UNIFORMLY ACCURATE NESTED PICARD ITERATIVE INTEGRATORS FOR THE KLEIN-GORDON EQUATION IN THE NONRELATIVISTIC REGIME

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Abstract. In this paper, a class of uniformly accurate nested Picard iterative integrator (NPI) Fourier pseudospectral methods is proposed for the nonlinear Klein-Gordon equation (NLKG) in the nonrelativistic regime, involving a dimensionless parameter $\varepsilon \ll 1$ inversely proportional to the speed of light. For $0 < \varepsilon \ll 1$, the solution propagates waves in time with $O(\varepsilon^2)$ wavelength, which brings significant difficulty in designing accurate and efficient numerical schemes. The idea of NPI methods can be applied to derive arbitrary higher-order methods in time with optimal and uniform accuracy (w.r.t. $\varepsilon \in (0, 1]$). Detailed constructions of the NPI methods up to the third order in time are presented for NLKG with a cubic/quadratic nonlinear term, where the corresponding error estimates are rigorously analyzed. In addition, the practical implementation of the second-order NPI method via Fourier pseupospectral discretization is clearly demonstrated. Some numerical examples are provided to support our theoretical results and show the accuracy and efficiency of the proposed schemes.

1. Introduction

Consider the nonlinear Klein-Gordon equation [1,5,12,18–21,28–30,32,33] (NLKG) in d-dimensions ($d = 1, 2, 3$)

$$\begin{aligned} &\varepsilon^2 \partial_{tt}\psi(x,t) - \Delta\psi(x,t) + \frac{1}{\varepsilon^2}\psi(x,t) = f(\psi),\ x \in \mathbb{R}^d, t > 0, \\ &\psi(x,0) = \psi_0(x),\ \partial_t\psi(x,0) = \frac{1}{\varepsilon^2}\psi_1(x), x \in \mathbb{R}^d, \end{aligned} \tag{1.1}$$

where $\psi(x,t)$ is a complex-valued scalar field, Δ is the d dimensional Laplace operator, $f(\cdot)$ is Gauge invariant satisfying $f(\omega\psi) = \omega f(\psi)$ ($\forall \omega \in \mathbb{C}$ with $|\omega| = 1$), $0 < \varepsilon \leq 1$ is a dimensionless parameter inversely proportional to the speed of light. Here, we will assume the nonlinear term $f(|\psi|^2) = \lambda|\psi|^2\psi$ ($\lambda \in \mathbb{R}$) to fix the idea if unspecified, and the discussion also holds for polynomial type function $f(\cdot)$ (in ψ and its complex conjugate $\overline{\psi}$).

The above NLKG equation has been extensively studied numerically in the relativistic regime $\varepsilon = 1$, see [8,10,13,14,16,22–26] and the references therein. In the 'non-relativistic regime' $\varepsilon \ll 1$, due to the highly-oscillatory behavior in time of the solution, it is challenging to construct efficient and uniformly accurate numerical

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methods. More precisely, the solution of (1.1) oscillates in time with $O(\varepsilon^2)$ wavelength, which is difficult to resolve numerically when $\varepsilon \ll 1$. To address this issue, Bao and Dong [3] proposed four finite difference time domain methods (FDTD) for the problem (1.1), and analyzed the error estimates which depends explicitly on ε as well as the mesh size h and time step τ. Based on the estimates, the meshing strategy (ε-scalability) requirement of FDTD methods is $\tau = O(\varepsilon^3)$ and $h = O(1)$. In order to improve the error convergence, by using Fourier pseudospectral approximation for spatial derivatives combined with the exponential integrator (EWI) for temporal derivatives in (1.1), they proposed the EWI Fourier pseudospectral method and shows the ε-scalability is $\tau = O(\varepsilon^2)$ and $h = O(1)$. At the same time, Dong et.al. [15] applied the time-splitting pseudospectral discretization to solve (1.1), and obtained the similar ε-scalability ($\tau = O(\varepsilon^2)$) as the EWI Fourier pseudospectral method. Later, in [17] Faou and Schratz presented a class of limit integrators (LI) for (1.1) via solving numerically the limiting model without imposing any $\varepsilon-$dependent step-size restriction. However, as this approach is based on the asymptotic expansion of the solution with respect to ε^2, the limit integration method only yields an accurate approximation of the exact solution for $\varepsilon \to 0$. Numerically, in order to resolve such high frequency in time, the meshing strategies of the above methods which depend on ε bring severe numerical burden.

To overcome this difficulty, various uniformly accurate methods haven been designed for solving the problem (1.1), e.g. the multiscale time integrator pseudospectral method [2, 4, 6, 34] (MTI-FP) via a multiscale decomposition by frequency to the solution at each time step and adopting the exponential wave integrator Fourier pseudospectral method for discretizing the decomposed sub-problems, and the uniformly accurate two-scale formulation (TSF) method [11] based on the Chapman-Enskog expansions, where (1.1) is embedded in a suitable "two-scale" reformulation by introducing an extra dimension, i.e. the fast variable $\xi = t/\varepsilon^2$. Recently, a second-order uniformly accurate iterative exponential integrator method (IEI) has been constructed [7] based on the integral form of the NLKG (1.1) and the 'twisted variable' formulation. The main point in the approximation is integrating the highly oscillatory phases $e^{\pm it/\varepsilon^2}$ and their interactions exactly. Noticing the fact that the leading oscillations in time are due to the linear differential operator in (1.1), the iteration techniques [7] were generalized to design arbitrary high order uniformly accurate nested Picard integrators (NPIs) for the Dirac equation in the nonrelativistic regime [9].

The main object of this paper is to present a general strategy to construct arbitrary k-th order ($k = 1, 2, \ldots,$) numerical schemes which are uniformly accurate with respect to ε, based on the ideas in [7, 9]. Our strategy enables to design k-th order uniformly accurate numerical schemes only by adding a $O(\tau^k)$ term to the previous constructed $(k-1)$-th order uniformly accurate numerical schemes. In the same spirit as in [9], we will propose NPI methods using the nested Picard iterative idea to the integral form of (1.1).

The rest of the paper is organized as follows. In section 2 and section 4, we construct the NPI methods and show the practical implementation of the first-order, second-order and third-order accurate NPI methods. Error estimates are rigorously analyzed for arbitrary higher-order semi-discrete-in-time NPI methods in section 3. Application to the real-valued quadratic NLKG is presented in section 5. Numerical examples are reported in section 6 to validate the efficiency and

uniform accuracy. Finally, we draw some conclusions in section 7. Throughout the paper, we will use $A \lesssim B$ to mean that there exists constant C independent of ε and time step τ, such that $|A| \leq CB$.

2. The Nested Picard method

In this section, based on the Duhamel's principle, we shall present the details for the construction of NPI methods in the semi-discrete-in-time form.

For the simplicity of notations, we denote

$$\mathcal{D}_\varepsilon = \sqrt{\frac{1-\varepsilon^2\Delta}{\varepsilon^4}} = \frac{1}{\varepsilon^2} + \mathcal{D},\ \mathcal{D} = \frac{\sqrt{1-\varepsilon^2\Delta}-1}{\varepsilon^2}, \tag{2.1}$$

where $\mathcal{D}$ is a uniformly bounded operator from $H^s(\mathbb{R}^d)$ to $H^{s-2}(\mathbb{R}^d)$ w.r.t ε. Then, we can rewrite the NLKG (1.1) as

$$\partial_{tt}\psi(x,t) + \mathcal{D}_\varepsilon^2\psi(x,t) = \frac{1}{\varepsilon^2}f(\psi), \quad f(\psi) = \lambda|\psi|^2\psi, \quad x \in \mathbb{R}^d,\ t \geq 0. \tag{2.2}$$

By Duhamel's principle, the solution $\psi(t) := \psi(x,t)$ of (2.2)/(1.1) can be expressed in the integral form as

$$\psi(t) = \cos(\mathcal{D}_\varepsilon t)\psi(0) + \frac{\sin(\mathcal{D}_\varepsilon t)}{\mathcal{D}_\varepsilon}\partial_t\psi(0) + \frac{1}{\varepsilon^2\mathcal{D}_\varepsilon}\int_0^t \sin(\mathcal{D}_\varepsilon(t-s))f(\psi(s))ds. \tag{2.3}$$

Differentiating (2.3) with respect to t, we obtain

$$\partial_t\psi(t) = -\mathcal{D}_\varepsilon \sin(\mathcal{D}_\varepsilon t)\psi(0) + \cos(\mathcal{D}_\varepsilon t)\partial_t\psi(0) + \frac{1}{\varepsilon^2}\int_0^t \cos(\mathcal{D}_\varepsilon(t-s))f(\psi(s))ds. \tag{2.4}$$

Inspired by the linear terms in (2.3) and (2.4), it is natural to introduce the auxiliary variables (twisted variables) as

$$\psi_\pm(t) := \psi_\pm(x,t) = \frac{1}{2}\left(\psi(x,t) \pm i\mathcal{D}_\varepsilon^{-1}\partial_t\psi(x,t)\right), \tag{2.5}$$

and the following equivalent integral form of (1.1)/(2.2) for $\psi_\pm(t)$ can be written as

$$\psi_\pm(t) = e^{\mp i\mathcal{D}_\varepsilon t}\psi_\pm(0) \pm \frac{i}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^t e^{\mp i\mathcal{D}_\varepsilon(t-s)}f(\psi_+(s)+\psi_-(s))\,ds. \tag{2.6}$$

For given initial data of NLKG (1.1), (2.5) defines the initial value for the integral equations (2.6) as

$$\psi_\pm(0) = \frac{1}{2}\left(\psi_0 \pm i\mathcal{D}_\varepsilon^{-1}\psi_1\right), \tag{2.7}$$

and the solution $\psi(t)$ to KG (1.1) can be recovered from $\psi_\pm(t)$ as

$$\psi(t) = \psi_+(t) + \psi_-(t), \quad \partial_t\psi(t) = -i\mathcal{D}_\varepsilon\left(\psi_+(t) - \psi_-(t)\right). \tag{2.8}$$

