overline{z_N^n}\psi_N^n)}_l(0) + d_l^-(\tau)\widehat{(\overline{z_N^n}\psi_N^n)}_l'(0)\\
&\quad + \frac{i\tau}{2}\left[\widehat{(A_1)}_l(\tau) + \tau\,\widehat{(A_2)}_l(\tau)\right],
\end{cases} \tag{3.14}$$

where $p_l(\tau)$, $q_l(\tau)$, $p_l'(\tau)$, $q_l'(\tau)$, $c_l^{\pm}(\tau)$ and $d_l^{\pm}(\tau)$ as well as their bounds are given in Appendix. For the derivatives, we can compute them as

$$\widehat{(|\psi_N^n|^2)}_l'(0) = 2\Big(\mathrm{Re}\{\widehat{\overline{\psi_N^n}\partial_s\psi_N^n}\}\Big)_l(0),$$
$$\widehat{(z_N^n\psi_N^n)}_l'(0) = \widehat{(\partial_s z_N^n\psi_N^n)}_l(0) + \widehat{(z_N^n\partial_s\psi_N^n)}_l(0),$$

where $\mathrm{Re}\{z\}$ denotes the real part of a complex number z, and for $-\frac{N}{2} \le l \le \frac{N}{2}-1$,

$$\widehat{(z_N^n)}_l'(0) = \frac{i}{2}\frac{\sin(\mu_l^2\tau)}{\tau}\widehat{(z_N^n)}_l(0),$$
$$\widehat{(\psi_N^n)}_l'(0) = -i\frac{\sin(\mu_l^2\tau)}{\tau}\widehat{(\psi_N^n)}_l(0) + i\widehat{(\phi_N^n\psi_N^n)}_l(0),$$

which are approximations of $\partial_s z^n(x,0) = -\frac{i}{2}\partial_{xx}z^n(x,0)$ and $\partial_s\psi^n(x,0) = i\partial_{xx}\psi^n(x,0) + i\phi^n(x,0)\psi^n(x,0)$, respectively [8]. Inserting (3.12) and (3.14) into (3.6) with setting $s=\tau$, and noticing (2.8), we immediately obtain a multiscale time integrator Fourier spectral method based on the MDF (3.2) for the problem (3.1).

In practice, the integrals for computing the Fourier transform coefficients in (3.5), (3.9) and (3.11) are usually approximated by the numerical quadratures [9,11,46]. Let $\Phi_j^n, \dot\Phi_j^n$ and Ψ_j^n be approximations of $\phi(x_j,t_n), \partial_t\phi(x_j,t_n)$ and $\psi(x_j,t_n)$, respectively; Z_j^{n+1}, $\dot Z_j^{n+1}$, R_j^{n+1} and $\dot R_j^{n+1}$ be approximations of $z^n(x_j,\tau)$, $\partial_s z^n(x_j,\tau)$, $r^n(x_j,\tau)$ and $\partial_s r^n(x_j,\tau)$, respectively, for $j=0,1,\ldots,N$. Choosing $\Phi_j^0 = \phi_0(x_j)$, $\dot\Phi_j^0 = \phi_1(x_j)/\varepsilon^2$ and $\Psi_j^0 = \psi_0(x_j)$ for $0\le j\le N$, a multiscale time integrator Fourier pseudospectral (MTI-FP) discretization for the problem (3.1) reads

$$\begin{cases} \Phi_j^{n+1} = \mathrm{e}^{i\tau/\varepsilon^2}Z_j^{n+1} + \mathrm{e}^{-i\tau/\varepsilon^2}\overline{Z_j^{n+1}} + R_j^{n+1}, \\ \dot\Phi_j^{n+1} = \mathrm{e}^{i\tau/\varepsilon^2}\left(\dot Z_j^{n+1} + \frac{i}{\varepsilon^2}Z_j^{n+1}\right) + \mathrm{e}^{-i\tau/\varepsilon^2}\left(\overline{\dot Z_j^{n+1}} - \frac{i}{\varepsilon^2}\overline{Z_j^{n+1}}\right) + \dot R_j^{n+1}, \\ \Psi_j^{n+1} = \displaystyle\sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1}\widetilde{(\Psi^{n+1})}_l\mathrm{e}^{i\mu_l(x_j-a)}, \quad j=0,1,\ldots,N, \quad n\ge 0, \end{cases} \tag{3.15}$$

where

$$\begin{cases} Z_j^{n+1} = \displaystyle\sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1}\widetilde{(Z^{n+1})}_l\mathrm{e}^{i\mu_l(x_j-a)}, \quad R_j^{n+1} = \sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1}\widetilde{(R^{n+1})}_l\mathrm{e}^{i\mu_l(x_j-a)}, \\ \dot Z_j^{n+1} = \displaystyle\sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1}\widetilde{(\dot Z^{n+1})}_l\mathrm{e}^{i\mu_l(x_j-a)}, \quad \dot R_j^{n+1} = \sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1}\widetilde{(\dot R^{n+1})}_l\mathrm{e}^{i\mu_l(x_j-a)}, \end{cases}$$

with

$$\widetilde{(Z^{n+1})}_l = a_l(\tau)\widetilde{(Z^0)}_l + \varepsilon^2 b_l(\tau)\widetilde{(\dot{Z}^0)}_l,\ \widetilde{(\dot{Z}^{n+1})}_l = a_l'(\tau)\widetilde{(Z^0)}_l + \varepsilon^2 b_l'(\tau)\widetilde{(\dot{Z}^0)}_l, \tag{3.16a}$$

$$\widetilde{(R^{n+1})}_l = \frac{\sin(\omega_l\tau)}{\omega_l}\widetilde{(\dot{R}^0)}_l + p_l(\tau)\widetilde{(|\Psi^n|^2)}_l + 2q_l(\tau)\widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot{\Psi}^n\})}_l, \tag{3.16b}$$

$$\widetilde{(\dot{R}^{n+1})}_l = \cos(\omega_l\tau)\widetilde{(\dot{R}^0)}_l + p_l'(\tau)\widetilde{(|\Psi^n|^2)}_l + 2q_l'(\tau)\widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot{\Psi}^n\})}_l, \tag{3.16c}$$

$$\begin{aligned}\widetilde{(\Psi^{n+1})}_l &= \mathrm{e}^{-i\mu_l^2\tau}\widetilde{(\Psi^n)}_l + c_l^+(\tau)\widetilde{(Z^0\Psi^n)}_l + d_l^+(\tau)\left[\widetilde{(\dot{Z}^0\Psi^n)}_l + \widetilde{(Z^0\dot{\Psi}^n)}_l\right]\\ &\quad + c_l^-(\tau)\widetilde{(\overline{Z^0}\Psi^n)}_l + d_l^-(\tau)\left[\widetilde{(\overline{\dot{Z}^0}\Psi^n)}_l + \widetilde{(\overline{Z^0}\dot{\Psi}^n)}_l\right] + \frac{i\tau}{2}\widetilde{(R^{n+1}\Psi^n)}_l\\ &\quad + \frac{i\tau^2}{2}\widetilde{(R^{n+1}\dot{\Psi}^n)}_l, \quad -N/2 \le l \le N/2-1,\end{aligned} \tag{3.16d}$$

and

$$\widetilde{(Z^0)}_l = \frac{1}{2}\left[\widetilde{(\Phi^n)}_l - i\varepsilon^2\widetilde{(\dot{\Phi}^n)}_l\right],\quad \widetilde{(\dot{Z}^0)}_l = \frac{i\sin\left(\mu_l^2\tau\right)}{2\tau}\widetilde{(Z^0)}_l, \tag{3.17a}$$

$$\widetilde{(\dot{R}^0)}_l = -\widetilde{(\dot{Z}^0)}_l - \widetilde{\left(\dot{Z}^0\right)}_l,\quad \widetilde{(\dot{\Psi}^n)}_l = -\frac{i\sin(\mu_l^2\tau)}{\tau}\widetilde{(\Psi^n)}_l + i\widetilde{(\Phi^n\Psi^n)}_l. \tag{3.17b}$$

This MTI-FP method for the KGS equations (3.1) (or (1.3)) is explicit, accurate, easy to be implemented and very efficient due to the discrete fast Fourier transform. The memory cost is $O(N)$ and the computational cost per time step is $O(N\log N)$.

4 Uniform convergence of MTI-FP

In this section, we establish an error bound for the MTI-FP method (3.15) of the KGS (3.1), which is uniformly accurate for $\varepsilon \in (0,1]$. Let $0 < T < T^*$ with T^* the maximum existence time of the solution of the problem (3.1). Motivated by the formal asymptotic results (1.8) and (1.9) as well as the numerical results (cf. Fig. 1), we make the following assumptions on the solution of the problem (3.1)—there exists an integer $m_0 \ge 4$ such that $\phi \in C^1([0,T]; H_p^{m_0+4}(\Omega))$, $\psi \in C([0,T]; H_p^{m_0+2}(\Omega)) \cap C^1([0,T]; H_p^{m_0}(\Omega)) \cap C^2([0,T]; H_p^{m_0-2}(\Omega))$ and

$$\begin{aligned}&\|\phi\|_{L^\infty([0,T];H^{m_0+4})} + \varepsilon^2\|\partial_t\phi\|_{L^\infty([0,T];H^{m_0+4})} \lesssim 1,\\ &\|\psi\|_{L^\infty([0,T];H^{m_0+2})} + \|\partial_t\psi\|_{L^\infty([0,T];H^{m_0})} + \varepsilon^2\|\partial_{tt}\psi\|_{L^\infty([0,T];H^{m_0-2})} \lesssim 1,\end{aligned} \tag{4.1}$$

where $H_p^m(\Omega) = \left\{f(x) \in H^m(\Omega) \mid f^{(k)}(a) = f^{(k)}(b), k = 0,1,\ldots,m-1\right\} \subset H^m(\Omega)$. From the nonlinear Schrödinger equation (NLSE) in (3.1), it is easy to see that

$$i\partial_t\rho(x,t) + \partial_x\left[\overline{\psi}\partial_x\psi(x,t) - \psi\partial_x\overline{\psi}(x,t)\right] = 0,\quad x \in \Omega,\quad t > 0,$$

where $\rho(x,t) := |\psi(x,t)|^2$. Then under the assumption (4.1), we have

$$\rho \in C\left([0,T];\, H_p^{m_0+2}(\Omega)\right) \cap C^1\left([0,T];\, H_p^{m_0}(\Omega)\right) \cap C^2\left([0,T];\, H_p^{m_0-2}(\Omega)\right),$$
$$\|\partial_t^k \rho\|_{L^\infty([0,T];H^{m_0+2-2k}(\Omega))} \lesssim 1, \quad k = 0,1,2. \tag{4.2}$$

Denote $C_\phi = \max_{0<\varepsilon\le 1}\{\|\phi\|_{L^\infty([0,T];H^{m_0+4}(\Omega))}, \varepsilon^2\|\partial_t\phi\|_{L^\infty([0,T];H^{m_0+4}(\Omega))}\}$ and $C_\psi = \max_{0<\varepsilon\le 1}\{\|\psi\|_{L^\infty([0,T];H^{m_0+2}(\Omega))}\}$.

Let $\Phi^n = (\Phi_0^n, \Phi_1^n, \ldots, \Phi_N^n) \in Y_N$, $\Psi^n = (\Psi_0^n, \Psi_1^n, \ldots, \Psi_N^n) \in Y_N$ and $\dot\Phi^n = (\dot\Phi_0^n, \dot\Phi_1^n, \ldots, \dot\Phi_N^n) \in Y_N$ $(n \ge 0)$ be the numerical solution obtained from the MTI-FP method (3.15)–(3.17). Denote their interpolations as

$$\phi_I^n(x) := (I_N\Phi^n)(x), \quad \psi_I^n(x) := (I_N\Psi^n)(x), \quad \dot\phi_I^n(x) := (I_N\dot\Phi^n)(x), \quad x \in \overline{\Omega}, \tag{4.3}$$

and define the error functions as

$$\begin{aligned} e_\phi^n(x) &:= \phi(x,t_n) - \phi_I^n(x), \qquad e_\psi^n(x) := \psi(x,t_n) - \psi_I^n(x), \\ \dot e_\phi^n(x) &:= \partial_t\phi(x,t_n) - \dot\phi_I^n(x), \qquad x \in \overline{\Omega}, \qquad 0 \le n \le \tfrac{T}{\tau}; \end{aligned} \tag{4.4}$$

then we have the following error estimates for the MTI-FP method (3.15)–(3.17).

Theorem 4.1 (Error bounds of MTI-FP) *Under the assumption* (4.1), *there exist two constants* $0 < h_0 \le 1$ *and* $0 < \tau_0 \le 1$ *sufficiently small and independent of* ε *such that for any* $0 < \varepsilon \le 1$, *when* $0 < h \le h_0$ *and* $0 < \tau \le \tau_0$, *we have*

$$\left\|e_\phi^n\right\|_{H^2} + \left\|e_\psi^n\right\|_{H^2} + \varepsilon^2\left\|\dot e_\phi^n\right\|_{H^2} \lesssim h^{m_0} + \frac{\tau^2}{\varepsilon^2}, \tag{4.5}$$

$$\left\|e_\phi^n\right\|_{H^2} + \left\|e_\psi^n\right\|_{H^2} + \varepsilon^2\left\|\dot e_\phi^n\right\|_{H^2} \lesssim h^{m_0} + \varepsilon^2, \qquad 0 \le n \le \frac{T}{\tau}, \tag{4.6}$$

$$\left\|\phi_I^n\right\|_{H^2} \le C_\phi + 1, \qquad \left\|\psi_I^n\right\|_{H^2} \le C_\psi + 1, \qquad \left\|\dot\phi_I^n\right\|_{H^2} \le \frac{C_\phi + 1}{\varepsilon^2}. \tag{4.7}$$

Thus, by taking the minimum of the two error bounds (4.5) *and* (4.6) *for* $\varepsilon \in (0,1]$, *we obtain a uniform error bound with respect to* $\varepsilon \in (0,1]$ *for* $0 \le n \le \frac{T}{\tau}$

$$\left\|e_\phi^n\right\|_{H^2} + \left\|e_\psi^n\right\|_{H^2} + \varepsilon^2\left\|\dot e_\phi^n\right\|_{H^2} \lesssim h^{m_0} + \min_{0<\varepsilon\le 1}\left\{\frac{\tau^2}{\varepsilon^2}, \varepsilon^2\right\} \lesssim h^{m_0} + \tau. \tag{4.8}$$

In order to prove the above theorem, we introduce

$$\begin{aligned} e_{\phi,N}^n(x) &:= (P_N\phi)(x,t_n) - \phi_I^n(x), \quad \dot e_{\phi,N}^n(x) := P_N(\partial_t\phi)(x,t_n) - \dot\phi_I^n(x), \\ e_{\psi,N}^n(x) &:= (P_N\psi)(x,t_n) - \psi_I^n(x), \qquad x \in \overline{\Omega}, \qquad 0 \le n \le \tfrac{T}{\tau}. \end{aligned} \tag{4.9}$$

Using the triangle inequality and noticing the assumption (4.1), we have

$$\begin{aligned}
&\|e_\phi^n\|_{H^2} \le \|\phi(x,t_n) - (P_N\phi)(x,t_n)\|_{H^2} + \|e_{\phi,N}^n\|_{H^2} \lesssim h^{m_0+2} + \|e_{\phi,N}^n\|_{H^2},\\
&\|e_\psi^n\|_{H^2} \le \|\psi(x,t_n) - (P_N\psi)(x,t_n)\|_{H^2} + \|e_{\psi,N}^n\|_{H^2} \lesssim h^{m_0} + \|e_{\psi,N}^n\|_{H^2},\\
&\|\dot{e}_\phi^n\|_{H^2} \le \|\dot{\phi}(x,t_n) - (P_N\dot{\phi})(x,t_n)\|_{H^2} + \|\dot{e}_{\phi,N}^n\|_{H^2} \lesssim \frac{h^{m_0+2}}{\varepsilon^2} + \|\dot{e}_{\phi,N}^n\|_{H^2}.
\end{aligned} \tag{4.10}$$

Thus we need only obtain estimates for $\|e_{\phi,N}^n\|_{H^2}$, $\|e_{\psi,N}^n\|_{H^2}$ and $\|\dot{e}_{\phi,N}^n\|_{H^2}$, which will be done by introducing the error energy functional

$$\begin{aligned}
\mathcal{E}\left(e_{\phi,N}^n, e_{\psi,N}^n, \dot{e}_{\phi,N}^n\right) := \varepsilon^2 \left\|\dot{e}_{\phi,N}^n\right\|_{H^2}^2 + \left\|\partial_x e_{\phi,N}^n\right\|_{H^2}^2 + \frac{1}{\varepsilon^2}\left(\left\|e_{\phi,N}^n\right\|_{H^2}^2\right.\\
\left. + \left\|e_{\psi,N}^n\right\|_{H^2}^2\right),
\end{aligned} \tag{4.11}$$

and establishing the following several lemmas.

For any $\mathbf{v} \in Y_N$, denote $v_{-1} = v_{N-1}$ and $v_{N+1} = v_1$, and define the difference operators $\delta_x^+\mathbf{v} \in Y_N$ and $\delta_x^2\mathbf{v} \in Y_N$ as

$$\delta_x^+ v_j = \frac{v_{j+1} - v_j}{h}, \qquad \delta_x^2 v_j = \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2}, \qquad j = 0, 1, \ldots, N,$$

and the norms as

$$\|\mathbf{v}\|_{Y,1}^2 = \|\mathbf{v}\|_{l^2}^2 + \|\delta_x^+\mathbf{v}\|_{l^2}^2, \qquad \|\mathbf{v}\|_{Y,2}^2 = \|\mathbf{v}\|_{l^2}^2 + \|\delta_x^+\mathbf{v}\|_{l^2}^2 + \|\delta_x^2\mathbf{v}\|_{l^2}^2, \tag{4.12}$$

with

$$\|\mathbf{v}\|_{l^2}^2 = h\sum_{j=0}^{N-1} |v_j|^2, \quad \|\delta_x^+\mathbf{v}\|_{l^2}^2 = h\sum_{j=0}^{N-1} |\delta_x^+ v_j|^2, \quad \|\delta_x^2\mathbf{v}\|_{l^2}^2 = h\sum_{j=0}^{N-1} |\delta_x^2 v_j|^2,$$

then we can have the following estimates [7,8]

$$\|I_N\mathbf{v}\|_{H^1} \lesssim \|\mathbf{v}\|_{Y,1} \lesssim \|I_N\mathbf{v}\|_{H^1}, \quad \|I_N\mathbf{v}\|_{H^2} \lesssim \|\mathbf{v}\|_{Y,2} \lesssim \|I_N\mathbf{v}\|_{H^2}, \quad \forall \mathbf{v} \in Y_N. \tag{4.13}$$

Lemma 4.1 (A new formulation of MTI-FP) *For the numerical solution ϕ_I^{n+1} and $\dot{\phi}_I^{n+1}$ ($n \ge 0$) obtained from the MTI-FP method (3.15)–(3.17), we have*

$$\phi_I^{n+1}(x) = \sum_{l=-N/2}^{N/2-1} \widetilde{(\Phi^{n+1})}_l e^{i\mu_l(x-a)}, \qquad \dot{\phi}_I^{n+1}(x) = \sum_{l=-N/2}^{N/2-1} \widetilde{(\dot{\Phi}^{n+1})}_l e^{i\mu_l(x-a)}, \tag{4.14}$$

where

$$\widetilde{(\Phi^{n+1})}_l = \cos(\omega_l\tau)\widetilde{(\Phi^n)}_l + \frac{\sin(\omega_l\tau)}{\omega_l}\widetilde{(\dot\Phi^n)}_l + p_l(\tau)\widetilde{(|\Psi^n|^2)}_l + 2q_l(\tau)\widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot\Psi^n\})}_l,$$
$$\widetilde{(\dot\Phi^{n+1})}_l = \cos(\omega_l\tau)\widetilde{(\dot\Phi^n)}_l - \omega_l\sin(\omega_l\tau)\widetilde{(\Phi^n)}_l + p_l'(\tau)\widetilde{(|\Psi^n|^2)}_l + 2q_l'(\tau)\widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot\Psi^n\})}_l.$$

Proof For $l = -\frac{N}{2}, \ldots, \frac{N}{2} - 1$, from (3.15), we get

$$\begin{cases} \widetilde{(\Phi^{n+1})}_l = \mathrm{e}^{\frac{i\tau}{\varepsilon^2}}\widetilde{(Z^{n+1})}_l + \mathrm{e}^{-\frac{i\tau}{\varepsilon^2}}\widetilde{\left(\overline{Z^{n+1}}\right)}_l + \widetilde{(R^{n+1})}_l, \\ \widetilde{(\dot\Phi^{n+1})}_l = \mathrm{e}^{\frac{i\tau}{\varepsilon^2}}\left[\widetilde{(\dot Z^{n+1})}_l + \frac{i}{\varepsilon^2}\widetilde{(Z^{n+1})}_l\right] + \mathrm{e}^{-\frac{i\tau}{\varepsilon^2}}\left[\widetilde{\left(\overline{\dot Z^{n+1}}\right)}_l - \frac{i}{\varepsilon^2}\widetilde{\left(\overline{Z^{n+1}}\right)}_l\right] + \widetilde{(\dot R^{n+1})}_l, \end{cases} \tag{4.15}$$

and from (3.17), we obtain

$$\widetilde{(Z^0)}_l = \frac{1}{2}\left[\widetilde{(\Phi^n)}_l - i\varepsilon^2\widetilde{(\dot\Phi^n)}_l\right], \quad \widetilde{(\dot R^0)}_l = -\widetilde{(\dot Z^0)}_l - \widetilde{\left(\overline{\dot Z^0}\right)}_l. \tag{4.16}$$

Noticing (3.10) and (3.4), for $\mathbf{v} \in Y_N$, we have

$$a_l(\tau) = a_{-l}(\tau), \quad b_l(\tau) = b_{-l}(\tau), \quad l = -\frac{N}{2}, \ldots, \frac{N}{2} - 1,$$
$$\widetilde{(\overline{\mathbf{v}})}_l = \begin{cases} \overline{\widetilde{\mathbf{v}}_{-l}}, & |l| \le \frac{N}{2} - 1, \\ \overline{\widetilde{\mathbf{v}}_l}, & l = -\frac{N}{2}. \end{cases}$$

Plugging (4.16) into (3.16a)–(3.16c), and (3.16) into (4.15), we get

$$\begin{aligned} \widetilde{(\Phi^{n+1})}_l &= \mathrm{Re}\left\{\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}a_l(\tau)\right\}\widetilde{(\Phi^n)}_l + \varepsilon^2\mathrm{Im}\left\{\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}a_l(\tau)\right\}\widetilde{(\dot\Phi^n)}_l + \varepsilon^2\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}b_l(\tau)\widetilde{(\dot Z^0)}_l \\ &\quad + \varepsilon^2\mathrm{e}^{-\frac{i\tau}{\varepsilon^2}}\overline{b_l}(\tau)\widetilde{\left(\overline{\dot Z^0}\right)}_l + \frac{\sin(\omega_l\tau)}{\omega_l}\widetilde{(\dot R^0)}_l + p_l(\tau)\widetilde{(|\Psi^n|^2)}_l \\ &\quad + 2q_l(\tau)\widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot\Psi^n\})}_l, \\ \widetilde{(\dot\Phi^{n+1})}_l &= \varepsilon^2\mathrm{Im}\left\{\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}a_l'(\tau) + \frac{i}{\varepsilon^2}\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}a_l(\tau)\right\}\widetilde{(\dot\Phi^n)}_l + \varepsilon^2\mathrm{e}^{-\frac{i\tau}{\varepsilon^2}}\left[\overline{b_l'}(\tau) - \frac{i}{\varepsilon^2}\overline{b_l}(\tau)\right]\widetilde{\left(\overline{\dot Z^0}\right)}_l \\ &\quad + \mathrm{Re}\left\{\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}a_l'(\tau) + \frac{i}{\varepsilon^2}\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}a_l(\tau)\right\}\widetilde{(\Phi^n)}_l + \varepsilon^2\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}\left[b_l'(\tau) + \frac{i}{\varepsilon^2}b_l(\tau)\right]\widetilde{(\dot Z^0)}_l \\ &\quad + \cos(\omega_l\tau)\widetilde{(\dot R^0)}_l + p_l'(\tau)\widetilde{(|\Psi^n|^2)}_l + 2q_l'(\tau)\widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot\Psi^n\})}_l, \end{aligned}$$

where $\mathrm{Im}\{z\}$ denotes the imaginary part of a complex number z. Then (4.14) can be obtained by combining the above equalities and (3.10). □

For the solution $\phi^n(x,s) := \phi(x,t_n+s)$, $\psi^n(x,s) := \psi(x,t_n+s)$ of (3.1), we have

$$\varepsilon^2\widehat{\phi}_l''(t_n+s)+\mu_l^2\widehat{\phi}_l(t_n+s)+\frac{1}{\varepsilon^2}\widehat{\phi}_l(t_n+s)=\widehat{(|\psi|^2)}_l(t_n+s),\quad s>0 \tag{4.17a}$$

$$i\widehat{\psi}_l'(t_n+s)-\mu_l^2\widehat{\phi}_l(t_n+s)+\widehat{(\phi\psi)}_l(t_n+s)=0,\quad l\in\mathbb{Z}. \tag{4.17b}$$

By applying the variation-of-constant formula to (4.17) and noticing the ansatz (2.2) with $\rho^n(x,s) := |\psi(x,t_n+s)|^2$, we get

$$\widehat{\phi}_l(t_{n+1})=\cos(\omega_l\tau)\widehat{\phi}_l(t_n)+\frac{\sin(\omega_l\tau)}{\omega_l}\widehat{\phi}_l'(t_n)+\int_0^\tau\frac{\sin(\omega_l(\tau-\theta))}{\varepsilon^2\omega_l}\widehat{(\rho^n)}_l(\theta)d\theta, \tag{4.18a}$$

$$\widehat{\phi}_l'(t_{n+1})=\cos(\omega_l\tau)\widehat{\phi}_l'(t_n)-\omega_l\sin(\omega_l\tau)\widehat{\phi}_l(t_n)+\int_0^\tau\frac{\cos(\omega_l(\tau-\theta))}{\varepsilon^2}\widehat{(\rho^n)}_l(\theta)d\theta, \tag{4.18b}$$

$$\begin{aligned}\widehat{\psi}_l(t_{n+1})=&\,\mathrm{e}^{-i\mu_l^2\tau}\widehat{\psi}_l(t_n)+i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau\mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\widehat{(z^n\psi^n)}_l(\theta)d\theta \\ &+i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau\mathrm{e}^{i\left(\mu_l^2-\frac{1}{\varepsilon^2}\right)\theta}\widehat{(\overline{z^n}\psi^n)}_l(\theta)d\theta+i\int_0^\tau\mathrm{e}^{i\mu_l^2(\theta-\tau)}\widehat{(r^n\psi^n)}_l(\theta)d\theta.\end{aligned} \tag{4.18c}$$

Combining the above results, we define local truncation error functions as

$$\begin{aligned}\xi_\phi^n(x)&=\sum_{l=-N/2}^{N/2-1}\widehat{(\xi_\phi^n)}_l\mathrm{e}^{i\mu_l(x-a)},\qquad \xi_\psi^n(x)=\sum_{l=-N/2}^{N/2-1}\widehat{(\xi_\psi^n)}_l\mathrm{e}^{i\mu_l(x-a)},\\ \dot{\xi}_\phi^n(x)&=\sum_{l=-N/2}^{N/2-1}\widehat{(\dot{\xi}_\phi^n)}_l\mathrm{e}^{i\mu_l(x-a)},\qquad x\in\Omega,\end{aligned} \tag{4.19}$$

where

$$\begin{aligned}\widehat{(\xi_\phi^n)}_l:=&\,\widehat{\phi}_l(t_{n+1})-\Big[\cos(\omega_l\tau)\widehat{\phi}_l(t_n)+\frac{\sin(\omega_l\tau)}{\omega_l}\widehat{\phi}_l'(t_n)+p_l(\tau)\widehat{(|\psi^n|^2)}_l(0)\\ &+2q_l(\tau)\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0)\Big],\end{aligned} \tag{4.20a}$$

$$\begin{aligned}\widehat{(\dot{\xi}_\phi^n)}_l:=&\,\widehat{\phi}_l'(t_{n+1})-\Big[-\omega_l\sin(\omega_l\tau)\widehat{\phi}_l(t_n)+\cos(\omega_l\tau)\widehat{\phi}_l'(t_n)+p_l'(\tau)\widehat{(|\psi^n|^2)}_l(0)\\ &+2q_l'(\tau)\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0)\Big],\end{aligned} \tag{4.20b}$$

$$\begin{aligned}\widehat{(\xi_\psi^n)}_l:=&\,\widehat{\psi}_l(t_{n+1})-\mathrm{e}^{-i\mu_l^2\tau}\widehat{\psi}_l(t_n)-c_l^+(\tau)\widehat{(z^n\psi^n)}_l(0)-c_l^-(\tau)\widehat{(\overline{z^n}\psi^n)}_l(0)\\ &-d_l^+(\tau)\Big[\widehat{(\mathfrak{z}^n\psi^n)}_l(0)+\widehat{(z^n\varphi^n)}_l(0)\Big]-d_l^-(\tau)\Big[\widehat{(\overline{\mathfrak{z}^n}\psi^n)}_l(0)+\widehat{(\overline{z^n}\varphi^n)}_l(0)\Big]\\ &-\frac{i\tau}{2}\widehat{(\gamma^{n+1}\psi^n)}_l(0)-\frac{i\tau^2}{2}\widehat{(\gamma^{n+1}\varphi^n)}_l.\end{aligned} \tag{4.20c}$$

Here we introduce three auxiliary functions as

$$\varphi^n(x) = \sum_{l\in\mathbb{Z}} \widehat{(\varphi^n)}_l e^{i\mu_l(x-a)}, \quad \mathfrak{z}^n(x) = \sum_{l\in\mathbb{Z}} \widehat{(\mathfrak{z}^n)}_l e^{i\mu_l(x-a)},$$
$$\gamma^{n+1}(x) = \sum_{l\in\mathbb{Z}} \widehat{(\gamma^{n+1})}_l e^{i\mu_l(x-a)},$$

with

$$\begin{cases} \widehat{(\varphi^n)}_l = -\frac{i}{\tau}\sin(\mu_l^2\tau)\widehat{(\psi^n)}_l(0) + i\widehat{(\phi^n\psi^n)}_l(0), \ \widehat{(\mathfrak{z}^n)}_l = \frac{i}{2\tau}\sin(\mu_l^2\tau)\widehat{(z^n)}_l(0), \\ \widehat{(\gamma^{n+1})}_l = p_l(\tau)\widehat{(|\psi^n|^2)}_l(0) + 2q_l(\tau)\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0) - \frac{\sin(\omega_l\tau)}{\omega_l}\left(\widehat{(\mathfrak{z}^n)}_l + \widehat{(\overline{\mathfrak{z}^n})}_l\right). \end{cases} \tag{4.21}$$

Similar to the case of the KG equation [8] with details omitted here for brevity, we can prove a prior estimates for the solution of the problem (3.2) with (3.3).

Lemma 4.2 (A prior estimates for MDF) *Let $z^n(x,s)$ and $r^n(x,s)$ be the solution of the MDF* (3.2) *with initial and boundary conditions* (3.3). *Under the assumption* (4.1), *there exists a constant $\tau_1 > 0$ independent of ε, h and τ (or n), such that*

$$\|z^n\|_{L^\infty([0,\tau];H^{m_0+2})} + \|\partial_s z^n\|_{L^\infty([0,\tau];H^{m_0+1})} + \left\|\partial_s^2 z_\pm^n\right\|_{L^\infty([0,\tau];H^{m_0})} \lesssim 1, \tag{4.22}$$
$$\left\|\partial_s^k r^n\right\|_{L^\infty([0,\tau];H^{6-k})} \lesssim \varepsilon^{2-2k}, \qquad 0<\tau\le\tau_1, \qquad k=0,1,2. \tag{4.23}$$

Based on this result, when $0 < \tau \le \tau_1$, it is easy to see that $\varphi^n, \mathfrak{z}^n \in H_p^{m_0}(\Omega)$, $\gamma^{n+1} \in H_p^4(\Omega)$ and we have the prior estimates

$$\|\varphi^n\|_{H^4} \lesssim 1, \quad \|\mathfrak{z}^n\|_{H^4} \lesssim 1, \quad \|\gamma^{n+1}\|_{H^4} \lesssim \varepsilon^2.$$

With the above a prior bounds, we can estimate the local truncation error functions.