From now on, it suffices to consider the integral equations (2.6) with (2.7). Choose time-step size $\tau = \Delta t > 0$ and denote time steps $t_n = n\tau$ $(n = 0, 1, 2, \dots)$. Let $\psi_\pm^n$ be the numerical approximations of $\psi_\pm(t_n)$. By Duhamel's principle, from

t_n to t_{n+1}, the solution $\psi_\pm(t_n+s) := \psi_\pm(x,t_n+s)$ $(s\in[0,\tau])$ of (2.6) can be represented as

(2.9)
$$\psi_\pm(t_n+s) = e^{\mp i\mathcal{D}_\varepsilon s}\psi_\pm(t_n) \pm \frac{i}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{\mp i\mathcal{D}_\varepsilon(s-w)} f(\psi_+(t_n+w)+\psi_-(t_n+w))dw.$$

From the theoretical results, we know $\psi_\pm(t)=O(1)$ and oscillations (w.r.t ε) are in time, i.e. $\|\psi_\pm(t)\|_{H^k}=O(1)$, $\|\partial_t^k\psi_\pm(t)\|_{H^k}=O(\varepsilon^{-2k})$ for sufficiently regular initial data. To construct uniformly accurate numerical schemes for solving (2.9), the key observation is that $e^{it\mathcal{D}_\varepsilon}$ is unitary in Hilbert space $H^k(\mathbb{R}^d)$ and the highly oscillatory phases can be separated by the decomposition (2.1) as

$$e^{i\mathcal{D}_\varepsilon t} = e^{it/\varepsilon^2}e^{it\mathcal{D}}. \tag{2.10}$$

Inspired by the works in [7, 9, 30], we can construct the following m-th order uniformly accurate method by applying nested Picard iterative idea to (2.9). From t_n to t_{n+1}, we follow the procedures below to update $\psi_\pm^{n+1}$ from $\psi_\pm^n$.

Step 1. In each time interval, i.e., from t_n to t_{n+1}, $n\geq 0$, starting from $\psi_\pm^n = \psi(t_n)$ (for simplicity of illustration), we construct the the numerical approximations $\psi_\pm^{n,k}(s)$ $(k\geq 1)$ of the exact solution $\psi_\pm(t_n+s)$ $(s\in[0,\tau])$. Choose

$$\psi_\pm^{n,0}(s) = e^{\mp i\mathcal{D}_\varepsilon s}\psi_\pm^n, \tag{2.11}$$

and $\psi_\pm^{n,0}(s)-\psi_\pm(t_n+s)=O(s)$.

Step 2. Calculate $\psi^{n,k}(s) := \psi^{n,k}(s,x)$ by the following nested Picard iteration:

(2.12)
$$\psi_\pm^{n,k}(s) = e^{\mp i\mathcal{D}_\varepsilon s}\psi_\pm^n \pm \frac{i}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{\mp i\mathcal{D}_\varepsilon(s-w)} f(\psi_+^{n,k-1}(w)+\psi_-^{n,k-1}(w)) + O(s^{k+1}),$$

and the error term $O(s^{k+1})$ allows suitable numerical approximation of the integral term to maintain the properties $\psi_\pm^{n,k}(s)-\psi_\pm(t_n+s)=O(s^{k+1})$.

Step 3. Update $\psi_\pm^{n+1}$ at the m-th iteration by $\psi_\pm^{n+1}(x)=\psi_\pm^{n,m}(\tau)=\psi_\pm^{n,m}(\tau,x)$. Then the local error of $\psi_\pm^{n+1}$ would be an $O(\tau^{m+1})$ and the global error of such scheme is $O(\tau^m)$ independent of ε.

To implement the above NPI methods in practice, we update $\psi_\pm^{n,k}$ based on lower order NPI as $\psi_\pm^{n,k}(s)=\psi_\pm^{n,k-1}(s)+\delta_\pm^k(s;\psi_+^n,\psi_-^n)$ $(k\geq 1)$, i.e.

$$\delta_\pm^{n,k}(s) := \delta_\pm^k(s;\psi_+^n,\psi_-^n) = \psi_\pm^{n,k}(s)-\psi_\pm^{n,k-1}(s), \quad k\geq 1,\ s\in[0,\tau],$$

where $\psi_\pm^{n,0}(s)=e^{\mp i\mathcal{D}_\varepsilon s}\psi_\pm^n$, and it is obvious that $\delta_\pm^{n,k}(s)=O(\tau^k)$. To be precise, we will update $\psi_\pm^{n,k}(s)$ by adding the $O(\tau^k)$ term $\delta_\pm^{n,k}(s)$ to the previous constructed $\psi_\pm^{n,k-1}(s)$, similar to Taylor expansion. Now, let's show the detailed construction of the uniform first-order and high-order NPI methods.

First order NPI: From (2.12), we have

$$\delta_\pm^{n,1}(s) = \pm\frac{i}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{\mp i\mathcal{D}_\varepsilon(s-w)} f(\psi_+^{n,0}(w)+\psi_-^{n,0}(w)) + O(s^2). \tag{2.13}$$

To make the minimal efforts, only zero-th order term (in s) in the integrand needs to be evaluated for the time integrals. Combining (2.10), $e^{\pm is\mathcal{D}_\varepsilon} = e^{\pm is/\varepsilon^2}(I+O(s\mathcal{D}))$

and, we get

$$\delta_{\pm}^{n,1}(s) = \pm\frac{i}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{\mp i(s-w)/\varepsilon^2} f(e^{-iw/\varepsilon^2}\psi_+^n + e^{iw/\varepsilon^2}\psi_-^n)\,dw. \tag{2.14}$$

The strategy is to approximate the non-oscillatory differential operator part $e^{is\mathcal{D}}$ by suitable polynomials and leave the oscillatory factor $e^{\mp iw/\varepsilon^2}$ exact, which will lead to an easily computable $\delta_{\pm}^{n,1}(s)$ $(s\in\mathbb{R})$:

$$\begin{aligned}
\delta_{\pm}^{n,1}(s) =& p_{-2}(\pm s)\mathcal{F}_{1,\pm}^n + p_0(\pm s)\mathcal{F}_{2,\pm}^n + p_2(\pm s)\mathcal{F}_{2,\mp}^n + p_4(\pm s)\mathcal{F}_{1,\mp}^n,\\
\mathcal{F}_{1,\pm}^n :=& \mathcal{F}_{1,\pm}(\psi_+^n,\psi_-^n) = \mathcal{A}(\overline{\psi_\mp^n}(\psi_\pm^n)^2),\\
\mathcal{F}_{2,\pm}^n :=& \mathcal{F}_{2,\pm}(\psi_+^n,\psi_-^n) = \mathcal{A}\left((2|\psi_\mp^n|^2+|\psi_\pm^n|^2)\psi_\pm^n\right),\ \mathcal{A} = i\frac{\lambda}{2\varepsilon^2}\mathcal{D}_\varepsilon^{-1},\\
p_0(s) =& e^{\frac{-is}{\varepsilon^2}}s,\ p_{\pm 2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{\pm 2iw}{\varepsilon^2}}dw,\ p_4(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{4iw}{\varepsilon^2}}dw.
\end{aligned} \tag{2.15}$$

We note that $\overline{p_k(s)} = -p_k(-s)$ $(k=0,\pm 2,4)$.

Higher order NPI: Assume now, we have computed $\delta_{\pm}^{n,m}(s)$ $(m=1,2,\cdots k-1$, $k\geq 2)$, to construct $\psi_{\pm}^{n,k}(s)$, we need only evaluate the integral

$$\psi_{\pm}^{n,k}(s) = \psi_{\pm}^{n,0}(s) \pm \frac{i}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{\mp i\mathcal{D}_\varepsilon(s-w)} f(\psi_+^{n,k-1}(w) + \psi_-^{n,k-1}(w))\,dw. \tag{2.16}$$

Using the strategy in the first order NPI case, one possible polynomial expansion for the integral kernel could be $e^{\pm is\mathcal{D}_\varepsilon} = e^{\pm is/\varepsilon^2}(I + \sum_{j=1}^{k-1}\frac{(\pm is\mathcal{D})^j}{j!}) + O((s\mathcal{D}))^k)$, but such expansion would yield regularity loss due to the $\mathcal{D}^j$ terms. Instead, we apply filters to $\mathcal{D}$ as $\frac{\sin(\mathcal{D}\tau)}{\tau} = \mathrm{sinc}(\tau\mathcal{D})\mathcal{D} = \mathcal{D} + O(\tau\mathcal{D})$ (sinc function is defined as $\mathrm{sinc}(s) = \frac{\sin s}{s}$ $(s\neq 0)$ and $\mathrm{sinc}(0)=1$). For $\mu = \sin(\tau\lambda)$, $\tau\lambda\in(-\pi/2,\pi/2)$, noticing

$$\tau\lambda = \arcsin(\mu) = \sum_{k=0}^{\infty}\frac{(2k)!}{2^{2k}(k!)^2}\frac{\mu^{2k+1}}{2k+1},\quad b_k = \frac{(2k)!}{2^{2k}(k!)^2}\frac{1}{2k+1},\quad k\geq 0, \tag{2.17}$$

we have the following expansion of $e^{\pm is\mathcal{D}}$ $(s\in[0,\tau])$ in terms of $\sin(\tau\mathcal{D})$

$$e^{\pm is\mathcal{D}_\varepsilon} = e^{\pm is/\varepsilon^2}\left(Id + \sum_{k=1}^{\infty} a_k^{\pm}(s)\left(\sin(\tau\mathcal{D})\right)^k\right), \tag{2.18}$$

where the coefficients $a_k^{\pm}(s)$ $(k=0,1,\cdots,\ a_0^{\pm}(s)=1)$ are polynomials of degree k given by

$$a_k^{\pm}(s) = \sum_{j=1}^{k}\frac{(\pm i)^j}{j!}\left(\frac{s}{\tau}\right)^j b_{kj},\quad b_{kj} = \begin{cases} 0, & k-j \text{ odd},\\ \sum\limits_{k_1+\cdots+k_j=\frac{k-j}{2}} b_{k_1}b_{k_2}\cdots b_{k_j}, & k-j \text{ even}.\end{cases} \tag{2.19}$$