Lemma 4.3 (Estimates for local errors) *Under the assumption* (4.1), *for any $0 < \tau \le \tau_1$ with τ_1 given in Lemma* 4.2, *we have two independent bounds as*

$$\mathscr{E}\left(\xi_\phi^n, \xi_\psi^n, \dot\xi_\phi^n\right) \lesssim \frac{\tau^6}{\varepsilon^6}, \quad \mathscr{E}\left(\xi_\phi^n, \xi_\psi^n, \dot\xi_\phi^n\right) \lesssim \tau^2\varepsilon^2, \qquad 0 \le n \le \frac{T}{\tau} - 1. \tag{4.24}$$

Proof Subtracting (4.20) from (4.18) and by using the Taylor's expansion, from (4.18a) and (4.20a), we get

$$\widehat{(\xi_\phi^n)}_l = \int_0^\tau \frac{\sin(\omega_l(\tau-\theta))}{\varepsilon^2\omega_l}\theta^2\left[\int_0^1 (1-s)\widehat{(|\psi^n|^2)}_l''(\theta s)ds\right]d\theta + 2q_l(\tau)\widehat{(B_0)}_l, \tag{4.25}$$

where

$$B_0(x) = \mathrm{Re}\{\overline{\psi^n(x,0)}(\partial_s\psi^n(x,0) - \varphi^n)\}, \qquad x \in \Omega.$$

Noticing (7.1), we obtain

$$|\widehat{(\xi_\phi^n)_l}| \lesssim \frac{\tau^2}{\varepsilon^2\omega_l}\int_0^\tau\int_0^1 \left|\widehat{(|\psi^n|^2)}_l''(\theta s)\right| ds d\theta + \frac{\tau^2}{\varepsilon^2\omega_l}\left|\widehat{(B_0)_l}\right|.$$

Noting $\frac{1}{\varepsilon^2\omega_l} = \frac{1}{\sqrt{1+\varepsilon^2\mu_l^2}} \le 1$ for $l = -\frac{N}{2}, \ldots, \frac{N}{2}-1$ and (4.1), (4.2), we get

$$\begin{aligned}\|\xi_\phi^n\|_{H^2}^2 &\lesssim \tau^6\|\partial_{ss}\rho\|_{L^\infty([0,T];H^2)}^2 + \tau^4\left\|\psi^n(\cdot,0)(\partial_s\psi^n(\cdot,0)-\varphi^n)\right\|_{H^2}^2\\ &\lesssim \tau^6 + \tau^4\left\|\partial_s\psi^n(\cdot,0)-\varphi^n\right\|_{H^2}^2, \qquad 0<\tau\le\tau_1. \end{aligned} \tag{4.26}$$

By Parseval's identity, we have

$$\begin{aligned}\left\|\partial_s\psi^n(\cdot,0)-\varphi^n\right\|_{H^2}^2 &= \sum_{l=-N/2}^{N/2-1}(1+\mu_l^2+\mu_l^4)\left|\widehat{(\partial_s\psi^n)}_l(0) - \widehat{(\varphi^n)}_l\right|^2\\ &\lesssim \sum_{l=-N/2}^{N/2-1}\mu_l^4\left|\frac{\sin(\mu_l^2\tau)}{\tau}-\mu_l^2\right|^2|\widehat{(\psi^n)}_l(0)|^2 \lesssim \tau^2\sum_{l=-N/2}^{N/2-1}\mu_l^{12}|\widehat{(\psi^n)}_l(0)|^2\\ &\lesssim \tau^2\|\psi\|_{L^\infty([0,T];H^6)}^2 \lesssim \tau^2. \end{aligned} \tag{4.27}$$

This together with (4.26), we get

$$\|\xi_\phi^n\|_{H^2}^2 \lesssim \tau^6, \quad 0<\tau\le\tau_1. \tag{4.28}$$

Similarly, noting $\frac{|\mu_l|}{\varepsilon^2\omega_l} = \frac{|\mu_l|}{\sqrt{1+\varepsilon^2\mu_l^2}} \le \frac{1}{\varepsilon}$ for $l = -\frac{N}{2}, \ldots, \frac{N}{2}-1$, we obtain

$$\|\partial_x\xi_\phi^n\|_{H^2}^2 \lesssim \frac{\tau^6}{\varepsilon^2} \quad \text{and} \quad \|\dot{\xi}_\phi^n\|_{H^2}^2 \lesssim \frac{\tau^6}{\varepsilon^4}, \quad 0<\tau\le\tau_1. \tag{4.29}$$

For ξ_ψ^n, from (4.18c) and (4.20c) and by the Taylor's expansion, we have

$$\begin{aligned}\widehat{(\xi_\psi^n)}_l &= i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta^2\Big[\int_0^1(1-s)\widehat{(z^n\psi^n)}_l''(\theta s)ds\Big]d\theta \\ &+ i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2-\frac{1}{\varepsilon^2}\right)\theta}\theta^2\left[\int_0^1(1-s)\widehat{(\overline{z^n}\psi^n)}_l''(\theta s)ds\right]d\theta \\ &+ d_l^+(\tau)\left[\widehat{(B_1)}_l+\widehat{(B_2)}_l\right]+d_l^-(\tau)\left[\widehat{(B_3)}_l+\widehat{(B_4)}_l\right]+\frac{i\tau^3}{4}\widehat{(B_5)}_l+\frac{i\tau}{2}\widehat{(B_6)}_l \\ &+ \frac{i\tau^2}{2}\left[\widehat{(B_7)}_l+\widehat{(B_8)}_l\right]-\frac{i\tau}{2}\widehat{(r^n\psi^n)}_l(\tau)+i\int_0^\tau \mathrm{e}^{i\mu_l^2(\theta-\tau)}\widehat{(r^n\psi^n)}_l(\theta)d\theta,\end{aligned} \tag{4.30}$$

where

$$\begin{aligned}&B_1(x)=\left[\partial_s z^n(x,0)-\mathfrak{z}^n(x)\right]\psi^n(x,0),\quad B_2(x)=z^n(x,0)\left[\partial_s\psi^n(x,0)-\varphi^n(x\right],\\ &B_3(x)=\left[\partial_s\overline{z^n}(x,0)-\overline{\mathfrak{z}^n}(x)\right]\psi^n(x,0),\quad B_4(x)=\overline{z^n}(x,0)\left[\partial_s\psi^n(x,0)-\varphi^n(x)\right],\\ &B_5(x)=r^n(x,\tau)\partial_{ss}\psi^n(x,\theta_0),\quad B_6(x)=\left[r^n(x,\tau)-\gamma^{n+1}(x)\right]\psi^n(x,0),\\ &B_7(x)=r^n(x,\tau)\left[\partial_s\psi^n(x,0)-\varphi^n(x)\right],\quad B_8(x)=\left[r^n(x,\tau)-\gamma^{n+1}(x)\right]\varphi^n(x),\end{aligned}$$

with $\theta_0\in[0,\tau]$. For the last two terms in (4.30), we have

$$\begin{aligned}&\left|i\int_0^\tau \mathrm{e}^{i\mu_l^2(\theta-\tau)}\widehat{(r^n\psi^n)}_l(\theta)d\theta-\frac{i\tau}{2}\widehat{(r^n\psi^n)}_l(\tau)\right|\\ &\lesssim\int_0^\tau\theta(\tau-\theta)\left|\frac{d^2}{d\theta^2}\left[\mathrm{e}^{i\mu_l^2(\theta-\tau)}\widehat{(r^n\psi^n)}_l(\theta)\right]\right|d\theta.\end{aligned}$$

Then by using the triangle inequality, we obtain

$$\begin{aligned}|\widehat{(\xi_\psi^n)}_l|&\lesssim\tau^2\int_0^\tau\int_0^1\left[\left|\widehat{(z^n\psi^n)}_l''(\theta s)\right|+\left|\widehat{(\overline{z^n}\psi^n)}_l''(\theta s)\right|\right]dsd\theta\\ &+\tau^2\left[\left|\widehat{(B_1)}_l\right|+\left|\widehat{(B_2)}_l\right|\right]+\tau^2\left[\left|\widehat{(B_3)}_l\right|+\left|\widehat{(B_4)}_l\right|\right]+\tau^3\left|\widehat{(B_5)}_l\right|+\tau\left|\widehat{(B_6)}_l\right|\\ &+\tau^2\left|\widehat{(B_7)}_l\right|+\tau^2\left|\widehat{(B_8)}_l\right|+\tau^2\int_0^\tau\left|\frac{d^2}{d\theta^2}\left[\mathrm{e}^{i\mu_l^2(\theta-\tau)}\widehat{(r^n\psi^n)}_l(\theta)\right]\right|d\theta.\end{aligned}$$

Similar to (4.27), we find from (4.21)

$$\|\partial_s z^n-\mathfrak{z}^n\|_{H^2}\lesssim\tau\|z^n(\cdot,0)\|_{H^6}\lesssim\tau\left(\|\phi\|_{L^\infty([0,T];H^6)}+\varepsilon^2\|\partial_t\phi\|_{L^\infty([0,T];H^6)}\right)\lesssim\tau.$$

Again, similar to (4.27) and noticing (3.9b), we have

$$\begin{aligned}\|\gamma^{n+1}-r^n(\cdot,\tau)\|_{H^2}^2&\lesssim\|\xi_\phi^n\|_{H^2}^2+\sum_{l\in\mathbb{Z}}(1+\mu_l^2+\mu_l^4)\left|\frac{\sin(\omega_l\tau)}{\omega_l}\right|^2\cdot\left|\widehat{(\mathfrak{z}^n)}_l-\widehat{(\partial_s z^n)}_l\right|^2\\ &\lesssim\tau^6+\tau^2\|\partial_s z^n-\mathfrak{z}^n\|_{H^2}^2\lesssim\tau^4.\end{aligned}$$

By the assumption (4.1) and Lemma 4.2, we get

$$\begin{aligned}\left\|\xi_{\psi}^{n}\right\|_{H^2}^2 \lesssim\ & \tau^6\left\|\partial_{ss}(z^n\psi^n)\right\|^2_{L^\infty([0,\tau];H^2)} + \tau^6\|z^n\|^2_{L^\infty([0,\tau];H^6)} + \tau^6\|\psi^n\|^2_{L^\infty([0,\tau];H^6)}\\ &+\tau^6\left\|r^n\partial_{ss}\psi^n\right\|^2_{L^\infty([0,\tau];H^2)} + \tau^2\|\gamma^{n+1}-r^n(\cdot,\tau)\|^2_{H^2}\\ &+\tau^6\left\|r^n\psi^n\right\|^2_{L^\infty([0,\tau];H^6)}\\ &+\tau^6\left\|\partial_s(r^n\psi^n)\right\|^2_{L^\infty([0,\tau];H^4)} + \tau^6\left\|\partial_{ss}(r^n\psi^n)\right\|^2_{L^\infty([0,\tau];H^2)} \lesssim \frac{\tau^6}{\varepsilon^4}.\end{aligned} \tag{4.31}$$

Plugging (4.28), (4.29) and (4.31) into (4.11) with $e^n_{\phi,N}=\xi^n_\phi$, $e^n_{\psi,N}=\xi^n_\psi$ and $\dot e^n_{\phi,N}=\dot\xi^n_\phi$, we immediately get the first inequality in (4.24).

Next we show how to get the second estimate in (4.24). By using Taylor's expansion, truncating at the first order term and integrating by parts, we have

$$\begin{aligned}\widehat{(\xi^n_\phi)}_l &= \int_0^\tau \frac{\sin(\omega_l(\tau-\theta))}{\varepsilon^2\omega_l}\theta\left[\int_0^1 \widehat{(|\psi^n|^2)}_l'(\theta s)ds\right]d\theta - 2q_l(\tau)\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0),\\ &= q_l(\tau)\int_0^1 \widehat{(|\psi^n|^2)}_l'(\tau s)ds - \int_0^\tau q_l(\theta)\left[\int_0^1 \widehat{(|\psi^n|^2)}_l''(\theta s)sds\right]d\theta\\ &\quad - q_l(0)\widehat{(|\psi^n|^2)}_l'(0) - 2q_l(\tau)\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0).\end{aligned}$$

From (7.1) and noticing $q_l(0)=0$ and $|q_l(\tau)|\lesssim\tau\varepsilon^2$, we find

$$\begin{aligned}\|\xi^n_\phi\|^2_{H^2} &\lesssim \tau^2\varepsilon^4\left[\|\partial_t\rho\|^2_{L^\infty([0,T],H^2)} + \|\partial_{tt}\rho\|^2_{L^\infty([0,T],H^2)} + \|\psi\varphi^n\|^2_{L^\infty([0,T],H^2)}\right]\\ &\lesssim \tau^2\varepsilon^4, \qquad 0<\tau\le\tau_1, \qquad 0\le\varepsilon\le 1.\end{aligned} \tag{4.32}$$

Similarly, we can get

$$\|\partial_x\xi^n_\phi\|^2_{H^2}\lesssim\tau^2\varepsilon^2 \quad\text{and}\quad \|\dot\xi^n_\phi\|^2_{H^2}\lesssim\tau^2, \quad 0<\tau\le\tau_1. \tag{4.33}$$

In order to estimate ξ^n_ψ, we introduce

$$I^n(x)=\sum_{l=-N/2}^{N/2-1}\widehat{I}^n_l e^{i\mu_l(x-a)}, \qquad J^n(x)=\sum_{l=-N/2}^{N/2-1}\widehat{J}^n_l e^{i\mu_l(x-a)}, \tag{4.34}$$

where

$$\begin{aligned}\widehat{I}^n_l &= G^n_{1,l} - d^+_l(\tau)\left[\widehat{(\mathfrak{z}^n\psi^n)}_l(0) + \widehat{(z^n\varphi^n)}_l(0)\right],\\ \widehat{J}^n_l &= G^n_{2,l} - d^-_l(\tau)\left[\widehat{(\overline{\mathfrak{z}^n}\psi^n)}_l(0) + \widehat{(\overline{z^n}\varphi^n)}_l(0)\right],\end{aligned} \tag{4.35}$$

with

$$\begin{aligned} G_{1,l}^n &= i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta\left[\int_0^1 \widehat{(z^n\psi^n)}_l'(\theta s)ds\right]d\theta,\\ G_{2,l}^n &= i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2-\frac{1}{\varepsilon^2}\right)\theta}\theta\left[\int_0^1 \widehat{(\overline{z^n}\psi^n)}_l'(\theta s)ds\right]d\theta. \end{aligned} \tag{4.36}$$

Applying the Taylor's expansion in (4.18c) and (4.20c) and truncating at the first order term, we obtain

$$\widehat{(\xi_\psi^n)}_l = \widehat{I}_l^n + \widehat{J}_l^n + i\int_0^\tau \mathrm{e}^{i\mu_l^2(\theta-\tau)}\widehat{(r^n\psi^n)}_l(\theta)d\theta - \frac{i\tau}{2}\left[\widehat{(\gamma^{n+1}\psi^n)}_l(0) + \tau\widehat{(\gamma^{n+1}\varphi^n)}_l\right]. \tag{4.37}$$

From (4.36), integration by parts, we get

$$\begin{aligned} G_{1,l}^n &= i\mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta\int_0^1\left[\widehat{(\partial_s z^n\psi^n)}_l(\theta s) + \widehat{(z^n\partial_s\psi^n)}_l(\theta s)\right]dsd\theta\\ &= d_l^+(\tau)\int_0^1 \widehat{(\partial_s z^n\psi^n)}_l(\tau s)ds - \int_0^\tau d_l^+(\theta)\int_0^1 \widehat{(\partial_s z^n\psi^n)}_l'(\theta s)sdsd\theta\\ &\quad - \mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta\int_0^1\left[\widehat{(z^n\partial_{xx}\psi^n)}_l(\theta s) + \widehat{(z^n\phi^n\psi^n)}_l(\theta s)\right]dsd\theta\\ &= d_l^+(\tau)\int_0^1\left[\widehat{(\partial_s z^n\psi^n)}_l(\tau s) + i\widehat{(z^n\partial_{xx}\psi^n)}_l(\tau s)\right]ds\\ &\quad - \int_0^\tau d_l^+(\theta)\int_0^1\left[\widehat{(\partial_s z^n\psi^n)}_l'(\theta s) + i\widehat{(z^n\partial_{xx}\psi^n)}_l'(\theta s)\right]sdsd\theta - G_{3,l}^n, \end{aligned} \tag{4.38}$$

where

$$G_{3,l}^n = \mathrm{e}^{-i\mu_l^2\tau}\int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta\int_0^1 \widehat{(z^n\phi^n\psi^n)}_l(\theta s)dsd\theta. \tag{4.39}$$

Noticing the ansatz (2.2), we get

$$\begin{aligned} G_{3,l}^n &= \mathrm{e}^{-i\mu_l^2\tau}\int_0^1\left[\int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1+s}{\varepsilon^2}\right)\theta}\theta\widehat{((z^n)^2\psi^n)}_l(\theta s)d\theta\right.\\ &\quad \left. + \int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1-s}{\varepsilon^2}\right)\theta}\theta\widehat{(|z^n|^2\psi^n)}_l(\theta s)d\theta + \int_0^\tau \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta\widehat{(z^n r^n\psi^n)}_l(\theta s)d\theta\right]ds. \end{aligned}$$

Using integration by parts and the triangle inequality, we have

$$\begin{aligned} \left|G_{3,l}^n\right| \lesssim \int_0^1\Bigg[&\tau\varepsilon^2\left|\widehat{((z^n)^2\psi^n)}_l(\tau s)\right| + \tau\varepsilon^2\left|\widehat{(|z^n|^2\psi^n)}_l(\tau s)\right|\\ &+ \varepsilon^2\int_0^\tau\left|\widehat{((z^n)^2\psi^n)}_l'(\theta s)\right|d\theta\\ &+ \varepsilon^2\int_0^\tau\left|\widehat{(|z^n|^2\psi^n)}_l'(\theta s)\right|d\theta + \int_0^\tau\left|\widehat{(z^n r^n\psi^n)}_l(\theta s)\right|d\theta\Bigg]ds. \end{aligned} \tag{4.40}$$

Combining (4.34)–(4.40) and noting $|d_l^+(\tau)| \lesssim \tau\varepsilon^2$ and Lemma 4.2, we get

$$\begin{aligned}\|I^n\|_{H^2} \lesssim\ & \tau\varepsilon^2\left[\|\partial_s z^n\psi^n\|_{L^\infty([0,\tau];H^2)} + \|z^n\partial_{xx}\psi^n\|_{L^\infty([0,\tau];H^2)} + \|\partial_{ss} z^n\psi^n\|_{L^\infty([0,\tau];H^2)}\right.\\ &+\|\partial_s z^n\partial_s\psi^n\|_{L^\infty([0,\tau];H^2)} + \|\partial_s z^n\partial_{xx}\psi^n\|_{L^\infty([0,\tau];H^2)} + \|z^n\partial_{sxx}\psi^n\|_{L^\infty([0,\tau];H^2)}\\ &\left.+\|(z^n)^2\psi^n\|_{L^\infty([0,\tau];H^2)}\right] + \tau\varepsilon^2\left[\|\mathfrak{z}^n\psi^n\|_{L^\infty([0,\tau];H^2)} + \|z^n\varphi^n\|_{L^\infty([0,\tau];H^2)}\right]\\ &+\tau\|z^n r^n\psi^n\|_{L^\infty([0,\tau];H^2)} \lesssim \tau\varepsilon^2. \end{aligned} \tag{4.41}$$

In order to estimate J^n, denote $N_\varepsilon := \frac{b-a}{2\sqrt{2}\pi\varepsilon}$. When $|l| \le N_\varepsilon$, we have $|\mu_l| \le \frac{1}{\sqrt{2}\varepsilon}$ which indicates that $|d_l^-(\tau)| \lesssim \tau\varepsilon^2$. Similar to the estimate of I^n, we have

$$\sum_{|l|\le N_\varepsilon}\left(1+\mu_l^2+\mu_l^4\right)|\widehat{J_l^n}|^2 \lesssim \tau^2\varepsilon^4. \tag{4.42}$$

On the other hand, when $|\mu_l| > \frac{1}{\sqrt{2}\varepsilon}$, we have $|d_l^-(\tau)| \lesssim \tau^2$. Due to the regularity of the solution, i.e. the assumption (4.1) and Lemma 4.2, we can get

$$\begin{aligned}&\sum_{|l|>N_\varepsilon}\left(1+\mu_l^2+\mu_l^4\right)|\widehat{J_l^n}|^2\\ &\lesssim \sum_{|l|>N_\varepsilon}\tau^3\mu_l^4\left[\int_0^\tau\int_0^1\left|\widehat{(\overline{z^n}\psi^n)}_l'(\theta s)\right|^2 ds d\theta + \tau\left(\left|\widehat{(\mathfrak{z}^n\psi^n)}_l(0)\right|^2 + \left|\widehat{(\overline{z^n}\varphi^n)}_l(0)\right|^2\right)\right]\\ &\lesssim \tau^4\varepsilon^4\left[\|\partial_s(z^n\psi^n)\|^2_{L^\infty([0,\tau];H^4)} + \|\mathfrak{z}^n\psi^n(\cdot,0)\|^2_{H^4} + \|z^n(\cdot,0)\varphi^n\|^2_{H^4}\right]\\ &\lesssim \tau^4\varepsilon^4\left[\|\partial_s(z^n\psi^n)\|^2_{L^\infty([0,\tau];H^4)} + \frac{1}{\tau^2}\|z^n\psi^n\|^2_{L^\infty([0,\tau];H^4)} + \|z^n\psi^n\phi^n\|^2_{L^\infty([0,\tau];H^4)}\right]\\ &\lesssim \tau^2\varepsilon^4. \end{aligned} \tag{4.43}$$

From (4.42) and (4.43), we obtain

$$\|J^n\|_{H^2} \lesssim \tau\varepsilon^2, \qquad 0<\tau\le\tau_1, \qquad 0<\varepsilon\le 1. \tag{4.44}$$

Combining the above estimates and noting (4.37), we have

$$\begin{aligned}\|\xi_\psi^n\|^2_{H^2} \lesssim\ & \|I^n\|^2_{H^2} + \|J^n\|^2_{H^2} + \tau^2\|r^n\psi^n\|^2_{L^\infty([0,\tau];H^2)} + \tau^4\|\gamma^{n+1}\psi^n\|^2_{L^\infty([0,\tau];H^2)}\\ &+\tau^4\|\gamma^{n+1}\varphi^n\|^2_{H^2} \lesssim \tau^2\varepsilon^4. \end{aligned} \tag{4.45}$$

Plugging (4.32), (4.33) and (4.45) into (4.11), we get the second estimate. □

Defining the errors from the nonlinear terms as

$$\begin{cases} \eta_\phi^n(x) := \displaystyle\sum_{l=-N/2}^{N/2-1}\widehat{(\eta_\phi^n)}_l e^{i\mu_l(x-a)}, \quad \dot\eta_\phi^n(x) := \sum_{l=-N/2}^{N/2-1}\widehat{(\dot\eta_\phi^n)}_l e^{i\mu_l(x-a)},\\ \eta_\psi^n(x) := \displaystyle\sum_{l=-N/2}^{N/2-1}\widehat{(\eta_\psi^n)}_l e^{i\mu_l(x-a)}, \quad x\in\overline{\Omega}, \quad n\ge 0, \end{cases} \tag{4.46}$$

where

$$\widehat{(\eta_\phi^n)}_l = p_l(\tau)\left[\widehat{(|\psi^n|^2)}_l(0) - \widetilde{(|\Psi^n|^2)}_l\right] + 2q_l(\tau)\left[\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0) - \widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot{\Psi}^n\})}_l\right], \tag{4.47a}$$

$$\widehat{(\dot{\eta}_\phi^n)}_l = p_l'(\tau)\left[\widehat{(|\psi^n|^2)}_l(0) - \widetilde{(|\Psi^n|^2)}_l\right] + 2q_l'(\tau)\left[\widehat{(\mathrm{Re}\{\overline{\psi^n}\varphi^n\})}_l(0) - \widetilde{(\mathrm{Re}\{\overline{\Psi^n}\dot{\Psi}^n\})}_l\right], \tag{4.47b}$$

$$\begin{aligned}\widehat{(\eta_\psi^n)}_l &= c_l^+(\tau)\left[\widehat{(z^n\psi^n)}_l(0) - \widetilde{(Z^0\Psi^n)}_l\right] + c_l^-(\tau)\left[\widehat{(\overline{z^n}\psi^n)}_l(0) - \widetilde{(\overline{Z^0}\Psi^n)}_l\right] \\ &+ d_l^+(\tau)\left[\widehat{(\mathfrak{z}^n\psi^n)}_l(0) - \widetilde{(\dot{Z}^0\Psi^n)}_l + \widehat{(z^n\varphi^n)}_l(0) - \widetilde{(Z^0\dot{\Psi}^n)}_l\right] \\ &+ d_l^-(\tau)\left[\widehat{(\overline{\mathfrak{z}^n}\psi^n)}_l(0) - \widetilde{(\overline{\dot{Z}^0}\Psi^n)}_l + \widehat{(\overline{z^n}\varphi^n)}_l(0) - \widetilde{(\overline{Z^0}\dot{\Psi}^n)}_l\right] \\ &+ \frac{i\tau}{2}\left[\widehat{(\gamma^{n+1}\psi^n)}_l(0) - \widetilde{(R^{n+1}\Psi^n)}_l + \tau\left(\widehat{(\gamma^{n+1}\varphi^n)}_l - \widetilde{(R^{n+1}\dot{\Psi}^n)}_l\right)\right],\end{aligned} \tag{4.47c}$$

then we have

Lemma 4.4 (Estimates for η_ϕ^n, η_ψ^n and $\dot{\eta}_\phi^n$) *Under the assumption* (4.1) *and assume* (4.7) *holds* (*which will be proved by induction later*), *we have for any* $0 < \tau \le \tau_1$,

$$\mathscr{E}\left(\eta_\phi^n, \eta_\psi^n, \dot{\eta}_\phi^n\right) \lesssim \tau^2 \mathscr{E}\left(e_{N,\phi}^n, e_{N,\psi}^n, \dot{e}_{N,\phi}^n\right) + \frac{\tau^2 h^{2m_0}}{\varepsilon^2}, \quad 0 \le n \le \frac{T}{\tau} - 1. \tag{4.48}$$

Proof From (4.46) and (4.47a), we have

$$\begin{aligned}\|\eta_\phi^n\|_{H^2} &\lesssim \tau\||\psi^n(\cdot,0)|^2 - I_N|\Psi^n|^2\|_{H^2} + \tau^2\|\overline{\psi^n}(\cdot,0)\varphi^n - I_N(\overline{\Psi^n}\dot{\Psi}^n)\|_{H^2} \\ &\lesssim \tau\|I_N|\psi^n(\cdot,0)|^2 - I_N|\Psi^n|^2\|_{H^2} + \tau^2\|I_N(\overline{\psi^n}(\cdot,0)\varphi^n) - I_N(\overline{\Psi^n}\dot{\Psi}^n)\|_{H^2} + \tau h^{m_0} \\ &\lesssim \tau\||\psi^n(\cdot,0)|^2 - |\Psi^n|^2\|_{Y,2} + \tau^2\|\overline{\psi^n}(\cdot,0)\varphi^n - \overline{\Psi^n}\dot{\Psi}^n\|_{Y,2} + \tau h^{m_0} \\ &\lesssim \tau\|e_\psi^n\|_{Y,2} + \tau^2\|\varphi^n - \dot{\Psi}^n\|_{Y,2} + \tau h^{m_0} \\ &\lesssim \tau\|e_\psi^n\|_{Y,2} + \tau^2\|\partial_{xx}^S\psi^n(\cdot,0) - \partial_{xx}^S\Psi^n\|_{Y,2} + \tau^2\|\phi^n\psi^n(\cdot,0) - \Phi^n\Psi^n\|_{Y,2} + \tau h^{m_0} \\ &\lesssim \tau\|e_\psi^n\|_{H^2} + \tau\|e_\phi^n\|_{H^2} + \tau^2\|\partial_{xx}^S\psi^n(\cdot,0) - \partial_{xx}^S\Psi^n\|_{H^2} + \tau h^{m_0} \\ &\lesssim \tau\|e_\psi^n\|_{H^2} + \tau\|e_\phi^n\|_{H^2} + \tau h^{m_0},\end{aligned} \tag{4.49}$$

where the operator ∂_{xx}^S on a function $f(x)$ is defined as

$$\partial_{xx}^S f(x) := -\sum_{l\in\mathbb{Z}} \frac{\sin(\mu_l^2\tau)}{\tau}\, \widehat{f}_l\, \mathrm{e}^{i\mu_l(x-a)}.$$

Combining (4.49) and (4.10), we get

$$\|\eta_\phi^n\|_{H^2} \lesssim \tau\|e_{\psi,N}^n\|_{H^2} + \tau\|e_{\phi,N}^n\|_{H^2} + \tau h^{m_0}. \tag{4.50}$$

In addition, we can obtain (by noting some estimates in Appendix)

$$\varepsilon^2\|\dot\eta_\phi^n\|_{H^2}^2 + \|\partial_x\eta_\phi^n\|_{H^2}^2 \lesssim \frac{\tau^2}{\varepsilon^2}\left[\|e_{\psi,N}^n\|_{H^2}^2 + \|e_{\phi,N}^n\|_{H^2}^2 + h^{2m_0}\right]. \tag{4.51}$$

Similarly, we can estimate all the terms of η_ψ^n in (4.47c) except the last term. For the last term, we have

$$\begin{aligned}
&\sum_{l=-N/2}^{N/2-1}(1+\mu_l^2+\mu_l^4)\left|\widehat{(\gamma^{n+1}\psi^n)}_l(0) - \widetilde{(R^{n+1}\Psi^n)}_l\right|^2 \\
&\lesssim \|I_N(\gamma^{n+1}\psi^n(\cdot,0)) - I_N(R^{n+1}\psi^n))\|_{H^2}^2 + h^{2m_0} \\
&\lesssim \|e_\psi^n\|_{H^2}^2 + \|\gamma^{n+1} - I_N R^{n+1}\|_{H^2}^2 + h^{2m_0}.
\end{aligned} \tag{4.52}$$

Noting (4.21) and (3.16b), we get

$$\begin{aligned}
\left|\widehat{(\gamma^{n+1})}_l - \widetilde{(R^{n+1})}_l\right| \lesssim{}& \left|\widehat{(z^n)}_l(0) - \widetilde{(Z^0)}_l\right| + |p_l(\tau)|\cdot\left|\widehat{(|\psi^n|^2)}_l(0) - \widetilde{(|\Psi^n|^2)}_l\right| \\
&+ |q_l(\tau)|\cdot\left|\widehat{(\overline{\psi^n}\varphi^n)}_l(0) - \widetilde{(\overline{\Psi^n}\dot\Psi^n)}_l\right|.
\end{aligned} \tag{4.53}$$

Combining the above two inequalities, we obtain

$$\|\gamma^{n+1} - I_N R^{n+1}\|_{H^2} \lesssim \|e_\phi^n\|_{H^2} + \varepsilon^2\|\dot e_\phi^n\|_{H^2} + \|e_\psi^n\|_{H^2} + h^{2m_0}. \tag{4.54}$$

Plugging (4.54) into (4.52), we get

$$\begin{aligned}
&\sum_{l=-N/2}^{N/2-1}(1+\mu_l^2+\mu_l^4)\left|\widehat{(\gamma^{n+1}\psi^n)}_l(0) - \widetilde{(R^{n+1}\Psi^n)}_l\right|^2 \\
&\lesssim \|e_\psi^n\|_{H^2}^2 + \|e_\phi^n\|_{H^2}^2 + \varepsilon^4\|\dot e_\phi^n\|_{H^2}^2 + h^{2m_0}.
\end{aligned} \tag{4.55}$$

Similarly, we can obtain

$$\begin{aligned}
&\sum_{l=-N/2+1}^{N/2}(1+\mu_l^2+\mu_l^4)\left|\widehat{(\gamma^{n+1}\varphi^n)}_l - \widetilde{(R^{n+1}\dot\Psi^n)}_l\right|^2 \\
&\lesssim \|e_\psi^n\|_{H^2}^2 + \|e_\phi^n\|_{H^2}^2 + \varepsilon^4\|\dot e_\phi^n\|_{H^2}^2 + h^{2m_0}.
\end{aligned} \tag{4.56}$$

Combining (4.55), (4.56) and (4.47c), we have

$$\begin{aligned}\|\eta_\psi^n\|_{H^2} &\lesssim \tau\left(\|e_\phi^n\|_{H^2}+\varepsilon^2\|\dot{e}_\phi^n\|_{H^2}+\|e_\psi^n\|_{H^2}+h^{m_0}\right)\\ &\lesssim \tau\left(\|e_{\phi,N}^n\|_{H^2}+\varepsilon^2\|\dot{e}_{\phi,N}^n\|_{H^2}+\|e_{\psi,N}^n\|_{H^2}+h^{m_0}\right).\end{aligned}\tag{4.57}$$

Plugging (4.50), (4.51) and (4.57) into (4.11), we get the estimate (4.48). □

Remark 4.1 As part of the error propagation, the term $\|\partial_x e_{\phi,N}^n\|_{H^2}$ is introduced in the error energy functional (4.11). While we do not have to estimate the related errors under this term directly. By noting the fact of the coefficients p_l, q_l as given in Appendix, the estimates of the local error $\partial_x \xi_\phi^n$ and the error of the nonlinear terms $\partial_x \eta_\phi^n$ can be converted as

$$\|\partial_x \xi_\phi^n\|_{H^2} \lesssim \frac{1}{\varepsilon}\|\xi_\phi^n\|_{H^2}, \quad \|\partial_x \eta_\phi^n\|_{H^2} \lesssim \frac{1}{\varepsilon}\|\eta_\phi^n\|_{H^2}.$$

Thus, throughout the proof, we do not require any bootstrap argument or induction assumptions on the boundedness of $\partial_x \phi_I^n$ in H^2.