The first three coefficients $a_k^{\pm}(s)$ $(k\geq 1)$ can be computed as

$$a_1^{\pm}(s) = \pm is/\tau,\quad a_2^{\pm}(s) = -\frac{1}{2\tau^2}s^2,\quad a_3^{\pm}(s) = \mp\frac{is^3}{6\tau^3}\pm\frac{is}{6\tau}. \tag{2.20}$$

On the other hand, we already have $\delta_{\pm}^{n,m}(s)$, which are the $O(\tau^m)$ terms of the integrals in (2.16). Therefore, we only need compute $\delta_{\pm}^{n,k}(s)$ as the $O(\tau^k)$ term in

the integral of (2.16) to get $\psi_\pm^{n,k}(s) = \psi_\pm^{n,k-1}(s) + \delta_\pm^{n,k}(s)$. Using expansions in (2.18) where the k-th term is of $O(\tau^k)$, we take the approximations

$$e^{\mp i\mathcal{D}_\varepsilon(s-w)} \approx e^{\mp i(s-w)/\varepsilon^2}\left(I + \sum_{j=1}^{k-1} a_j^{\mp}(s-w)\left(\sin(\tau\mathcal{D})\right)^j\right),$$

$$\psi_+^{n,k-1}(w) + \psi_-^{n,k-1}(w) \approx e^{-iw/\varepsilon^2}\psi_+^n + e^{iw/\varepsilon^2}\psi_-^n + \sum_{j=1}^{k-1}\sum_{\sigma=\pm}\left(\delta_\sigma^{n,j}(w) + e^{\frac{-\sigma iw}{\varepsilon^2}} a_j^{-\sigma}(w)(\sin(\tau\mathcal{D}))^j\psi_\sigma^n\right).$$

Denoting $\delta^{n,0}(w) := \delta^0(w;\psi_+^n,\psi_-^n) = \sum_{\sigma=\pm} e^{-\sigma iw/\varepsilon^2}\psi_\sigma^n$ and $\delta^{n,j}(w) := \delta^j(w;\psi_+^n,\psi_-^n)$ $(j \geq 1)$ as

$$\delta^{n,j}(w) = \sum_{\sigma=\pm}\left(\delta_\sigma^{n,j}(w) + e^{\frac{-\sigma iw}{\varepsilon^2}} a_j^{-\sigma}(w)(\sin(\tau\mathcal{D}))^j\psi_\sigma^n\right), \tag{2.21}$$

we can derive the $O(\tau^{k-1})$ term in the integrand and $\delta_\pm^{n,k}(s)$ can be constructed as $(f(\psi) = \lambda|\psi|^2\psi)$

$$\delta_\pm^{n,k}(s) = \pm\frac{i\lambda}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{\mp\frac{i(s-w)}{\varepsilon^2}}\sum_{j=0}^{k-1}\Bigg(a_j^{\mp}(s-w)\big(\sin(\tau\mathcal{D})\big)^j \sum_{(j_1,j_2,j_3)\in\mathcal{I}_j^k}\delta^{n,j_1}(w)\delta^{n,j_2}(w)\overline{\delta^{n,j_3}(w)}\Bigg)dw, \tag{2.22}$$

where the index set $\mathcal{I}_j^k = \left\{(j_1,j_2,j_3)\in\mathbb{Z}^3 | \sum_{l=1}^3 j_l = k-1-j, j_1,j_2,j_3 \geq 0,\right\}$ for $j = 0,\cdots,k-1$, and the time integral can be evaluated exactly. For k-th order NPI, $\psi_\pm^{n+1} := \psi_\pm^{n,k}(\tau)$ is then given by $\psi_\pm^{n+1} = \psi_\pm^{n,0}(\tau) + \delta_\pm^{n,1}(\tau) + \cdots \delta_\pm^{n,k}(\tau)$.

Remark 2.1. From the constructions of $\delta_\pm^{n,k}(s)$, it is easy to verify that $\delta_\pm^{n,k}$ has the form

$$\delta_\pm^{n,k}(s) = \sum_\alpha p_{m,\alpha}(s)\mathcal{F}_{m,\alpha}(\psi_+^n,\psi_-^n),\ \alpha = (\alpha_1,\ldots,\alpha_m) \text{ can be a multi-index,}$$

where $p_{k,\alpha}(s)$ are the scalar coefficients (integrals of the products of trigonometric polynomials and polynomials) and $\mathcal{F}_{m,\alpha}(\psi_+^n,\psi_-^n)$ only depends on the initial values $\psi_\pm^n$ on the interval $[t_n,t_{n+1}]$. Therefore, based on the proposed scheme, $\delta_\pm^{n,k}(s)$ can be computed exactly, i.e. the time integrals in (2.22) can be evaluated exactly.

Applying the above results, the **k-th order NPI method** can be proposed as follows. For $\psi_\pm^0 = \psi_\pm(0)$, the numerical approximations $\psi_\pm^{n+1}$ $(n \geq 0)$ are updated according to

$$\psi_\pm^{n+1} = e^{\mp i\mathcal{D}_\varepsilon\tau}\psi_\pm^n + \delta_\pm^{n,1}(\tau) + \cdots + \delta_\pm^{n,k}(\tau), \tag{2.23}$$

where $\delta_\pm^{n,m}(s) := \delta_\pm^m(s;\psi_+^n,\psi_-^n)$ $(s\in[0,\tau],\ m = 1,\cdots,k)$ are defined in (2.22) and (2.21). The numerical approximation ψ^n of the solution $\psi(x,t_n)$ to the original KG equation (1.1) is then recovered from (2.8) as $\psi^n = \psi_+^n + \psi_-^n$. The **first oder NPI** is constructed in (2.15) as $\psi_\pm^{n+1} = \psi_\pm^{n,1} := e^{\mp i\mathcal{D}_\varepsilon\tau}\psi_\pm^n + \delta_\pm^{n,1}(\tau)$.

The **second order NPI**, $\psi_\pm^{n+1} = \psi_\pm^{n,2} := e^{\mp i\mathcal{D}_\varepsilon \tau}\psi_\pm^n + \delta_\pm^{n,1}(\tau) + \delta_\pm^{n,2}(\tau)$, can be stated as below by specifying $\delta_\pm^{n,2}$, i.e. evaluating (2.22) for $k = 2$,

$$\begin{aligned}\delta_\pm^{n,2}(s) &= p_{-2,1}(\pm s)(\mathcal{G}_{1,\pm}^n \pm \mathcal{G}_{3,\pm}^n) + p_{0,1}(\pm s)(\mathcal{G}_{2,\pm}^n \pm \mathcal{G}_{4,\pm}^n) + p_{2,1}(\pm s)(\mathcal{G}_{2,\mp}^n \pm \mathcal{G}_{4,\mp}^n)\\ &\quad + p_{4,1}(\pm s)(\mathcal{G}_{1,\mp}^n \pm \mathcal{G}_{3,\mp}^n) + \sum_{k=1}^{6}\sum_{\sigma=\pm} q_{k,\sigma}(\pm s)\mathcal{F}_{2,k,\pm\sigma}^n \mp s p_{-2}(\pm s)\mathcal{B}\mathcal{F}_{1,\pm}^n\\ &\quad \mp s p_0(\pm s)\mathcal{B}\mathcal{F}_{2,\pm}^n \mp s p_2(\pm s)\mathcal{B}\mathcal{F}_{2,\mp}^n \mp s p_4(\pm s)\mathcal{B}\mathcal{F}_{1,\mp}^n,\end{aligned}$$

and we use the notation $\sigma_1\sigma_2 = +$ if $\sigma_1 = \sigma_2$ and $\sigma_1\sigma_2 = +$ if $\sigma_1 \neq \sigma_2$ ($\sigma_1, \sigma_2 = +, -$). The nonlinear terms are

$$\begin{aligned}
&\mathcal{G}_{1,\pm}^n = \mathcal{A}\mathcal{B}((\psi_\pm^n)^2\overline{\psi_\mp^n}), \quad \mathcal{G}_{2,\pm}^n = \mathcal{A}\mathcal{B}((2|\psi_\mp^n|^2 + |\psi_\pm^n|^2)\psi_\pm^n),\\
&\mathcal{G}_{3,\pm}^n = \pm\mathcal{A}\left((\psi_\pm^n)^2\overline{\mathcal{B}\psi_\mp^n} - 2(\mathcal{B}\psi_\pm^n)\psi_\pm^n\overline{\psi_\mp^n}\right), \quad \mathcal{B} = \frac{i}{\tau}\sin(\tau\mathcal{D}),\\
&\mathcal{G}_{4,\pm}^n = \pm\mathcal{A}(2\psi_\pm^n\overline{\psi_\mp^n}(\mathcal{B}\psi_\mp^n) - 2(|\psi_\pm^n|^2 + |\psi_\mp^n|^2)(\mathcal{B}\psi_\pm^n) - (\psi_\pm^n)^2\overline{\mathcal{B}\psi_\pm^n}\\
&\qquad\qquad + 2\psi_\pm^n\psi_\mp^n\overline{(\mathcal{B}\psi_\mp^n)}),\\
&\mathcal{F}_{2,m,\pm}^n = \mathcal{A}\left(2\psi_\mp^n\overline{\psi_\pm^n}\mathcal{F}_{m,\mp}^n - (\psi_\mp^n)^2\overline{\mathcal{F}_{m,\pm}^n}\right),\ m = 1,2,\\
&\mathcal{F}_{2,m+2,\pm}^n = \mathcal{A}\left(2(|\psi_+^n|^2 + |\psi_-^n|^2)\mathcal{F}_{m,\mp}^n - 2\psi_+^n\psi_-^n\overline{\mathcal{F}_{m,\pm}^n}\right),\ m = 1,2,\\
&\mathcal{F}_{2,m+4,\pm}^n = \mathcal{A}\left(2\psi_\pm^n\overline{\psi_\mp^n}\mathcal{F}_{m,\mp}^n - (\psi_\pm^n)^2\overline{\mathcal{F}_{m,\pm}^n}\right),\ m = 1,2,
\end{aligned} \tag{2.24}$$

with the coefficient functions given below

$$\begin{aligned}
&p_{0,1}(s) = e^{\frac{-is}{\varepsilon^2}}\frac{s^2}{2}, \quad p_{\pm2,1}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s we^{\frac{\pm2iw}{\varepsilon^2}}dw, \quad p_{4,1}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s we^{\frac{4iw}{\varepsilon^2}}dw,\\
&q_{1+k,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}}e^{\frac{\pm(2-k)iw}{\varepsilon^2}}(p_{-2}(\mp w) + p_4(\pm w))\,dw, \quad k = 0,2,4,\\
&q_{2+k,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}}e^{\frac{\pm(2-k)iw}{\varepsilon^2}}(p_2(\pm w) + p_0(\mp w))\,dw, \quad k = 0,2,4.
\end{aligned}$$