Proof of Theorem 4.1. The proof will be proceeded by the energy method and the method of mathematical induction [6,7,9,11,12]. For $n = 0$, from the initial data in the MTI-FP method (3.15)–(3.17) and noticing the assumption (4.1), we have

$$\begin{aligned}&\|e_\phi^0\|_{H^2}+\|e_\psi^0\|_{H^2}+\varepsilon^2\|\dot{e}_\phi^0\|_{H^2}\\ &\quad=\|\phi_0-I_N\phi_0\|_{H^2}+\|\psi_0-I_N\psi_0\|_{H^2}+\|\phi_1-I_N\phi_1\|_{H^2}\lesssim h^{m_0+2}\lesssim h^{m_0}.\end{aligned}$$

In addition, using the triangle inequality, we know that there exists $h_1 > 0$ independent of ε such that

$$\begin{aligned}&\|\phi_I^0\|_{H^2}\le\|\phi_0\|_{H^2}+\|e_\phi^0\|_{H^2}\le C_\phi+1, \quad \|\dot{\phi}_I^0\|_{H^2}\le\frac{\|\phi_1\|_{H^2}}{\varepsilon^2}+\|\dot{e}_\phi^0\|_{H^2}\le\frac{C_\phi+1}{\varepsilon^2},\\ &\|\psi_I^0\|_{H^2}\le\|\psi_0\|_{H^2}+\|e_\psi^0\|_{H^2}\le C_\psi+1, \qquad 0<h\le h_1.\end{aligned}$$

Thus (4.5)–(4.7) are valid for $n = 0$. Now we assume that (4.5)–(4.7) are valid for $0 \le n \le m-1 \le T/\tau - 1$. Adding (4.20) and (4.14), we have

$$\widehat{(e_\phi^{n+1})}_l = \cos(\omega_l\tau)\widehat{(e_\phi^n)}_l+\frac{\sin(\omega_l\tau)}{\omega_l}\widehat{(\dot{e}_\phi^n)}_l+\widehat{(\xi_\phi^n)}_l+\widehat{(\eta_\phi^n)}_l,\tag{4.58a}$$

$$\widehat{(\dot{e}_\phi^{n+1})}_l = -\omega_l\sin(\omega_l\tau)\widehat{(e_\phi^n)}_l+\cos(\omega_l\tau)\widehat{(\dot{e}_\phi^n)}_l+\widehat{(\dot{\xi}_\phi^n)}_l+\widehat{(\dot{\eta}_\phi^n)}_l,\tag{4.58b}$$

$$\widehat{(e_\psi^{n+1})}_l = \mathrm{e}^{-i\mu_l^2\tau}\widehat{(e_\psi^n)}_l+\widehat{(\xi_\psi^n)}_l+\widehat{(\eta_\psi^n)}_l.\tag{4.58c}$$

Using the Cauchy's inequality, we obtain

$$\left|\widehat{(e_\phi^{n+1})}_l\right|^2 \le (1+\tau)\left|\cos(\omega_l\tau)\widehat{(e_\phi^n)}_l + \frac{\sin(\omega_l\tau)}{\omega_l}\widehat{(\dot e_\phi^n)}_l\right|^2 + \frac{1+\tau}{\tau}\left|\widehat{(\xi_\phi^n)}_l + \widehat{(\eta_\phi^n)}_l\right|^2, \tag{4.59a}$$

$$\left|\widehat{(\dot e_\phi^{n+1})}_l\right|^2 \le (1+\tau)\left|\cos(\omega_l\tau)\widehat{(\dot e_\phi^n)}_l - \omega_l\sin(\omega_l\tau)\widehat{(e_\phi^n)}_l\right|^2 + \frac{1+\tau}{\tau}\left|\widehat{(\dot\xi_\phi^n)}_l + \widehat{(\dot\eta_\phi^n)}_l\right|^2, \tag{4.59b}$$

$$\left|\widehat{(e_\psi^{n+1})}_l\right|^2 \le (1+\tau)\left|\widehat{(e_\psi^n)}_l\right|^2 + \frac{1+\tau}{\tau}\left|\widehat{(\xi_\psi^n)}_l + \widehat{(\eta_\psi^n)}_l\right|^2. \tag{4.59c}$$

Multiplying (4.59a)–(4.59c) by $(\mu_l^2 + \frac{1}{\varepsilon^2})(1+\mu_l^2+\mu_l^4)$, $\varepsilon^2(1+\mu_l^2+\mu_l^4)$ and $\frac{1}{\varepsilon^2}(1+\mu_l^2+\mu_l^4)$, respectively, then adding them together and summing up for $l = -N/2, \dots, N/2-1$, we obtain

$$\begin{aligned}\mathcal{E}(e_{\phi,N}^{n+1}, e_{\psi,N}^{n+1}, \dot e_{\phi,N}^{n+1}) \le{}& (1+\tau)\mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_N^n)\\ &+\frac{1+\tau}{\tau}\mathcal{E}(\xi_\phi^n+\eta_\phi^n, \xi_\psi^n+\eta_\psi^n, \dot\xi_\phi^n+\dot\eta_\phi^n).\end{aligned}$$

Using the Cauchy's inequality, we get

$$\begin{aligned}&\mathcal{E}(e_{\phi,N}^{n+1}, e_{\psi,N}^{n+1}, \dot e_{\phi,N}^{n+1}) - \mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_{\phi,N}^n)\\ &\lesssim \tau\mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_{\phi,N}^n) + \frac{1+\tau}{\tau}\left[\mathcal{E}(\xi_\phi^n, \xi_\psi^n, \dot\xi_\phi^n) + \mathcal{E}(\eta_\phi^n, \eta_\psi^n, \dot\eta_\phi^n)\right].\end{aligned} \tag{4.60}$$

Inserting (4.48) and the second inequality in (4.24) into (4.60), we get

$$\begin{aligned}&\mathcal{E}(e_{\phi,N}^{n+1}, e_{\psi,N}^{n+1}, \dot e_{\phi,N}^{n+1}) - \mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_{\phi,N}^n)\\ &\lesssim \tau\mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_{\phi,N}^n) + \frac{\tau h^{2m_0}}{\varepsilon^2} + \frac{\tau^5}{\varepsilon^6}.\end{aligned} \tag{4.61}$$

Summing the above inequality for $0 \le n \le m-1$ and then applying the discrete Gronwall's inequality, we have

$$\mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_{\phi,N}^n) \lesssim \frac{h^{2m_0}}{\varepsilon^2} + \frac{\tau^4}{\varepsilon^6}. \tag{4.62}$$

Similarly, by using the first inequality in (4.24), we obtain

$$\mathcal{E}(e_{\phi,N}^n, e_{\psi,N}^n, \dot e_{\phi,N}^n) \lesssim \frac{h^{2m_0}}{\varepsilon^2} + \varepsilon^2. \tag{4.63}$$

Combining (4.11), (4.62) and (4.63), we get that (4.5) is valid for $n = m$, which implies

$$\|e_\phi^m\|_{H^2} + \|e_\psi^m\|_{H^2} + \varepsilon^2 \|\dot{e}_\phi^m\|_{H^2} \le h^{m_0} + \tau.$$

Using the triangle inequality, we obtain that there exist $h_2 > 0$ and $\tau_2 > 0$ independent of ε such that

$$\begin{aligned}
&\|\phi_I^m\|_{H^2} \le \|\phi(\cdot, t_m)\|_{H^2} + \|e_\phi^m\|_{H^2} \le C_\phi + 1,\\
&\|\psi_I^m\|_{H^2} \le \|\psi(\cdot, t_m)\|_{H^2} + \|e_\psi^m\|_{H^2} \le C_\psi + 1, \qquad 0 < h \le h_2, \quad 0 < \tau \le \tau_2,\\
&\|\dot{\phi}_I^m\|_{H^2} \le \|\partial_t \phi(\cdot, t_m)\|_{H^2} + \|\dot{e}_\phi^m\|_{H^2} \le \frac{C_\phi + 1}{\varepsilon^2}.
\end{aligned}$$

Thus (4.7) is also valid for $n = m$. Then the proof is completed by choosing $\tau_0 = \min\{\tau_1, \tau_2\}$ and $h_0 = \min\{h_1, h_2\}$. □

Remark 4.2 Here we emphasize that Theorem 4.1 holds in two/three dimensions (2D/3D) and the above approach can be directly extended to 2D/3D without extra effort. The only thing needs to be taken care of is the Sobolev inequality used in Lemma 4.4 in 2D/3D

$$\|u\|_{L^\infty(\Omega)} \lesssim \|u\|_{H^2(\Omega)}, \qquad \|u\|_{W^{1,p}(\Omega)} \lesssim \|u\|_{H^2(\Omega)}, \quad 1 < p < 6, \tag{4.64}$$

where Ω is a bounded domain in 2D/3D. By using the assumption (4.7), Lemma 4.4 still holds in 2D/3D. Thus (4.7) and the error bounds can be proved by the method of mathematical induction since our scheme is explicit.

Remark 4.3 Under a weaker assumption on the regularity of the solution, i.e. there exists an integer $m_0 \ge 4$ such that $\phi \in C^1([0,T]; H_p^{m_0+3}(\Omega))$, $\psi \in C([0,T]; H_p^{m_0+1}(\Omega)) \cap C^1([0,T]; H_p^{m_0-1}(\Omega)) \cap C^2([0,T]; H_p^{m_0-3}(\Omega))$ and

$$\begin{aligned}
&\|\phi\|_{L^\infty([0,T]; H^{m_0+3})} + \varepsilon^2 \|\partial_t \phi\|_{L^\infty([0,T]; H^{m_0+3})} \lesssim 1,\\
&\|\psi\|_{L^\infty([0,T]; H^{m_0+1})} + \|\partial_t \psi\|_{L^\infty([0,T]; H^{m_0-1})} + \varepsilon^2 \|\partial_{tt} \psi\|_{L^\infty([0,T]; H^{m_0-3})} \lesssim 1,
\end{aligned} \tag{4.65}$$

we can establish an H^1-norm estimate of the MTI-FP method in Theorem 4.1 by a very similar proof with all the H^2-norm in the proof being replaced by H^1-norm. In 1D case, the H^1-norm estimate of the MTI-FP method holds without any stability (or CFL) condition. However in 2D/3D, due to the use of the inverse inequality to provide the bound in l^∞-norm of the numerical solution [5–8], we need impose the technical condition

$$0 < \tau \lesssim C_d(h), \qquad \text{with} \quad C_d(h) = \begin{cases} 1/|\ln h|, & d = 2,\\ \sqrt{h}, & d = 3. \end{cases} \tag{4.66}$$

Of course, if the solution of the KGS is smooth enough, we can always adapt the H^2-norm estimate in Theorem 4.1 and thus there is no need to assume the stability (or CFL) condition (4.66).

Remark 4.4 An MTI-FP method with higher order uniform accuracy in time could be designed in the same spirit. For example, to get a second order UA scheme, we can separate the $O(\varepsilon^2)$ terms explicitly out from the remainder term r^n in the ansatz (2.2), which pushes the new remainder to $O(\varepsilon^4)$ [22]. After that, we need to integrate the $O(1)$ term z^n, the $O(\varepsilon^2)$ term and the remainder by a fourth order EWI [51]. Then error bounds at $O(\tau^4/\varepsilon^4)$ and $O(\varepsilon^4)$ can be obtained, which imply a second order uniform error bound in time. Of course, the scheme and its corresponding analysis would become much more complicated.

5 Numerical results

In this section, we report numerical results to demonstrate the uniform convergence of the MTI-FP method for $\varepsilon \in (0, 1]$ and apply it to numerically study convergence rates of the KGS equations to its limiting models (1.9) and (1.11) in the nonrelativistic limit regime. In order to do so, we take $d = 1$ and $\mu = \lambda = 1$ in (1.3) and choose the initial data in (1.5) with $d = 1$ as

$$\psi_0(x) = \frac{1+i}{2}\operatorname{sech}\left(x^2\right), \quad \phi_0(x) = \frac{1}{2}\mathrm{e}^{-x^2}, \quad \phi_1(x) = \frac{1}{\sqrt{2}}\mathrm{e}^{-x^2}, \quad x \in \mathbb{R}. \tag{5.1}$$

5.1 Accuracy test

The KGS equations (1.3) with $d = 1$ and (5.1) is solved on a bounded interval $\Omega = [-32, 32]$, i.e. $b = -a = 32$, which is large enough to guarantee that the periodic boundary condition does not introduce a significant aliasing error relative to the original problem. To quantify the error, we introduce two error functions:

$$\mathrm{e}^{\tau,h}_{\phi,\varepsilon}(t = t_n) := \left\|\phi(\cdot, t_n) - \phi^n_I\right\|_{H^2}, \quad \mathrm{e}^{\tau,h}_{\phi,\infty}(t) := \max_{0<\varepsilon\le 1}\left\{\mathrm{e}^{\tau,h}_{\phi,\varepsilon}(t)\right\},$$
$$\mathrm{e}^{\tau,h}_{\psi,\varepsilon}(t = t_n) := \left\|\psi(\cdot, t_n) - \psi^n_I\right\|_{H^2}, \quad \mathrm{e}^{\tau,h}_{\psi,\infty}(t) := \max_{0<\varepsilon\le 1}\left\{\mathrm{e}^{\tau,h}_{\psi,\varepsilon}(t)\right\}.$$

Since the analytical solution of this problem is not available, so the 'reference' solution here is obtained numerically by the MTI-FP method (3.15)–(3.17) with very fine mesh $h = 1/32$ and time step $\tau = 5 \times 10^{-6}$. Tables 1 and 2 show the spatial errors of the MTI-FP method for ψ and ϕ, respectively, at $t = 1$ under different ε and h with a very small time step $\tau = 5 \times 10^{-6}$ such that the discretization error in time is negligible. Tables 3 and 4 list the temporal errors of the MTI-FP method for ψ and ϕ, respectively, at $t = 1$ under different ε and τ with a small mesh size $h = 1/16$ such that the discretization error in space is negligible.

From Tables 1, 2, 3 and 4, we can draw the following observations:

(i) The MTI-FP method is spectrally accurate in space, which is uniformly for $0 < \varepsilon \le 1$ (cf. Tables 1, 2). The approximation in ϕ is more accurate than ψ.
(ii) The MTI-FP method converges uniformly in time for $\varepsilon \in (0, 1]$ with linear and quadratical convergence rates for ψ and ϕ, respectively (cf. last rows in Tables

Table 1 Spatial error analysis: $e_{\psi,\varepsilon}^{\tau,h}(t=1)$ with $\tau = 5 \times 10^{-6}$ for different ε and h

$e_{\psi,\varepsilon}^{\tau,h}(t=1)$	$h_0 = 1$	$h_0/2$	$h_0/4$	$h_0/8$	$h_0/16$
$\varepsilon_0 = 1$	6.90E−1	1.39E−1	1.70E−3	2.44E−7	8.96E−11
$\varepsilon_0/2$	7.57E−1	1.40E−1	1.70E−3	2.40E−7	8.37E−11
$\varepsilon_0/2^2$	6.37E−1	1.45E−1	1.70E−3	2.40E−7	9.19E−11
$\varepsilon_0/2^3$	6.46E−1	1.30E−1	1.90E−3	2.40E−7	8.89E−11
$\varepsilon_0/2^4$	6.47E−1	1.31E−1	1.80E−3	2.38E−7	9.26E−11
$\varepsilon_0/2^5$	6.47E−1	1.31E−1	1.80E−3	2.38E−7	9.66E−11
$\varepsilon_0/2^6$	6.46E−1	1.27E−1	1.70E−3	2.52E−7	8.76E−11
$\varepsilon_0/2^7$	6.46E−1	1.31E−1	1.80E−3	2.38E−7	9.08E−11
$\varepsilon_0/2^8$	6.46E−1	1.27E−1	1.70E−3	2.52E−7	9.08E−11
$\varepsilon_0/2^9$	6.46E−1	1.31E−1	1.80E−3	2.38E−7	1.02E−10
$\varepsilon_0/2^{10}$	6.45E−1	1.26E−1	1.80E−3	2.52E−7	4.42E−11
$\varepsilon_0/2^{11}$	6.46E−1	1.31E−1	1.80E−3	2.38E−7	9.07E−11

Table 2 Spatial error analysis: $e_{\phi,\varepsilon}^{\tau,h}(t=1)$ with $\tau = 5 \times 10^{-6}$ for different ε and h

$e_{\phi,\varepsilon}^{\tau,h}(t=1)$	$h_0 = 1$	$h_0/2$	$h_0/4$	$h_0/8$	$h_0/16$
$\varepsilon_0 = 1$	4.74E−2	1.60E−3	3.64E−6	3.57E−10	9.23E−11
$\varepsilon_0/2$	8.29E−2	1.90E−3	1.23E−5	3.92E−10	6.18E−11
$\varepsilon_0/2^2$	2.32E−1	1.12E−2	4.61E−5	1.46E−9	5.24E−11
$\varepsilon_0/2^3$	3.49E−1	1.30E−3	9.31E−5	5.33E−10	4.58E−11
$\varepsilon_0/2^4$	2.64E−1	1.20E−3	3.35E−5	5.16E−9	4.49E−11
$\varepsilon_0/2^5$	2.71E−1	2.09E−4	6.92E−6	8.76E−10	5.49E−11
$\varepsilon_0/2^6$	1.13E−1	5.27E−4	2.56E−6	1.73E−10	6.04E−11
$\varepsilon_0/2^7$	3.99E−1	4.29E−4	6.28E−7	4.23E−11	6.20E−11
$\varepsilon_0/2^8$	6.74E−2	5.90E−4	7.20E−8	2.38E−11	6.20E−11
$\varepsilon_0/2^9$	3.37E−1	5.13E−5	2.78E−8	1.86E−11	6.51E−11
$\varepsilon_0/2^{10}$	3.81E−1	2.46E−4	9.80E−9	8.39E−12	3.09E−11
$\varepsilon_0/2^{11}$	3.09E−1	7.75E−4	2.98E−9	1.73E−11	6.19E−11

3, 4, respectively). In addition, when $0 < \tau \lesssim \varepsilon^2$, it converges quadratically in time (cf. each row in the upper triangle above the diagonal with values in italics of Tables 3, 4); when $0 < \varepsilon \lesssim \tau^{1/2}$, the error is at $O(\varepsilon^2)$ which is independent of τ (cf. each row in the lower triangle of Tables 3, 4) and it converges quadratically in term of ε (cf. each column in the lower triangle of Tables 3, 4).

(iii) The practical temporal uniform convergence order of the MTI-FP in ϕ is better than the theoretical error estimate result. In fact, the temporal local truncation error of the MTI-FP in ϕ is at $O(\tau^3)$, but due to the nonlinear coupling with ψ,

Table 3 Temporal error analysis: $e^{\tau,h}_{\psi,\varepsilon}(t=1)$ and $e^{\tau,h}_{\psi,\infty}(t=1)$ with $h = 1/16$ for different ε and τ

$e^{\tau,h}_{\psi,\varepsilon}(t=1)$	$\tau_0 = 0.2$	$\tau_0/2^2$	$\tau_0/2^4$	$\tau_0/2^6$	$\tau_0/2^8$	$\tau_0/2^{10}$	$\tau_0/2^{12}$
$\varepsilon_0 = 1$	1.31E−1	1.60E−2	1.00E−3	6.20E−5	3.84E−6	2.35E−7	1.77E−8
Rate	–	1.52	2.00	2.01	2.01	2.02	1.87
$\varepsilon_0/2$	*1.59E−1*	2.05E−2	1.30E−3	7.70E−5	4.76E−6	2.92E−7	1.37E−8
Rate	–	1.48	1.99	2.04	2.01	2.01	2.20
$\varepsilon_0/2^2$	1.20E−1	*1.48E−2*	1.20E−3	7.65E−5	4.79E−6	2.95E−7	1.38E−8
Rate	–	1.35	1.81	1.99	2.00	2.01	2.20
$\varepsilon_0/2^3$	2.23E−2	5.30E−3	*5.19E−4*	3.20E−5	2.00E−6	1.23E−7	5.77E−9
Rate	–	1.04	1.68	2.00	2.00	2.01	2.20
$\varepsilon_0/2^4$	9.50E−3	3.50E−3	2.20E−3	*1.32E−4*	8.06E−6	4.94E−7	2.31E−8
Rate	–	0.72	0.33	2.03	2.02	2.01	2.20
$\varepsilon_0/2^5$	1.40E−3	1.00E−3	6.34E−4	4.67E−4	*3.35E−5*	2.02E−6	9.41E−8
Rate	–	0.24	0.33	0.22	1.91	2.02	2.20
$\varepsilon_0/2^6$	3.82E−4	5.65E−5	1.43E−4	1.51E−4	1.16E−4	*8.29E−6*	3.80E−7
Rate	–	–	−0.67	−0.18	0.19	1.90	2.22
$\varepsilon_0/2^7$	5.64E−5	2.30E−5	1.28E−5	3.61E−5	3.83E−5	2.89E−5	*1.58E−6*
Rate	–	–	–	−0.75	−0.04	0.20	2.10
$\varepsilon_0/2^8$	2.10E−5	5.60E−6	6.41E−6	2.61E−6	1.10E−5	1.12E−5	5.70E−6
Rate	–	–	–	–	−1.00	−0.01	0.49
$\varepsilon_0/2^9$	5.82E−6	4.05E−6	2.40E−6	2.00E−6	2.41E−6	8.49E−7	2.50E−7
Rate	–	–	–	–	–	0.75	0.88
$\varepsilon_0/2^{10}$	2.25E−6	3.40E−7	2.19E−7	5.47E−7	3.46E−7	6.29E−7	5.07E−8
Rate	–	–	–	–	–	–	1.81
$\varepsilon_0/2^{11}$	2.09E−7	2.19E−7	1.67E−7	1.58E−7	8.48E−8	1.43E−7	4.63E−8
Rate	–	–	–	–	–	–	–
$\varepsilon_0/2^{13}$	1.75E−8	8.01E−9	7.32E−9	4.13E−9	6.27E−9	1.64E−10	7.53E−9
Rate	–	–	–	–	–	–	–
$e^{\tau,h}_{\psi,\infty}(t=1)$	1.59E−1	2.05E−2	2.20E−3	4.67E−4	1.16E−4	2.89E−5	5.70E−6
Rate	–	1.48	1.61	1.11	1.00	1.00	1.17

the theoretical error bound drops down to uniform linear convergence rate. The rigorous mathematical analysis is still on-going.

(iv) In the nonrelativistic limit regime, i.e. $0 < \varepsilon \ll 1$, the mesh strategy (or ε-scalability) of the MTI-FP method is $\tau = O(1)$ and $h = O(1)$.

To compare with existing numerical methods for the KGS [13], Table 5 shows the temporal errors of the phase-space analytical solver time-splitting spectral method (PSAS-TSSP), in which the time-splitting spectral method was used to discretize the NLSE [4,13] and the exponential wave integrator spectral method was used to discretize the KG equation [9,13], at $t = 1$ under different ε and τ with a small mesh

Table 4 Temporal error analysis: $e_{\phi,\varepsilon}^{\tau,h}(t=1)$ and $e_{\phi,\infty}^{\tau,h}(t=1)$ with $h = 1/16$ for different ε and τ

$e_{\phi,\varepsilon}^{\tau,h}(t=1)$	$\tau_0 = 0.2$	$\tau_0/2^2$	$\tau_0/2^4$	$\tau_0/2^6$	$\tau_0/2^8$	$\tau_0/2^{10}$	$\tau_0/2^{12}$
$\varepsilon_0 = 1$	3.74E−2	1.50E−3	3.82E−5	1.78E−6	1.09E−7	6.73E−9	3.32E−10
Rate	–	2.32	2.65	2.21	2.01	2.01	2.17
$\varepsilon_0/2$	*9.32E−2*	4.80E−3	2.29E−4	1.35E−5	8.32E−7	5.11E−8	2.39E−9
Rate	–	2.14	2.19	2.04	2.01	2.01	2.20
$\varepsilon_0/2^2$	9.65E−2	*1.26E−2*	7.09E−4	4.23E−5	2.61E−6	1.60E−7	7.51E−9
Rate	–	1.47	2.07	2.03	2.01	2.01	2.20
$\varepsilon_0/2^3$	2.33E−2	4.10E−3	*3.02E−4*	1.95E−5	1.21E−6	7.47E−8	3.50E−9
Rate	–	1.25	1.88	1.98	2.00	2.01	2.20
$\varepsilon_0/2^4$	8.70E−3	3.30E−3	9.09E−5	*6.00E−6*	3.82E−7	2.36E−8	1.11E−9
Rate	–	0.70	2.59	1.96	1.99	2.00	2.20
$\varepsilon_0/2^5$	9.59E−4	8.29E−4	2.42E−4	3.73E−6	*2.89E−7*	1.81E−8	8.53E−10
Rate	–	0.11	0.89	3.01	1.85	2.00	2.20
$\varepsilon_0/2^6$	4.71E−4	1.19E−4	1.33E−5	3.80E−6	2.13E−7	*1.67E−8*	8.01E−10
Rate	–	–	1.58	0.90	2.07	1.84	2.19
$\varepsilon_0/2^7$	8.27E−5	2.88E−5	2.49E−6	1.76E−7	4.95E−8	1.30E−8	*7.86E−10*
Rate	–	–	–	1.91	0.92	0.96	2.02
$\varepsilon_0/2^8$	3.33E−5	5.69E−6	3.28E−7	2.18E−8	3.37E−9	1.70E−9	6.57E−10
Rate	–	–	–	–	1.35	0.49	0.69
$\varepsilon_0/2^9$	8.92E−6	3.98E−6	1.04E−7	5.46E−9	3.66E−10	5.75E−11	2.04E−11
Rate	–	–	–	–	–	1.34	0.75
$\varepsilon_0/2^{10}$	2.30E−6	5.26E−7	1.59E−7	1.29E−9	8.97E−11	2.51E−11	2.34E−11
Rate	–	–	–	–	–	–	0.01
$\varepsilon_0/2^{11}$	3.05E−7	1.59E−7	5.64E−9	1.32E−9	7.21E−11	7.09E−11	7.43E−11
Rate	–	–	–	–	–	–	–
$\varepsilon_0/2^{13}$	2.30E−8	7.26E−9	2.21E−9	7.75E−10	7.72E−10	7.72E−10	7.71E−10
Rate	–	–	–	–	–	–	–
$e_{\phi,\infty}^{\tau,h}(t=1)$	9.65E−2	1.26E−2	7.09E−4	4.23E−5	2.61E−6	1.60E−7	7.51E−9
Rate	–	1.46	2.00	2.00	2.00	2.00	2.00

size $h = 1/16$ such that the discretization error in space is negligible; and Table 6 lists similar results for the Crank–Nicolson leap-frog time-splitting spectral method (CN-LF-TSSP), in which the time-splitting spectral method was used to discretize the NLSE [4,13] and the Crank-Nicolson and leap-frog schemes were used to discretize the linear and nonlinear terms in the KG equation, respectively [9,13].

From Tables 5 and 6, we can draw the following observations: (i) the ε-scalability of the PSAS-TSSP method is $h = O(1)$ and $\tau = O(\varepsilon^2)$ (cf. upper triangle above the diagonal with values in italics of Table 5); and (ii) the ε-scalability of the CN-LF-TSSP method is $h = O(1)$ and $\tau = O(\varepsilon^3)$ (cf. upper triangle above the diagonal with values in italics of Table 6). In fact, similar to the proofs in [4,9] for establishing error bounds

Table 5 Temporal error $\mathrm{e}_{\psi,\varepsilon}^{\tau,h}(t=1)$ of PSAS-TSFP with $h = 1/16$ for different ε and τ

$\mathrm{e}_{\psi,\varepsilon}^{\tau,h}(t=1)$	$\tau_0 = 0.2$	$\tau_0/2^2$	$\tau_0/2^4$	$\tau_0/2^6$	$\tau_0/2^8$	$\tau_0/2^{10}$	$\tau_0/2^{12}$
$\varepsilon_0 = 1$	3.51E−2	8.40E−4	5.14E−5	3.19E−6	1.89E−7	1.21E−8	1.00E−9
Rate	–	2.69	2.01	2.00	2.03	1.98	1.80
$\varepsilon_0/2$	*7.79E−2*	4.50E−3	2.82E−4	1.76E−5	1.10E−6	6.85E−8	4.90E−9
Rate	–	2.05	2.00	2.00	2.00	2.00	1.90
$\varepsilon_0/2^2$	2.13E−1	*1.75E−2*	1.10E−3	6.96E−5	4.34E−6	2.75E−7	1.83E−8
Rate	–	1.80	2.00	1.99	2.00	2.00	1.94
$\varepsilon_0/2^3$	8.47E−1	2.88E−2	*1.50E−3*	9.39E−5	5.88E−6	3.78E−7	2.42E−8
Rate	–	2.43	2.13	2.00	2.00	1.98	1.98
$\varepsilon_0/2^4$	6.21E−1	7.41E−1	7.20E−3	*3.71E−4*	2.30E−5	1.49E−6	9.21E−8
Rate	–	-0.13	3.34	2.13	1.99	2.00	2.00
$\varepsilon_0/2^5$	1.46E−1	1.12E−1	1.27E−1	1.70E−3	*8.64E−5*	5.55E−6	3.42E−7
Rate	–	0.19	−0.09	3.11	2.14	1.98	2.01

Table 6 Temporal error $\mathrm{e}_{\phi,\varepsilon}^{\tau,h}(t=1)$ of CN-LF-TSFP with $h = 1/16$ for different ε and τ

$\mathrm{e}_{\phi,\varepsilon}^{\tau,h}(t=1)$	$\tau_0 = 0.2$	$\tau_0/2^3$	$\tau_0/2^6$	$\tau_0/2^9$	$\tau_0/2^{12}$
$\varepsilon_0 = 1$	*1.29E−1*	2.30E−3	3.65E−5	5.71E−7	9.78E−9
Rate	–	1.94	2.00	2.00	1.95
$\varepsilon_0/2$	1.31	*3.26E−2*	5.19E−4	8.12E−6	1.36E−8
Rate	–	1.77	1.99	2.00	1.97
$\varepsilon_0/2^2$	2.56	9.55E−1	*1.64E−2*	2.57E−4	4.10E−6
Rate	–	0.71	1.95	2.00	2.00
$\varepsilon_0/2^3$	2.09	2.49	8.42E−1	*1.40E−2*	2.18E−4
Rate	–	−0.13	0.78	1.97	2.00
$\varepsilon_0/2^4$	2.28	2.39	2.60	8.46E−1	*1.38E−2*
Rate	–	−0.34	−0.06	0.81	1.98
$\varepsilon_0/2^5$	1.64	1.35	2.72	1.82	7.99E−1
Rate	–	0.14	−0.50	0.29	0.59

of the NLSE and KG equation, we can establish an error bound for the PSAS-TSSP method under the condition $0 < \tau \lesssim \varepsilon^2$ (details omitted here for brevity)

$$\left\| e_\phi^n \right\|_{H^1} + \left\| e_\psi^n \right\|_{H^1} \lesssim h^{m_0} + \frac{\tau^2}{\varepsilon^2}, \qquad 0 \le n \le \frac{T}{\tau}, \tag{5.2}$$

and respectively, an error bound for the CN-LF-TSSP method

$$\left\| e_\phi^n \right\|_{H^1} + \left\| e_\psi^n \right\|_{H^1} \lesssim h^{m_0} + \frac{\tau^2}{\varepsilon^6}, \qquad 0 \le n \le \frac{T}{\tau}, \tag{5.3}$$

provided that the exact solution satisfy $\phi \in C([0,T]; H_p^{m_0+1}(\Omega)) \cap C^2([0,T]; H^1(\Omega))$ and $\psi \in C([0,T]; H_p^{m_0+1}(\Omega)) \cap C^1([0,T]; H^1(\Omega))$ with $m_0 \geq 2$. Here e_ϕ^n and e_ψ^n are defined in (4.4).