Recalling the definitions of $\mathcal{A}$ in (2.15) and $\mathcal{B}$ in the equation above, we know these operators are uniformly bounded w.r.t ε. The third order NPI method is described in Appendix.(the codes can be found at `https://github.com/xuanxuanzhou/NPI-method-matlab-code-for-KG`)

Remark 2.2. Though we present the NPI for KG equation (1.1) on the whole space, the discussion also works for the rectangular domain case under the periodic boundary conditions or homogeneous Dirichlet/Neumann boundary conditions. When spatial domain and boundary conditions change, one only need to properly treat the domain of the operator $\mathcal{D}_\varepsilon$.

3. Uniform error analysis for the semi-discrete-in-time NPI

Here, we shall rigorously establish error estimates of the NPI scheme (2.23) in the semi-discrete-in-time form. Let $0 < T < T^*$ with T^* being the uniform maximum existence time of the solution $\psi(x,t)$ to the KG equation (1.1) for $\varepsilon \in (0,1]$. Motivated by the results in [9,31], we assume for some positive integer $j > 0$,

$$(A): \psi_0(x), \psi_1(x) \in H^j(\mathbb{R}^d), \quad \sup_{\varepsilon\in(0,1]} \|\psi(x,t)\|_{L^\infty([0,T];H^j(\mathbb{R}^d))} \leq C_j,$$

For $\alpha > \frac{d}{2}$, under the above assumption (A) with $j \geq \alpha$, we have

$$M_0 = \sup_{\varepsilon\in(0,1]} \|\psi(x,t)\|_{L^\infty([0,T];H^\alpha(\mathbb{R}^d))} < \infty. \tag{3.1}$$

Recalling the auxiliary (twisted) variables $\psi_\pm(x,t)$ (2.5), under assumption (A), we have $\psi_\pm(x,t) = \frac{1}{2}(\psi(x,t) \pm i\mathcal{D}_\varepsilon^{-1}\partial_t\psi(x,t))$ satisfy (2.6) and $\psi_\pm(x,0) \in H^j(\mathbb{R}^d)$, which implies

$$\sup_{\varepsilon\in(0,1]} \|\psi_\pm(x,t)\|_{L^\infty([0,T];H^j(\mathbb{R}^d))} \lesssim 1, \quad M_1 = \sup_{\varepsilon\in(0,1]} \|\psi_\pm(x,t)\|_{L^\infty([0,T];H^\alpha(\mathbb{R}^d))} < \infty. \tag{3.2}$$

Let $\psi_\pm^n(x)$ and $\psi^n(x)$ $(n \geq 0)$ be the numerical approximations of $\psi_\pm(x,t_n)$ and $\psi(x,t_n)$ obtained by k-th order NPI ($\psi_\pm^0 = \psi_\pm(x,t_0)$), respectively. The following error estimates hold.

Theorem 3.1. *Under assumptions (A) with $j = 2k+\alpha$ ($\alpha > \frac{d}{2}$), there exists $\tau_0 \geq 0$ which is sufficiently small, when $0 \leq \tau \leq \tau_0$, the NPI scheme* (2.23) *satisfies the following optimal error estimates:*

$$\|\psi_\pm(x,t_n) - \psi_\pm^n(x)\|_{H^\alpha} \lesssim \tau^k, \quad \|\psi_\pm^n(\cdot)\|_{H^\alpha} \leq M_1 + 1,\ 0 \leq n \leq \frac{T}{\tau}, \tag{3.3}$$

and $\|\psi(x,t_n) - \psi^n(x)\|_{H^\alpha} \lesssim \tau^k$ ($0 \leq n \leq \frac{T}{\tau} - 1$).

Recalling the definitions of $\delta_\pm^{n,m}(s) := \delta_\pm^m(s;\psi_+^n,\psi_-^n)$ $(s \in [0,\tau],\ m = 0,1,\cdots,k)$ in (2.22) and (2.21) and replacing $\psi_\pm^n$ by $\psi_\pm(t_n)$, we define the local error function $\xi_\pm^n(x)$ for k-th order NPI at t_n $(n \geq)$ as

$$\xi_\pm^n(x) = \psi_\pm(x,t_{n+1}) - \left(e^{\mp i\mathcal{D}_\varepsilon\tau}\psi_\pm(x,t_n) + \sum_{j=1}^{k} \delta_\pm^j(\tau;\psi_+(t_n),\psi_-(t_n)) \right). \tag{3.4}$$

The following lemma regarding the local error is important.

Lemma 3.2. *Under assumption (A) with $j = 2k+\alpha$ ($\alpha > \frac{d}{2}$), we have the local error bounds for* (3.4) *as*

$$\|\xi_\pm^n(\cdot)\|_{H^\alpha} \lesssim \tau^{k+1}, \quad 0 \leq n \leq \frac{T}{\tau} - 1. \tag{3.5}$$

Proof. The local error bounds could be directly verified from the construction of NPI (2.23) and we omit the details here for brevity. Noticing that we use $\sin(\tau\mathcal{D})$ instead of $\mathcal{D}$ in the expansion (2.18), by expanding $\sin(\tau\mathcal{D})$ into the series of $\mathcal{D}$ (understood in the phase space), we would recover the usual Taylor expansion of $e^{\pm is\mathcal{D}}$. For k-th NPI, the next order residue in the expansion is $O(\mathcal{D}^k)$, which leads to the local error bounds with assumed regularity in view of the fact that $\mathcal{D} : H^s(\mathbb{R}^d) \to H^{s-2}(\mathbb{R}^d)$ is uniformly bounded w.r.t. ε. □

To control the nonlinearity, for the iterations in NPI (2.23), we have the following estimates regarding $\delta_\pm^m(s;\phi_+,\phi_-)$ (2.22) and $\delta^m(s;\phi_+,\phi_-)$ (2.21) for $\phi_\pm(x) \in H^\alpha(\mathbb{R}^d)$.

Lemma 3.3. *Assuming $\|\phi_\pm(\cdot)\|_{H^\alpha} \leq M_1 + 1$ and $\tau < 1$, there exists a positive constant C_{M_1} only depending on M_1, k, α and λ such that*

$$\|\delta_\pm^m(s;\phi_+,\phi_-)\|_{H^\alpha} \leq C_{M_1}, s \in [0,\tau], m = 0,1,\ldots,k. \tag{3.6}$$

In addition, for $\|\varphi_\pm(\cdot)\|_{H^\alpha} \le M_1 + 1$, *we have the (local) Lipschitz properties for* $m = 1, \ldots, k$,

$$\|\delta_\pm^m(s;\phi_+,\phi_-) - \delta_\pm^m(s;\varphi_+,\varphi_-)\|_{H^\alpha} \le \tau L_{M_1} \sum_{\sigma=\pm} \|\phi_\sigma - \varphi_\sigma\|_{H^\alpha}, s \in [0,\tau], \tag{3.7}$$

where $L_{M_1} > 0$ *only depends on* M_1, k, α *and* λ.

Proof. Noticing $\sin(\tau\mathcal{D}) : H^\alpha \to H^\alpha$ and $\varepsilon^{-2}\mathcal{D}_\varepsilon^{-1} : H^\alpha \to H^\alpha$ are bounded (1 is an upper bound), recalling the fact that $H^\alpha(\mathbb{R}^d)$ $(\alpha > d/2)$ is an algebra, we obtain from (2.21) and (2.22) that $\|\delta^0(s;\phi_+,\phi_-)\|_{H^\alpha} \le 2(M_1+1)$ $(s \in [0,\tau])$,

$$\|\delta_\pm^1(s;\phi_+,\phi_-)\| \le \frac{|\lambda| C_\alpha \tau}{2} \|\delta^0(\cdot;\phi_+,\phi_-)\|^3_{L^\infty([0,\tau];H^\alpha)} \le 4C_\alpha|\lambda|\tau(M_1+1)^3,$$

where C_α is a constant depending on d and α for the inequality $\|\phi_1\phi_2\phi_3\|_{H^\alpha} \le C_\alpha\|\phi_1\|_{H^\alpha}\|\phi_2\|_{H^\alpha}\|\phi_3\|_{H^\alpha}$. Continuing the above estimates for $m = 2, \cdots, k$ from (2.21) and (2.22), it is easy to derive (3.6). In particular, the upper bounds in (3.6) for $\delta_\pm^m(s;\cdot,\cdot)$ $(m = 1, \cdots, k)$ is proportional to τ and can be made arbitrary small by choosing small enough τ.

For the (local) Lipschitz property, we could similarly obtain

$$\|\delta^0(s;\phi_+,\phi_-) - \delta^0(s;\varphi_+,\varphi_-)\|_{H^\alpha} \le \sum_{\sigma=\pm} \|\phi_\sigma - \varphi_\sigma\|_{H^\alpha}, \quad s \in [0,\tau],$$

and (2.22) would yield for $\delta_\pm^1(s;\cdot,\cdot)$

$$\begin{aligned}
&\|\delta_\pm^1(s;\phi_+,\phi_-) - \delta_\pm^1(s;\varphi_+,\varphi_-)\|_{H^\alpha} \\
&\le |\lambda|\tau C_\alpha \|\delta^0(\cdot;\phi_+,\phi_-) - \delta^0(\cdot;\varphi_+,\varphi_-)\|_{L^\infty([0,\tau];H^\alpha)} \\
&\quad \times \Big(\|\delta^0(\cdot;\phi_+,\phi_-)\|^2_{L^\infty([0,\tau];H^\alpha)} + \|\delta^0(\cdot;\varphi_+,\varphi_-)\|^2_{L^\infty([0,\tau];H^\alpha)} \Big) \\
&\le 2|\lambda| C_\alpha \tau (M_1+1)^2 \sum_{\sigma=\pm} \|\phi_\sigma - \varphi_\sigma\|_{H^\alpha},
\end{aligned}$$

i.e. (3.7) holds for $m = 1$. The cases with $m = 2, \cdots, k$ can be verified in the same way using (2.22) and the established stability results for $0, 1, \cdots, m-1$. The detail is omitted here. □

We are now ready to prove Theorem 3.1.

Proof of Theorem 3.1. Introducing the error functions $e_\pm^n(x)$ for $n \ge 0$ as

$$e_\pm^n(x) = \psi_\pm(x,t_n) - \psi_\pm^n(x), \tag{3.8}$$

then subtracting (2.23) from (3.4), we have the error equation for $n \ge 0$ as

$$e_\pm^{n+1}(x) = e^{\mp i\mathcal{D}_\varepsilon\tau} e_\pm^n(x) + \sum_{m=1}^{k} \big(\delta_\pm^m(\tau;\psi_+(t_n),\psi_-(t_n)) - \delta_\pm^m(\tau;\psi_+^n,\psi_-^n)\big) + \xi_\pm^n(x). \tag{3.9}$$

We will prove (3.3) in Theorem 3.1 by induction. For $n = 0$, it is clear $e_\pm^0 = 0$ and the estimates in (3.3) hold for $n = 0$.

Assume the estimates in (3.3) hold for $n = 0, \cdots, N \le \frac{T}{\tau} - 1$, we are going to prove the case $n = N+1$ is also true in (3.3). By induction hypothesis, from Lemma 3.3, recalling the error equation (3.9), we have

$$\|e_\pm^{n+1}(\cdot)\|_{H^\alpha} \le \|e_\pm^n(\cdot)\|_{H^\alpha} + \tau L_{M_1} \sum_{m=1}^{k} \sum_{\sigma=\pm} \|\psi_\sigma(x,t_n) - \psi_\sigma^n(x)\|_{H^\alpha} + \|\xi_\pm^n(x)\|_{H^\alpha}$$

$$\leq \|e_{\pm}^n(\cdot)\|_{H^\alpha} + \tau k L_{M_1} \sum_{\sigma=\pm} \|e_\sigma^n(x)\|_{H^\alpha} + \|\xi_\pm^n(x)\|_{H^\alpha}, \quad n = 0, \cdots, N.$$

Denoting $S^n = \|e_+^n(x)\|_{H^\alpha} + \|e_-^n(x)\|_{H^\alpha}$, we have for $n = 0, \cdots, N$

$$S^{n+1} \leq S^n + \tau k L_{M_1} S^n + \|\xi_+^n(x)\|_{H^\alpha} + \|\xi_-^n(x)\|_{H^\alpha}, \tag{3.10}$$

and

$$S^{n+1} \leq \tau k L_{M_1} \sum_{m=0}^{n} S^m + \sum_{m=0}^{n} \left(\|\xi_+^m(x)\|_{H^\alpha} + \|\xi_-^m(x)\|_{H^\alpha} \right). \tag{3.11}$$

Using local truncation error estimates in Lemma 3.2 and discrete Gronwall inequality, we derive for some constant C independent of ε (depending on k, τ, L_{M_1}, T and the constants in the local error (3.4)) that

$$S^{n+1} \leq Cn\tau^{k+1} \leq CT\tau^k, \quad n = 0, 1, \cdots, N. \tag{3.12}$$

Thus $\|e_\pm^{N+1}(x)\|_{H^\alpha} \leq CT\tau^k$ and for $\tau < \frac{1}{(CT)^{1/k}}$, we know

$$\|\psi_\pm^{N+1}\|_{H^\alpha} \leq \|\psi_\pm(x, t_{N+1})\|_{H^\alpha} + \|e_\pm^{N+1}(x)\|_{H^\alpha} \leq M_1 + 1, \tag{3.13}$$

which verifies (3.3) for $n = N+1$. The induction process is complete and the results in Theorem 3.1 follow. □

4. Practical implementation and Fourier pseudospectral discretization

In practice, the KG equation (1.1) is usually truncated onto a large enough bounded computational domain, e.g. an interval in 1D, a rectangle in 2D or a box in 3D, with periodic boundary conditions (or homogeneous Dirchlet boundary conditions), such that the truncation error is negligible. Here, we take 1D ($d = 1$) for example. The KG equation (1.1) is truncated on a bounded interval $[a, b]$ with periodic boundary conditions:

$$\begin{aligned} &\varepsilon^2 \partial_{tt}\psi(x,t) - \Delta\psi(x,t) + \frac{1}{\varepsilon^2}\psi(x,t) = f(\psi), \ x \in [a,b], t > 0, \\ &\psi(a,t) = \psi(b,t), \quad \partial_x\psi(a,t) = \partial_x\psi(b,t), \quad t > 0 \\ &\psi(x,0) = \psi_0(x), \ \partial_t\psi(x,0) = \frac{1}{\varepsilon^2}\psi_1(x), \quad x \in [a,b]. \end{aligned} \tag{4.1}$$

As mentioned in Remark (2.2), the NPI (2.23) is directly applicable and the similar estimates in Theorem 3.1 hold. The choices of periodic truncation make the differential operators $\mathcal{D}_\varepsilon$ and $e^{\pm it\mathcal{D}_\varepsilon}$ easily and efficiently computable in phase space via Fast Fourier Transform in practice, which is crucial for efficient implementation of the NPI methods.

Below, we describe the fully discretized NPI for solving (4.1). It can be viewed by applying the Fourier spectral approximation to the time-discrete NPI schemes (2.23). In addition to the temporal discretization with time steps as $t_n = n\tau$ ($n = 0, 1, \ldots$), the interval $[a, b]$ is divided into M (even number) uniform subintervals with mesh size $h = (b-a)/M$ and grids points $x_j = a + jh$ ($j = 0, \ldots, M$). Let ψ_j^n, and $\dot{\psi}_j^n (j = 0, \ldots, M, \ n = 0, 1, \ldots)$ be the approximations to $\psi(x_j, t_n)$ and $\partial_t\psi(x_j, t_n)$, respectively. Denote the solution vector $\psi^n = (\psi_0^n, \psi_1^n, \cdots, \psi_M^n)^T$

($\psi_0^n = \psi_M^n$) and $\psi^n(x) = I_M(\psi^n)$ being the standard Fourier interpolation ($\psi^n(x_j) = \psi_j^n$)as

$$\psi^n(x) = \sum_{l=-M/2}^{M/2-1} \widetilde{\psi}_l^n e^{i\mu_l(x-a)}, \quad \widetilde{\psi}_l^n = \frac{1}{M}\sum_{j=0}^{M-1} \psi_j^n e^{-i\mu_l(x_j-a)}, \quad \mu_l = \frac{2\pi l}{b-a}, \tag{4.2}$$

where $\tilde{\psi}_l^n$ ($l = -M/2, \ldots, M/2-1$) are the discrete Fourier transform coefficients of the vector ψ^n.

Choose $\psi_j^0 = \psi_0(x_j)$, $\dot{\psi}_j^0 = \psi_1(x_j)/\varepsilon^2$, and let $\psi_\pm^0(x) = I_M(\psi_\pm^0)$ be given as

$$\psi_\pm^0(x) = \sum_{l=-\frac{M}{2}}^{\frac{M}{2}-1} \widetilde{\psi}_{\pm,l}^0 e^{i\mu_l(x-a)}, \quad \psi_{\pm,l}^0 = \frac{1}{2}\left(\widetilde{\psi}_l^0 \pm i\mathcal{D}_{\varepsilon,l}^{-1}\widetilde{\dot{\psi}_l^0}\right), \quad -\frac{M}{2} \le l \le \frac{M}{2}-1,$$

where $\mathcal{D}_{\varepsilon,l} = \sqrt{\frac{1+\varepsilon^2\mu_l^2}{\varepsilon^4}}$. The practical second-order NPI Fourier pseudospectral scheme updates $\psi_j^{n+1} = \sum_{l=-M/2}^{M/2-1} \widetilde{\psi}_l^{n+1} e^{i\mu_l(x_j-a)}$, $j = 0, 1, \ldots, M$, for $n \ge 0$ as

$$\widetilde{\psi}_l^{n+1} = \widetilde{\psi}_{+,l}^{n+1} + \widetilde{\psi}_{-,l}^{n+1}, \quad \widetilde{\psi}_{\pm,l}^{n+1} = e^{\mp i\mathcal{D}_{\varepsilon,l}\tau}\widetilde{\psi}_{\pm,l}^n + \widetilde{\delta}_{\pm,l}^{n,1} + \widetilde{\delta}_{\pm,l}^{n,2},$$

where for $-\frac{M}{2} \le l \le \frac{M}{2}-1$ and $\tilde{B}_l = \frac{i}{\tau}\sin(\tau(\frac{\sqrt{1+\varepsilon^2\mu_l^2}-1}{\varepsilon^2}))$,