5.2 Convergence rates of KGS to its limiting models

Let (ψ, ϕ) be the solution of the KGS equations (1.3) with $d = \mu = \lambda = 1$ and (5.1), which is obtained numerically on a bounded interval $\Omega = [-512, 512]$ by the MTI-FP method (3.15)–(3.17) with very fine mesh $h = 1/16$ and time step $\tau = 10^{-4}$. Similarly, let $(\psi_{\rm sw}, z_{\rm sw})$ be the solution of the Schrödinger equations with wave operator (1.9) with $d = \mu = \lambda = 1$ and (1.10) and (5.1), which is obtained numerically on the bounded interval Ω by the EWI-FP method [7] with very fine mesh $h = 1/16$ and time step $\tau = 10^{-4}$; and let $(\psi_{\rm s}, z_{\rm s})$ be the solution of the Schrödinger equations (1.11) with $d = \mu = \lambda = 1$ and (1.12) and (5.1), which is obtained numerically on the bounded interval Ω by the TSFP method [4] with very fine mesh $h = 1/16$ and time step $\tau = 10^{-4}$. It is easy to see that $\psi_{\rm sw} = \psi_{\rm s}$. Denote

$$\phi_{\rm sw}(x,t) = \mathrm{e}^{it/\varepsilon^2} z_{\rm sw}(x,t) + \mathrm{e}^{-it/\varepsilon^2} \overline{z_{\rm sw}}(x,t),$$
$$\phi_{\rm s}(x,t) = \mathrm{e}^{it/\varepsilon^2} z_{\rm s}(x,t) + \mathrm{e}^{-it/\varepsilon^2} \overline{z_{\rm s}}(x,t),$$

and define the error functions as

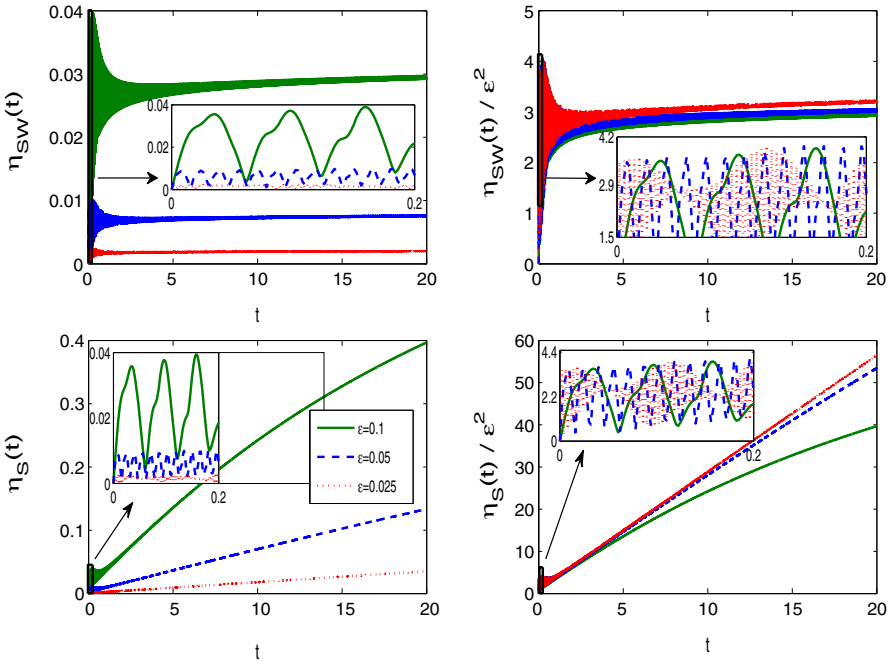

Fig. 2 Time evolution of $\eta_{\rm sw}(t)$ and $\eta_{\rm s}(t)$ for the smooth initial data (5.1) under different ε

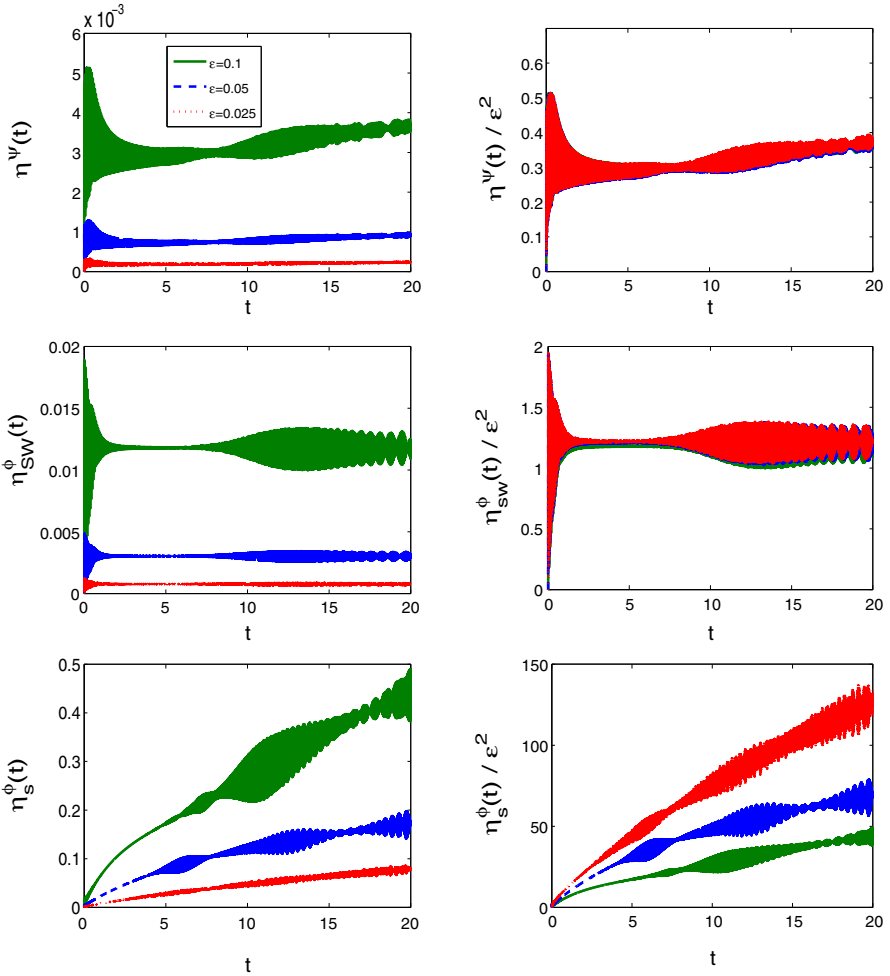

Fig. 3 Time evolution of $\eta^{\psi}(t)$, $\eta^{\phi}_{\rm sw}(t)$ and $\eta^{\phi}_{\rm s}(t)$ with nonsmooth data (5.5) for $m = 2$ under different ε

$$\eta_{\rm sw}(t) := \|\phi(\cdot,t) - \phi_{\rm sw}(\cdot,t)\|_{H^1} + \|\psi(\cdot,t) - \psi_{\rm sw}(\cdot,t)\|_{H^1},$$
$$\eta_{\rm s}(t) := \|\phi(\cdot,t) - \phi_{\rm s}(\cdot,t)\|_{H^1} + \|\psi(\cdot,t) - \psi_{\rm s}(\cdot,t)\|_{H^1}. \tag{5.4}$$

Figure 2 depicts $\eta_{\rm sw}(t)$ and $\eta_{\rm s}(t)$ for different ε. In addition, here we also study numerically convergence rates of the KGS equations (1.3) with $d = \mu = \lambda = 1$ to its limiting models when the initial data in (1.5) is not smooth. For this purpose, we take the initial data in (1.5) as

$$\psi_0(x) = \frac{x^m|x|}{2}\,\mathrm{sech}\left(x^2\right), \quad \phi_0(x) = \frac{x^m|x|}{2}\mathrm{e}^{-x^2}, \quad \phi_1(x) = \frac{1}{\sqrt{2}}\mathrm{e}^{-x^2}, \quad x \in \mathbb{R}, \tag{5.5}$$

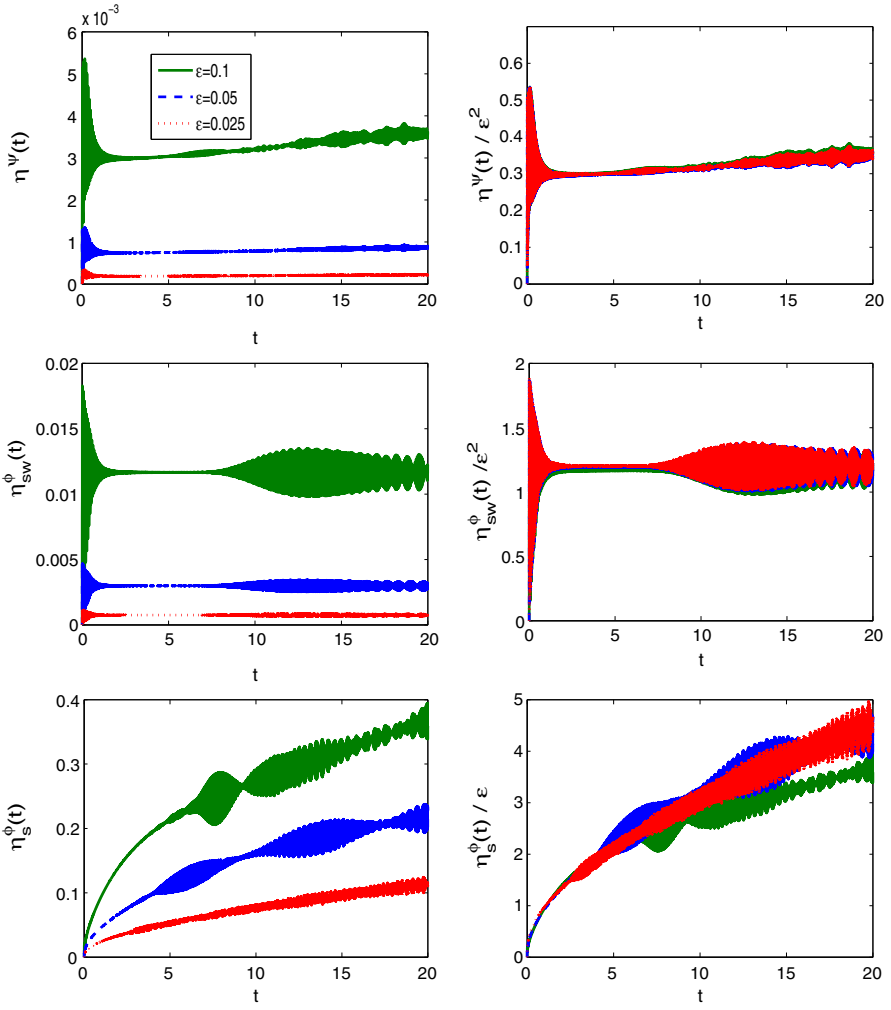

Fig. 4 Time evolution of $\eta^{\psi}(t)$, $\eta^{\phi}_{\rm sw}(t)$ and $\eta^{\phi}_{\rm s}(t)$ with nonsmooth data (5.5) for $m = 1$ under different ε

where $m = 1$ or 2. In order to see the convergence rate to the semi-limiting model (1.9) or limiting model (1.11) in each component ψ and ϕ more clearly, we define the error functions

$$\eta^{\phi}_{\rm sw}(t) := \|\phi(\cdot,t) - \phi_{\rm sw}(\cdot,t)\|_{H^1}, \quad \eta^{\phi}_{\rm s}(t) := \|\phi(\cdot,t) - \phi_{\rm s}(\cdot,t)\|_{H^1},$$
$$\eta^{\psi}(t) := \|\psi(\cdot,t) - \psi_{\rm sw}(\cdot,t)\|_{H^1} = \|\psi(\cdot,t) - \psi_{\rm s}(\cdot,t)\|_{H^1}.$$

Figure 3 depicts $\eta^{\psi}(t)$, $\eta^{\phi}_{\rm sw}(t)$ and $\eta^{\phi}_{\rm s}(t)$ for the nonsmooth initial data (5.5) with $m = 2$ under different ε and Fig. 4 shows similar results when $m = 1$ in (5.5).

From Figs. 2, 3, 4, we can draw the following conclusions:

(i) The solution of the KGS equations (1.3) with (1.5) converges to that of the Schrödinger equations with wave operator (1.9) with (1.10) quadratically in ε (and uniformly in time) provided that the initial data in (1.5) is smooth or at least satisfies ψ_0, ψ_1, ϕ_0 and $\phi_1 \in H^2(\mathbb{R}^d)$, i.e.

$$\|\psi(\cdot,t)-\psi_{\rm sw}(\cdot,t)\|_{H^1(\Omega)}+\|\phi(\cdot,t)-\phi_{\rm sw}(\cdot,t)\|_{H^1(\Omega)}\le C_0\varepsilon^2, \qquad t\ge 0,$$

where the constant $C_0>0$ is independent of ε and time $t\ge 0$.

(ii) The solution of the KGS equations (1.3) with (1.5) converges to that of the Schrödinger equations (1.11) with (1.12) quadratically in ε (in general, not uniformly in time) provided that the initial data in (1.5) is smooth or at least satisfies ψ_0, ψ_1, ϕ_0 and $\phi_1 \in H^3(\mathbb{R}^d)$, i.e.

$$\|\psi(\cdot,t)-\psi_{\rm s}(\cdot,t)\|_{H^1(\Omega)}+\|\phi(\cdot,t)-\phi_{\rm s}(\cdot,t)\|_{H^1(\Omega)}\le (C_1+C_2T)\varepsilon^2,\quad 0\le t\le T,$$

where C_1 and $C_2>0$ are two positive constants which are independent of ε and T. On the contrary, if the regularity of the initial data is weaker, e.g. ψ_0, ψ_1, ϕ_0 and $\phi_1 \in H^2(\mathbb{R}^d)$, then the convergence rate in ϕ collapses to linear rate while the convergence rate in ψ is still quadratic rate (and uniformly in time), i.e.

$$\begin{aligned}&\|\psi(\cdot,t)-\psi_{\rm s}(\cdot,t)\|_{H^1(\Omega)}\le C_0\varepsilon^2,\\ &\|\phi(\cdot,t)-\phi_{\rm s}(\cdot,t)\|_{H^1(\Omega)}\le (C_3+C_4T)\varepsilon,\quad 0\le t\le T,\end{aligned}$$

where C_3 and C_4 are two positive constants which are independent of ε and T. Rigorous mathematical justification for these numerical observations is on-going.