$$\begin{aligned}
\tilde{\delta}_{\pm,l}^{n,1} &= p_{-2}(\pm\tau)\tilde{\mathcal{F}}_{1,\pm,l}^n + p_0(\pm\tau)\tilde{\mathcal{F}}_{2,\pm,l}^n + p_2(\pm\tau)\tilde{\mathcal{F}}_{2,\mp,l}^n + p_4(\pm\tau)\tilde{\mathcal{F}}_{1,\mp,l}^n,\\
\tilde{\delta}_{\pm,l}^{n,2} &= p_{-2,1}(\pm\tau)(\tilde{\mathcal{G}}_{1,\pm,l}^n \pm \tilde{\mathcal{G}}_{3,\pm,l}^n) + p_{0,1}(\pm\tau)(\tilde{\mathcal{G}}_{2,\pm,l}^n \pm \tilde{\mathcal{G}}_{4,\pm,l}^n)\\
&\quad + p_{2,1}(\pm\tau)(\tilde{\mathcal{G}}_{2,\mp,l}^n \pm \tilde{\mathcal{G}}_{4,\mp,l}^n) + p_{4,1}(\pm\tau)(\tilde{\mathcal{G}}_{1,\mp,l}^n \pm \tilde{\mathcal{G}}_{3,\mp,l}^n)\\
&\quad \mp \tau p_{-2}(\pm\tau)\tilde{\mathcal{B}}_l\tilde{\mathcal{F}}_{1,\pm,l}^n \mp \tau p_0(\pm\tau)\tilde{\mathcal{B}}_l\tilde{\mathcal{F}}_{2,\pm,l}^n \mp \tau p_2(\pm\tau)\tilde{\mathcal{B}}_l\tilde{\mathcal{F}}_{2,\mp,l}^n\\
&\quad \mp \tau p_4(\pm\tau)\tilde{\mathcal{B}}_l\tilde{\mathcal{F}}_{1,\mp,l}^n + \sum_{k=1}^{6}\sum_{\sigma=\pm} q_{k,\sigma}(\pm\tau)\tilde{\mathcal{F}}_{2,k,\pm\sigma,l}^n.
\end{aligned}$$

In the above equalities, the nonlinear $\mathcal{F}$ and $\mathcal{G}$ terms are given in (2.24) and understood as vectors, e.g. $\mathcal{G}_{1,\pm}^n = (\mathcal{G}_{1,\pm,0}^n, \mathcal{G}_{1,\pm,1}^n, \ldots, \mathcal{G}_{1,\pm,M}^n)^T$ ($\mathcal{G}_{1,\pm,0}^n = \mathcal{G}_{1,\pm,M}^n$) and $I_M(\mathcal{G}_{1,\pm}^n)(x) = \mathcal{A}\mathcal{B}I_M((\psi_\pm^n)^2\overline{\psi_\pm^n})(x)$. We remark that the Fourier multiplier of the operator $\mathcal{A}$ at l-th Fourier mode is $\mathcal{A}_l = i\frac{\lambda}{2\sqrt{1+\varepsilon^2\mu_l^2}}$.

5. Application to a real-valued quadratic NLKG

The aforementioned NPI constructions are valid for NLKG (1.1) with general polynomial type nonlinearities. Moreover, if the scalar field in NLKG (1.1) is real, i.e. $\psi(x,t) \in \mathbb{R}$ and the initial data $\psi_0, \psi_1 \in \mathbb{R}$, the computations will be simplified since $\psi_+(x,t) = \overline{\psi_-(x,t)}$ in (2.5). Here, we show the application of our general NPI strategy applied to a real-valued quadratic NLKG:

$$\begin{aligned}
&\varepsilon^2\partial_{tt}\psi(x,t) - \Delta\psi(x,t) + \frac{1}{\varepsilon^2}\psi(x,t) = f(\psi), \qquad x \in \mathbb{R}^d, t > 0,\\
&\psi(x,0) = \psi_0(x) \in \mathbb{R}, \quad \partial_t\psi(x,0) = \frac{1}{\varepsilon^2}\psi_1(x) \in \mathbb{R}, \qquad x \in \mathbb{R}^d,
\end{aligned} \tag{5.1}$$

where $\psi(x,t) \in \mathbb{R}$ is a real scalar field and the nonlinear term is $f(\psi) = \lambda\psi^2$. It has been shown that NLKG (5.1) converges to the linear Schrödinger system in the limit $\varepsilon \to 0^+$ [27], which is different from the cubic nonlinearity case. We will

construct NPI methods for (5.1) and study the corresponding nonrelativistic limit $\varepsilon \to 0^+$ numerically.

As a consequence of the real-valued scalar field $\psi(x,t)$, a k-th otder NPI (2.23) would be formulated as $\psi^n = \psi_+^n + \psi_-^n = 2\mathrm{Re}(\psi_+^n)$ with $\psi_+^n = \overline{\psi_-^n}$ and $\delta_+^{n,k}(\cdot) = \overline{\delta_-^{n,k}(\cdot)}$,

$$\psi_+^{n+1} = e^{-i\mathcal{D}_\varepsilon \tau}\psi_+^n + \delta_+^{n,1}(\tau) + \cdots + \delta_+^{n,k}(\tau). \tag{5.2}$$

Adopting the same notations as those in Section 2, we shall construct the NPI methods up to third oder in time for the NLKG (5.1), and only $\delta_+^{n,1}(\tau), \delta_+^{n,2}(\tau)$ and $\delta_+^{n,3}(\tau)$ are needed. By direct computation, we find

$$\delta_+^{n,k}(s) = \frac{i\lambda}{2\varepsilon^2\mathcal{D}_\varepsilon}\int_0^s e^{-\frac{i(s-w)}{\varepsilon^2}}\sum_{j=0}^{k-1} a_j^-(s-w)\left(\sin(\tau\mathcal{D})\right)^j \sum_{(j_1,j_2)\in\mathcal{I}_j^k}\delta^{n,j_1}(w)\delta^{n,j_2}(w)dw,$$

$$\delta^{n,0}(w) = 2\mathrm{Re}\left(e^{-iw/\varepsilon^2}\psi_+^n\right), \quad \delta^{n,j}(w) = 2\mathrm{Re}\left(\delta_+^{n,j}(w) + e^{\frac{-iw}{\varepsilon^2}}a_j^-(w)(\sin(\tau\mathcal{D}))^j\psi_+^n\right),$$

where the index set $\mathcal{I}_j^k = \left\{(j_1,j_2)\in\mathbb{Z}^2 | j_1\geq 0, j_2\geq 0, j_1+j_2 = k-1-j\right\}$.

In detail, for the first order term $\delta_+^{n,1}(s)$ $(s\in[0,\tau])$, we have

$$\delta_+^{n,1}(s) = p_1(s)\mathcal{F}_1^n + p_2(s)\mathcal{F}_2^n + p_3(s)\mathcal{F}_3^n, \tag{5.3}$$

with

$$\mathcal{F}_1^n = \mathcal{A}(\overline{\psi_+^n})^2,\ \mathcal{F}_2^n = 2\mathcal{A}|\psi_+^n|^2,\ \mathcal{F}_3^n = \mathcal{A}(\psi_+^n)^2,$$
$$p_1(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{3iw}{\varepsilon^2}}\,dw,\ p_2(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{iw}{\varepsilon^2}}\,dw,\ p_3(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{-iw}{\varepsilon^2}}\,dw.$$

For the second order term $\delta_+^{n,2}(s)$ $(s\in[0,\tau])$, we obtain

$$\begin{aligned}\delta_+^{n,2}(s) = &\sum_{k=1}^3\left[p_{k,1}(s)\mathcal{F}_{k,1}^n + (p_{k,1}(s) - sp_k(s))\mathcal{B}\mathcal{F}_k^n\right]\\ &+\sum_{k=1}^6[q_{2,k}(s)\mathcal{A}\mathcal{E}_{2,k}^n + q_{0,k}(s)\mathcal{A}\overline{\mathcal{E}_{2,k}^n}],\end{aligned}$$

where the new coefficients and the nonlinear terms are given by

$$\mathcal{F}_{1,1}^n = 2\mathcal{A}(\overline{\psi_+^n}(\mathcal{B}\overline{\psi_+^n})),\quad \mathcal{F}_{2,1}^n = 2\mathcal{A}(\overline{\psi_+^n}(\overline{\mathcal{B}}\psi_+^n) + \psi_+^n(\mathcal{B}\overline{\psi_+^n})),\ \mathcal{F}_{3,1}^n = 2\mathcal{A}(\psi_+^n(\overline{\mathcal{B}}\psi_+^n)),$$
$$\mathcal{E}_{2,k}^n = 2\overline{\psi_+^n}\mathcal{F}_k^n,\ \mathcal{E}_{2,k+3}^n = 2\overline{\psi_+^n\mathcal{F}_k^n},\ p_{k,1}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{(5-2k)iw}{\varepsilon^2}}w\,dw,\ k=1,2,3,$$
$$q_{0,k+3}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s p_k(w)\,dw,\ q_{0,k}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s \overline{p_k(w)}\,dw,\ k=1,2,3,$$
$$q_{2,k}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{2iw}{\varepsilon^2}}p_k(w)\,dw,\ q_{2,k+3}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{2iw}{\varepsilon^2}}\overline{p_k(w)}\,dw,\ k=1,2,3.$$