6 Conclusion

A multiscale time integrator Fourier pseudospectral (MTI-FP) method was proposed and analyzed for solving the Klein–Gordon–Schrödinger (KGS) equations with a dimensionless parameter $0<\varepsilon\le 1$ which is inversely proportional to the speed of light. The key ideas for designing the MTI-FP method are based on (1) carrying out a multiscale decomposition by frequency at each time step with proper choice of transmission conditions between adjacent time intervals, and (2) adapting the Fourier spectral method for spatial discretization and the EWI for integrating second-order highly oscillating ODEs. Rigorous error bounds for the MTI-FP method were established, which imply that the MTI-FP method converges uniformly and optimally in space with spectral convergence rate, and uniformly in time with linear convergence rate for $\varepsilon\in(0,1]$ and optimally with quadratic convergence rate at $O(\tau^2)$ in the regime when $0<\tau\lesssim\varepsilon^2$ and the error is at $O(\varepsilon^2)$ independent of τ in the regime when $0<\varepsilon\lesssim\tau^{1/2}$. Numerical results confirmed these error bounds and showed that the MTI-FP method offers compelling advantages over classical methods in the nonrelativistic regime $0<\varepsilon\ll 1$. Numerical results suggest that the solution of the KGS equations converges quadratically to that of its limiting models when $\varepsilon\to 0$.

Acknowledgements This work was supported by the Ministry of Education of Singapore Grant R-146-000-196-112. Part of this work was done when the authors were visiting the Institute for Mathematical Science at the National University of Singapore in 2015.

Appendix: Explicit formulas and estimates for the coefficients used in (3.14)

Define the functions

$$\begin{cases} p_l(s) := \int_0^s \frac{\sin(\omega_l(s-\theta))}{\varepsilon^2\omega_l}d\theta, \quad p_l'(s) := \int_0^s \frac{\cos(\omega_l(s-\theta))}{\varepsilon^2}d\theta, \\ q_l(s) := \int_0^s \frac{\sin(\omega_l(s-\theta))}{\varepsilon^2\omega_l}\theta d\theta, \quad q_l'(s) := \int_0^s \frac{\cos(\omega_l(s-\theta))}{\varepsilon^2}\theta d\theta, \\ c_l^+(s) := i\mathrm{e}^{-i\mu_l^2 s}\int_0^s \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}d\theta, \quad c_l^-(s) := i\mathrm{e}^{-i\mu_l^2 s}\int_0^s \mathrm{e}^{i\left(\mu_l^2-\frac{1}{\varepsilon^2}\right)\theta}d\theta, \\ d_l^+(s) := i\mathrm{e}^{-i\mu_l^2 s}\int_0^s \mathrm{e}^{i\left(\mu_l^2+\frac{1}{\varepsilon^2}\right)\theta}\theta d\theta, \quad d_l^-(s) := i\mathrm{e}^{-i\mu_l^2 s}\int_0^s \mathrm{e}^{i\left(\mu_l^2-\frac{1}{\varepsilon^2}\right)\theta}\theta d\theta. \end{cases} \tag{7.1}$$

Taking $s = \tau$ in (7.1), after a detailed computation, we have

$$\begin{aligned} p_l(\tau) &= \frac{1-\cos(\omega_l\tau)}{\varepsilon^2\omega_l^2}, \quad p_l'(\tau) = \frac{\sin(\omega_l\tau)}{\varepsilon^2\omega_l}, \\ q_l(\tau) &= \frac{\tau\omega_l - \sin(\omega_l\tau)}{\varepsilon^2\omega_l^3}, \quad q_l'(\tau) = \frac{1-\cos(\omega_l\tau)}{\varepsilon^2\omega_l^2}, \\ c_l^+(\tau) &= \frac{\varepsilon^2\mathrm{e}^{-i\mu_l^2\tau}\left(\mathrm{e}^{i\tau(\mu_l^2+\frac{1}{\varepsilon^2})}-1\right)}{1+\varepsilon^2\mu_l^2}, \quad c_l^-(\tau) = \frac{\varepsilon^2\left(\mathrm{e}^{-i\tau\mu_l^2}-\mathrm{e}^{-i\frac{\tau}{\varepsilon^2}}\right)}{1-\varepsilon^2\mu_l^2}, \\ d_l^+(\tau) &= \frac{i\varepsilon^2}{(1+\varepsilon^2\mu_l^2)^2}\left[\mathrm{e}^{\frac{i\tau}{\varepsilon^2}}\left(\varepsilon^2 - i\tau\left(1+\varepsilon^2\mu_l^2\right)\right) - \varepsilon^2\mathrm{e}^{-i\mu_l^2\tau}\right], \\ d_l^-(\tau) &= \frac{i\varepsilon^2}{(1-\varepsilon^2\mu_l^2)^2}\left[\mathrm{e}^{-\frac{i\tau}{\varepsilon^2}}\left(\varepsilon^2 - i\tau\left(\varepsilon^2\mu_l^2-1\right)\right) - \varepsilon^2\mathrm{e}^{-i\mu_l^2\tau}\right]. \end{aligned}$$

Based on (7.1) and noting $\varepsilon^2\omega_l^2 = \sqrt{1+\varepsilon^2\mu_l^2} \geq 1$, we have

$$|p_l(\tau)| = \left|\int_0^\tau \frac{\sin(\omega_l(\tau-\theta))}{\varepsilon^2\omega_l}d\theta\right| \leq \int_0^\tau \frac{|\sin(\omega_l(s-\theta))|}{\sqrt{1+\varepsilon^2\mu_l^2}}d\theta \leq \int_0^\tau 1\, d\theta \lesssim \tau.$$

Similarly, we can get

$$|q_l(\tau)| \lesssim \tau^2, \quad |p_l'(\tau)| \lesssim \frac{\tau}{\varepsilon^2}, \quad |q_l'(\tau)| \lesssim \frac{\tau^2}{\varepsilon^2}, \quad l = -\frac{N}{2}, \ldots, \frac{N}{2}-1.$$

Again, based on (7.1) and noting $\varepsilon^2\omega_l^2 = \sqrt{1+\varepsilon^2\mu_l^2} \geq \varepsilon|\mu_l|$, we get

$$|p_l(\tau)\mu_l| \leq \int_0^\tau \frac{|\mu_l|\,|\sin(\omega_l(\tau-\theta))|}{\sqrt{1+\varepsilon^2\mu_l^2}}d\theta \leq \int_0^\tau \frac{1}{\varepsilon}d\theta \lesssim \frac{\tau}{\varepsilon},$$
$$|q_l(\tau)\mu_l| \leq \int_0^\tau \frac{\theta\,|\mu_l|\,|\sin(\omega_l(\tau-\theta))|}{\sqrt{1+\varepsilon^2\mu_l^2}}d\theta \leq \int_0^\tau \frac{\theta}{\varepsilon}d\theta \lesssim \frac{\tau^2}{\varepsilon}.$$

References

1. Adams, R.: Sobolev Spaces. Academic Press, Boston (1975)
2. Added, H., Added, S.: Equations of Langmuir turbulence and nonlinear Schrödinger equation: smoothness and approximation. J. Funct. Anal. **79**, 183–210 (1988)
3. Banquet, C., Ferreira, L.C.F., Villamizar-Roa, E.J.: On existence and scattering theory for the Klein–Gordon–Schrödinger system in an infinite L^2-norm setting. Ann. Mat. Pura Appl. (2014). doi:10.1007/s10231-013-0398-7
4. Bao, W., Cai, Y.: Mathematical theory and numerical methods for Bose–Einstein condensation. Kinet. Relat. Models **6**, 1–135 (2013)
5. Bao, W., Cai, Y.: Optimal error estimates of finite difference methods for the Gross–Pitaevskii equation with angular momentum rotation. Math. Comput. **82**, 99–128 (2013)
6. Bao, W., Cai, Y.: Uniform error estimates of finite difference methods for the nonlinear Schrödinger equation with wave operator. SIAM J. Numer. Anal. **50**, 492–521 (2012)
7. Bao, W., Cai, Y.: Uniform and optimal error estimates of an exponential wave integrator sine pseudospectral method for the nonlinear Schrödinger equation with wave operator. SIAM J. Numer. Anal. **52**, 1103–1127 (2014)
8. Bao, W., Cai, Y., Zhao, X.: A uniformly accurate multiscale time integrator pseudospectral method for the Klein–Gordon equation in the nonrelativistic limit regime. SIAM J. Numer. Anal. **52**, 2488–2511 (2014)
9. Bao, W., Dong, X.: Analysis and comparison of numerical methods for the Klein–Gordon equation in the nonrelativistic limit regime. Numer. Math. **120**, 189–229 (2012)
10. Bao, W., Dong, X., Wang, S.: Singular limits of Klein–Gordon–Schrödinger equations to Schrödinger–Yukawa equations. Multiscale Model. Simul. **8**, 1742–1769 (2010)
11. Bao, W., Dong, X., Zhao, X.: An exponential wave integrator sine pseudospectral method for the Klein–Gordon–Zakharov system. SIAM J. Sci. Comput. **25**, A2903–A2927 (2013)
12. Bao, W., Dong, X., Zhao, X.: Uniformly accurate multiscale time integrators for highly oscillatory second order differential equations. J. Math. Study **47**, 111–150 (2014)
13. Bao, W., Yang, L.: Efficient and accurate numerical methods for the Klein–Gordon–Schrödinger equations. J. Comput. Phys. **225**, 1863–1893 (2007)
14. Biler, P.: Attractors for the system of Schrödinger and Klein–Gordon equations with Yukawa coupling. SIAM J. Math. Anal. **21**, 1190–1212 (1990)
15. Chartier, Ph., Crouseilles, N., Lemou, M., Méhats, F.: Uniformly accurate numerical schemes for highly oscillatory Klein–Gordon and nonlinear Schrödinger equations. Numer. Math. **129**, 211–250 (2015)
16. Chartier, Ph., Mauser, N.J., Méhats, F., Zhang, Y.: Solving highly-oscillatory NLS with SAM: numerical efficiency and geometric properties. Discrete Contin. Dyn. Syst. Ser. S. To appear. arXiv:1308.1217
17. Cohen, D.: Analysis and numerical treatment of highly oscillatory differential equations. PhD thesis, Université de Genève (2004)
18. Cohen, D.: Conservation properties of numerical integrators for highly oscillatory Hamiltonian systems. IMA J. Numer. Anal. **26**, 34–59 (2005)
19. Cohen, D., Hairer, E., Lubich, Ch.: Modulated Fourier expansions of highly oscillatory differential equations. Found. Comput. Math. **3**, 327–345 (2003)
20. Cohen, D., Hairer, E., Lubich, Ch.: Conservation of energy, momentum and actions in numerical discretizations of non-linear wave equations. Numer. Math. **110**, 113–143 (2008)

21. Deuflhard, P.: A study of extrapolation methods based on multistep schemes without parasitic solutions. ZAMP **30**, 177–189 (1979)
22. Faou, E., Schratz, K.: Asympotic preserving schemes for the Klein–Gordon equation in the nonrelativistic limit regime. Numer. Math. **126**, 441–469 (2014)
23. Fukuda, I., Tsutsumi, M.: On the Yukawa-coupled Klein–Gordon–Schrödinger equations in three space dimensions. Proc. Jpn. Acad. **51**, 402–405 (1975)
24. Fukuda, I., Tsutsumi, M.: On coupled Klein–Gordon–Schrödinger equations II. J. Math. Anal. Appl. **66**, 358–378 (1978)
25. Fukuda, I., Tsutsumi, M.: On coupled Klein–Gordon–Schrödinger equations III. Math. Jpn. **24**, 307–321 (1979)
26. Garcia-Archilla, B., Sanz-Serna, J.M., Skeel, R.D.: Long-time-step methods for oscillatory differential equations. SIAM J. Sci. Comput. **20**, 930–963 (1998)
27. Gautschi, W.: Numerical integration of ordinary differential equations based on trigonometric polynomials. Numer. Math. **3**, 381–397 (1961)
28. Grimm, V.: A note on the Gautschi-type method for oscillatory second-order differential equations. Numer. Math. **102**, 61–66 (2005)
29. Grimm, V., Hochbruck, M.: Error analysis of exponential integrators for oscillatory second-order differential equations. J. Phys. A: Math. Gen. **39**, 5495–5507 (2006)
30. Gottlieb, D., Orszag, S.A.: Numerical Analysis of Spectral Methods: Theory and Applications. Society for Industrial and Applied Mathematics, Philadelphia (1993)
31. Guo, B.L.: Global solution for some problem of a class of equations in interaction of complex Schrödinger field and real Klein–Gordon field. Sci. China Ser. A **25**, 97–107 (1982)
32. Guo, B.L., Li, Y.S.: Attractor for dissipative Klein–Gordon–Schrödinger equations in $\mathbb{R}^3$. J. Differ. Equ. **136**, 356–377 (1997)
33. Guo, B.L., Miao, C.X.: Asymptotic behavior of coupled Klein–Gordon–Schrödinger equations. Sci. China Ser. A **25**, 705–714 (1995)
34. Hairer, E., Lubich, Ch.: Long-time energy conservation of numerical methods for oscillatory differential equations. SIAM J. Numer. Anal. **38**, 414–441 (2000)
35. Hairer, E., Lubich, Ch.: On the energy disctribution in Fermi–Pasta–Ulam lattices. Arch. Ration. Mech. Anal. **205**, 993–1029 (2012)
36. Hairer, E., Lubich, Ch., Wanner, G.: Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. Springer, Berlin (2006)
37. Hayashi, N., von Wahl, W.: On the global strong solutions of coupled Klein–Gordon–Schrödinger equations. J. Math. Soc. Jpn. **39**, 489–497 (1987)
38. Hochbruck, M., Lubich, Ch.: A Gautschi-type method for oscillatory second-order differential equations. Numer. Math. **83**, 403–426 (1999)
39. Lu, Y., Zhang, Z.: Long time behavior of the quadratic Klein–Gordon equation in the nonrelativistic limit regime. arXiv:1412.2787
40. Machihara, S., Nakanishi, K., Ozawa, T.: Nonrelativistic limit in the energy space for nonlinear Klein–Gordon equations. Math. Ann. **322**, 603–621 (2002)
41. Makhankov, V.G.: Dynamics of classical solitons (in non-integrable systems). Phys. Lett. C **35**, 1–128 (1978)
42. Masmoudi, N., Nakanishi, K.: From nonlinear Klein–Gordon equation to a system of coupled nonlinear Schrödinger equations. Math. Ann. **324**, 359–389 (2002)
43. Masmoudi, N., Nakanishi, K.: From the Klein–Gordon–Zakharov system to the nonlinear Schrödinger equation. J. Hyperbolic Differ. Equ. **2**, 975–1008 (2005)
44. Missaoui, S., Zahrouni, E.: Regularity of the attractor for a coupled Klein–Gordon–Schrödinger system with cubic nonlinearities in R^2. Commun. Pure Appl. Anal. **14**, 695–716 (2015)
45. Sanz-Serna, J.M.: Mollified impulse methods for highly oscillatory differential equations. SIAM J. Numer. Anal. **46**, 1040–1059 (1998)
46. Shen, J., Tang, T.: Spectral and High-Order Methods with Applications. Science Press, Beijing (2006)
47. Shi, Q.H., Li, W.T., Wang, S.: Wellposedness in energy space for the nonlinear Klein–Gordon–Schrödinger system. Appl. Math. Comput. **251**, 55–64 (2015)
48. Shi, Q.H., Wang, S., Li, Y.: Existence and uniqueness of energy solution to Klein–Gordon–Schrödinger equations. J. Differ. Equ. **252**, 168–180 (2012)
49. Wang, M.L., Zhou, Y.B.: The periodic wave solutions for the Klein–Gordon–Schrödinger equations. Phys. Lett. A **318**, 84–92 (2003)

50. Wang, T.C.: Optimal point-wise error estimate of a compact difference scheme for the Klein–Gordon–Schrödinger equation. J. Math. Anal. Appl. **412**, 155–167 (2014)
51. Wang, Y., Zhao, X.: Symmetric high order Gautschi-type exponential wave integrators spectral method for the Klein–Gordon equation in the nonrelativistic limit regime (preprint)
52. Xiang, X.M.: Spectral method for solving the system of equations of Schrödinger–Klein–Gordon field. J. Comput. Appl. Math. **21**, 161–171 (1988)
53. Zhang, L.M.: Convergence of a conservative difference scheme for a class of Klein–Gordon–Schrödinger equations in one space dimension. Appl. Math. Comput. **163**, 343–355 (2005)