The third order term $\delta_+^{n,3}(s)$ $(s\in[0,\tau])$ is more complicated and can be explicitly expressed as

$$\delta_+^{n,3}(s) = \sum_{k=1}^3\left[\frac{1}{2}(p_k(s)s^2 + p_{k,2}(s) - 2sp_{k,1}(s))\mathcal{B}^2\mathcal{F}_k^n - p_{k,1}(s)s\mathcal{F}_{k,1}^n\right]$$

$$
\begin{aligned}
&- \sum_{k=1}^{6} \Big[(s q_{2,k}(s) + q_{2,k,1}(s)) \mathcal{A}\mathcal{B}\mathcal{E}_{2,k}^n + (s q_{0,k}(s) + q_{0,k,1}(s)) \mathcal{A}\mathcal{B}\overline{\mathcal{E}_{2,k}^n} \Big] \\
&+ \sum_{k=1}^{3} p_{k,2}(s)(\mathcal{B}\mathcal{F}_{k,1}^n + \mathcal{F}_{k,2}^n + \mathcal{F}_{k,3}^n) + \sum_{k=1}^{6} \Big[q_{2,k,1}(s) \mathcal{A}\mathcal{E}_{3,k}^n + q_{0,k,1}(s) \mathcal{A}\overline{\mathcal{E}_{3,k}^n} \Big] \\
&+ \sum_{k=1}^{12} \Big[m_{2,k}(s) \mathcal{A}\mathcal{H}_{2,k}^n + m_{0,k}(s) \mathcal{A}\overline{\mathcal{H}_{2,k}^n} + r_{2,k}(s) \mathcal{G}_{2,k}^n + r_{0,k} \overline{\mathcal{G}_{2,k}^n} \Big] \\
&+ \sum_{k,l=1}^{3} \mathcal{A} \Big[r_{k,l}(s) \mathcal{G}_{k,l}^n + r_{k+3,l}(s) \mathcal{G}_{k+3,l+3}^n + r_{k,l+3}(s) \overline{\mathcal{G}_{k+3,l+3}^n} + r_{k+3,l+3}(s) \overline{\mathcal{G}_{k,l}^n} \Big],
\end{aligned}
$$

where the nonlinear terms are given by

$$
\begin{aligned}
&\mathcal{F}_{1,2}^n = \mathcal{A}(\mathcal{B}\overline{\psi_+^n})^2, \quad \mathcal{F}_{2,2}^n = 2\mathcal{A}|\mathcal{B}\overline{\psi_+^n}|^2, \quad \mathcal{F}_{3,2}^n = \mathcal{A}(\overline{\mathcal{B}}\psi_+^n)^2, \\
&\mathcal{F}_{1,3}^n = \mathcal{A}(\overline{\psi_+^n}(\mathcal{B}^2\overline{\psi_+^n})),\ \mathcal{F}_{3,3}^n = \mathcal{A}(\psi_+^n(\mathcal{B}^2\psi_+^n)),\ \mathcal{F}_{2,3}^n = \mathcal{A}(\overline{\psi_+^n}(\mathcal{B}^2\psi_+^n) + \psi_+^n(\mathcal{B}^2\overline{\psi_+^n})), \\
&\mathcal{E}_{3,k}^n = 2(\mathcal{B}\overline{\psi_+^n})\mathcal{F}_k^n,\ \mathcal{E}_{3,3+k}^n = 2(\mathcal{B}\overline{\psi_+^n})\overline{\mathcal{F}_k^n},\ \mathcal{H}_{2,k}^n = 2\overline{\psi_+^n}\mathcal{F}_{k,1}^n,\ k = 1,2,3, \\
&\mathcal{H}_{2,k+6}^n = 2\overline{\psi_+^n}(\mathcal{B}\mathcal{F}_k^n),\ \mathcal{H}_{2,3+k}^n = 2\overline{\psi_+^n}\,\overline{\mathcal{F}_{k,1}^n},\ \mathcal{H}_{2,k+9}^n = 2\overline{\psi_+^n}(\overline{\mathcal{B}\mathcal{F}_k^n}),\ k = 1,2,3, \\
&\mathcal{G}_{2,k}^n = 2\overline{\psi_+^n}(\mathcal{A}\mathcal{E}_{2,k}^n),\ \mathcal{G}_{2,3+k}^n = 2\overline{\psi_+^n}(\overline{\mathcal{A}\mathcal{E}_{2,k}^n}),\ \mathcal{G}_{2,k+6}^n = 2\overline{\psi_+^n}(\mathcal{A}\mathcal{E}_{2,k+3}^n),\ k = 1,2,3, \\
&\mathcal{G}_{2,k+9}^n = 2\overline{\psi_+^n}(\overline{\mathcal{A}\mathcal{E}_{2,k+3}^n}),\ \mathcal{G}_{k,l}^n = \mathcal{F}_k^n\mathcal{F}_l^n,\ \mathcal{G}_{k+3,l+3}^n = \overline{\mathcal{F}_k^n}\mathcal{F}_l^n,\ k,l = 1,2,3,
\end{aligned}
$$

and the coefficients for $k, l = 1, 2, 3$ are described below

$$
\begin{aligned}
&q_{2,k,1}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} p_k(w) w\, dw,\ q_{2,k+3,1}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} \overline{p_k(w)} w\, dw, \\
&q_{0,k+3,1}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s p_k(w) w\, dw,\ q_{0,k,1}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s \overline{p_k(w)} w\, dw, \\
&r_{k,l}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} p_k(w) p_l(w)\, dw,\ r_{k+3,l}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} \overline{p_k(w)} p_l(w)\, dw, \\
&r_{k,l+3}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} p_k(w) \overline{p_l(w)}\, dw,\ r_{k+3,l+3}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} \overline{p_k(w) p_l(w)}\, dw, \\
&m_{2,k}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} p_{k,1}(w)\, dw, \quad m_{2,k+3}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} \overline{p_{k,1}(w)}\, dw, \\
&m_{0,k+3}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s p_{k,1}(w)\, dw, \quad m_{0,k}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s \overline{p_{k,1}(w)}\, dw, \\
&m_{2,k+6}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} g_{k,1}(w)\, dw,\ m_{2,k+9}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} \overline{g_{k,1}(w)}\, dw, \\
&m_{0,k+9}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s g_{k,1}(w)\, dw,\ m_{0,k+6}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s \overline{g_{k,1}(w)}\, dw, \\
&r_{2,k}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} g_{k,2}(w)\, dw,\ r_{2,k+3}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} \overline{g_{k,2}(w)}\, dw, \\
&r_{2,k+6}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} g_{k,3}(w)\, dw,\ r_{2,k+9}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{2iw}{\varepsilon^2}} \overline{g_{k,3}(w)}\, dw, \\
&r_{0,k+3}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s g_{k,2}(w)\, dw,\ r_{0,k}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s \overline{g_{k,2}(w)}\, dw,
\end{aligned}
$$

$$r_{0,k+9}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s g_{k,3}(w)\,dw,\ r_{0,k+6}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s \overline{g_{k,3}(w)}\,dw,$$
$$p_{k,2}(s) = e^{\frac{-is}{\varepsilon^2}} \int_0^s e^{\frac{(5-2k)iw}{\varepsilon^2}} w^2\,dw,\ g_{k,1}(w) = p_{k,1}(w) - wp_k(w),$$
$$g_{k,2}(w) = q_{2,k}(w) - \overline{q_{0,k}(w)}, \quad g_{k,3}(w) = q_{2,k+3}(w) - \overline{q_{0,k+3}(w)}.$$

From the first order terms in $\delta_+^{n,1}$ (5.3), we can directly verify that the coefficients $p_k(s) = O(\varepsilon^2)$ $(k = 1, 2, 3)$ and formally $\delta_+^{n,1}(s) = O(\varepsilon^2)$. Noticing the coefficients in the next order terms $\delta_+^{n,2}$ and $\delta_+^{n,3}$, we could similarly obtain that $\delta_+^{n,2}(s), \delta_+^{n,3}(s) = O(\varepsilon^2)$. Therefore, we could observe that the NPI methods converge to the linear term $\psi_+^{n+1} \approx e^{-i\mathcal{D}_\varepsilon \tau}\psi_+^n$ in the limit $\varepsilon \to 0^+$, which coincides with the analysis in [27].

We remark here that all the coefficients can be evaluated exactly and precomputed in practical simulations. Compared with third order NPI (see Appendix) for the cubic NLKG with general initial data, the above third order NPI is much simpler for the real-valued quadratic NLKG.

6. Numerical experiments

In this section, we present numerical tests on the proposed NPI methods and compare the performances of different numerical methods. In addition, we apply the NPI method investigate the nonrelativisitic limits of cubic NLKG (1.1) and quadratic NLKG (5.1).

For numerical purpose, we focus on the equations (1.1) and (5.1) in 1D, and the numerical methods are programmed using Matlab and executed on an Intel i5-5200U 2.7GHz CPU laptop.

6.1. Spatial/temporal resolution.

We first test the temporal and spatial discretization error of the proposed NPI method, including the first-order NPI, second-order NPI and the third-order NPI. The two sets of initial data for NLKG are considered, i.e. the real-valued initial data ($\lambda = 1$)

$$\psi_0(x) = \frac{1}{2}\frac{\cos(3x)^2\sin(2x)}{2-\cos(x)}, \quad \psi_1(x) = \frac{1}{2}\frac{\sin(x)\cos(2x)}{2-\cos(x)}, \tag{6.1}$$

and the complex-valued initial data ($\lambda = -1$)

$$\psi_0(x) = \frac{2+i}{\sqrt{5}}\cos(x), \quad \psi_1(x) = \frac{1+i}{\sqrt{2}}\sin(x) + \frac{1}{2}\cos(x). \tag{6.2}$$

The computational domain is set as the interval $\Omega = [-\pi, \pi]$ with periodic boundary conditions on $\partial\Omega$. The discretization is prescribed in section 4. The 'exact' solution ψ_e is obtained numerically by the third-order NPI method with very fine mesh sizes, e.g. $\tau = 10^{-4},\ h = 2\pi/2^8$.

Denote $\psi_{h,\tau}^n$ as the numerical solution obtained by a numerical method with mesh size h and time step τ. In order to quantify the numerical solutions, we introduce the l^2 error function at time t_n as

$$e_{h,\tau}(t_n) = \sqrt{h\sum_{j=0}^{M-1} |(\psi_{h,\tau})_j^n - (\psi_e)_j^n|^2}. \tag{6.3}$$

Tables 1&2 list the spatial errors of the second order NPI for the cubic NLKG (1.1) with complex-valued initial data (6.2) and the quadratic NLKG (2) with real-valued initial data (6.1), respectively. Spatial spectral accuracies are clear. Similar results have been observed for the first and the third order NPI methods, and details are omitted here for brevity.

For temporal error analysis, the mesh size h is fixed as $h = 2\pi/2^8$ ($M = 256$) such that the spatial discretization error is negligible. Figures 1, 2 and 3 depict the errors $e_{h,\tau}(T = 1)$ (6.3) of the proposed NPI methods applied to the cubic NLKG (1.1) with initial value (6.1)(Fig. A) and (6.2)(Fig. B) for different τ and ε, where uniform convergence rates are confirmed.

For the quadratic NLKG (5.1), it has been shown that the equation converges to the linear Schrödinger equations in the limit $\varepsilon \to 0^+$ [27], and we expect the temporal errors of NPI methods for the quadratic NLKG (5.1) would behave as $O(\varepsilon^2)$ for $0 < \varepsilon \ll 1$. Tables 3, 4 and 5 show the temporal errors of the first-order, second-order and third-order NPI methods for the quadratic NLKG (5.1) with (6.1), respectively. From the top rows in Tables 3, we could verify the convergence rate for the first-order NPI method; from the bottom rows, due to the fact that the temporal errors are bounded by $\min\{O(\tau), O(\varepsilon^2)\}$, the errors tend to zero when either $\varepsilon \to 0^+$ or $\tau \to 0^+$. Similar phenomenon is observed for the second-order and third-order NPI methods.

TABLE 1. Spatial errors of the second-order NPI method for the cubic NLKG (1.1) with (6.2) at $T = 1$ under $\tau = \frac{1}{10^5}$, $h = 2\pi/M$.

$e_{h,\tau}(T)$	$M = 8$	$M = 16$	$M = 32$
$\varepsilon = 1$	2.40E-3	1.82E-6	1.20E-11
$\varepsilon = 1/2^2$	5.00E-3	3.82E-7	3.10E-11
$\varepsilon = 1/2^4$	3.30E-3	4.44E-7	5.57E-11
$\varepsilon = 1/2^6$	5.70E-3	6.36E-7	3.36E-11
$\varepsilon = 1/2^8$	5.30E-3	6.39E-7	3.32E-11
$\varepsilon = 1/2^{10}$	6.50E-3	3.88E-7	8.26E-11

TABLE 2. Spatial errors of the second-order NPI method for the quadratic NLKG (5.1) with (6.1) at $T = 1$ under $\tau = \frac{1}{10^5}$, $h = 2\pi/M$.

$e_{h,\tau}(T)$	$M = 8$	$M = 16$	$M = 32$	$M = 64$
$\varepsilon = 1$	6.88E-2	5.83E-2	3.06E-5	6.19E-12
$\varepsilon = 1/2^2$	3.10E-2	3.07E-2	7.56E-6	1.41E-11
$\varepsilon = 1/2^4$	4.59E-2	3.75E-2	2.07E-6	4.46E-12
$\varepsilon = 1/2^6$	4.63E-2	2.13E-2	2.14E-7	3.57E-12
$\varepsilon = 1/2^8$	4.92E-2	2.15E-2	4.43E-7	4.81E-12
$\varepsilon = 1/2^{10}$	6.77E-2	6.68E-2	2.79E-7	1.09E-11

6.2. **Comparison of different methods.** We consider the cubic NLKG (1.1) with $\lambda = 1$ and the initial data

$$u_0(x) = \frac{3\sin(x)}{e^{\frac{x^2}{2}} + e^{-\frac{x^2}{2}}}, \quad u_1(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}, \quad x \in \mathbb{R}, \tag{6.4}$$

TABLE 3. Temporal errors of the first-order NPI method for the quadratic NLKG (5.1) with (6.1) at $T = 1$ under $h = 2\pi/2^8$.

$e_{h,\tau}(T)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon = 1$	1.10E-3	5.30E-4	2.62E-4	1.30E-4	6.46E-5	3.22E-5	1.61E-5
$\varepsilon = 1/2^2$	1.90E-3	5.32E-4	2.52E-4	1.24E-4	6.16E-5	3.06E-5	1.53E-5
$\varepsilon = 1/2^4$	3.33E-4	2.39E-4	2.22E-4	4.46E-5	2.25E-5	9.35E-6	4.38E-6
$\varepsilon = 1/2^6$	1.36E-5	1.36E-5	1.06E-5	5.46E-6	4.95E-6	4.32E-6	3.98E-6
$\varepsilon = 1/2^8$	8.31E-7	7.37E-7	9.06E-7	2.31E-7	1.94E-7	1.84E-7	1.78E-7
$\varepsilon = 1/2^{10}$	1.42E-7	1.23E-7	3.47E-8	1.96E-8	1.91E-8	9.25E-9	9.10E-9

TABLE 4. Temporal errors of the second-order NPI method for the quadratic NLKG (5.1) with (6.1) at $T = 1$ under $h = 2\pi/2^8$.

$e_{h,\tau}(T)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon = 1$	1.51E-4	2.80E-5	7.19E-6	1.93E-6	5.06E-7	1.30E-7	3.28E-8
$\varepsilon = 1/2^2$	1.30E-3	2.16E-4	6.29E-5	1.54E-5	3.78E-6	9.37E-7	2.33E-7
$\varepsilon = 1/2^4$	3.47E-4	1.85E-4	1.03E-4	7.74E-6	1.24E-6	2.83E-7	6.85E-8
$\varepsilon = 1/2^6$	1.73E-5	1.40E-5	3.00E-6	4.66E-6	7.63E-7	8.40E-7	5.34E-7
$\varepsilon = 1/2^8$	7.06E-7	1.11E-6	7.72E-7	4.27E-8	1.56E-8	5.66E-9	2.69E-9
$\varepsilon = 1/2^{10}$	1.34E-7	1.57E-7	1.88E-8	1.59E-8	9.81E-9	3.26E-10	1.42E-10

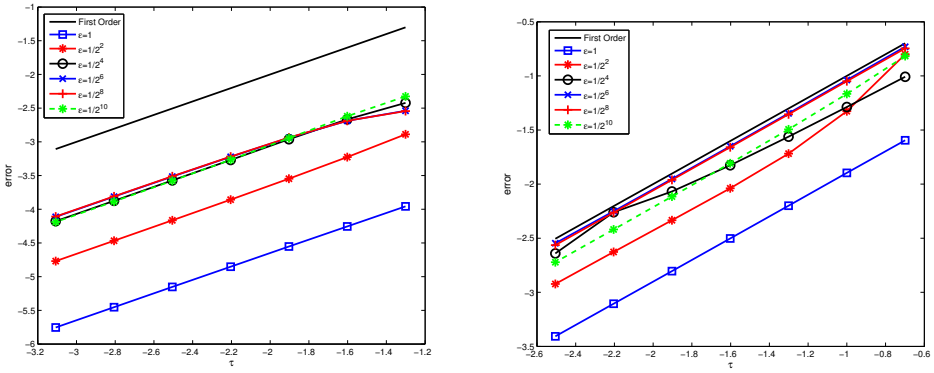
TABLE 5. Temporal errors of the third-order NPI method for quadratic NLKG (5.1) with (6.1) at $T = 1$ under $h = 2\pi/2^8$.

$e_{h,\tau}(T)$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon = 1$	2.49E-5	3.14E-6	4.38E-7	5.56E-8	6.93E-9	8.64E-10	1.08E-10
$\varepsilon = 1/2^2$	1.00E-3	8.26E-5	7.56E-6	6.07E-7	7.06E-8	8.67E-9	1.07E-9
$\varepsilon = 1/2^4$	2.81E-4	1.40E-4	3.14E-5	1.66E-6	1.17E-7	1.00E-8	1.17E-9
$\varepsilon = 1/2^6$	1.41E-5	9.28E-6	2.47E-6	2.86E-6	2.28E-7	7.71E-8	1.89E-8
$\varepsilon = 1/2^8$	6.31E-7	8.22E-7	2.42E-7	1.42E-8	1.48E-9	1.62E-10	3.57E-11
$\varepsilon = 1/2^{10}$	1.21E-7	1.44E-7	7.26E-9	5.78E-9	9.45E-10	2.88E-11	2.10E-11

where the computational domain is chosen as $[-32, 32]$ with periodic boundary conditions. Table 6 compares the performances of the four numerical methods (including EWI-FP [3],TS-FP [15],IEI-FP [7] and second-order NPI method) in classical regime i.e. $\varepsilon = 1$ and the limit regime($\varepsilon = 10^{-4}$), together with the computational time. For ease of comparison, we present the efficiency plots in Figure 4.

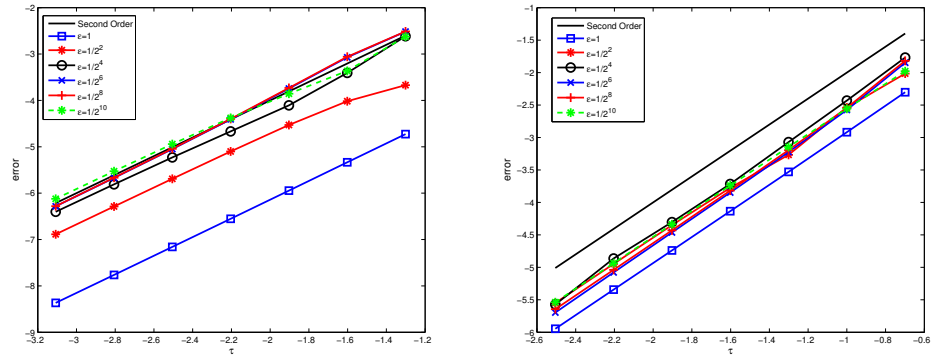
Based on the results in Table 6 and Figure 4, we can draw the following conclusions:
(1). Among all the four methods, for the relativistic regime ($\varepsilon = 1$), EWI-FP and TSFP are the most accurate and efficient methods(cf. Fig. 4(A)).
(2). IEI-FP and NPI methods are uniformly accurate and more efficient (cf. Fig. 4(B)) for varying $\varepsilon \in (0, 1]$.
(3). Compared to IEI-FP, NPI method is more accurate under the same CPU time.

6.3. **Convergence of the NLKG** (1.1)/(5.1) **to the limit models.** Here, we apply the third-order NPI method to study numerically the convergence rate from the problem (1.1)/ (5.1) to its limiting system [7] as $\varepsilon \to 0$, i.e., $\psi(x,t) \to z(x,t) = \frac{1}{2}(e^{it/\varepsilon^2} u_\infty(x,t) + e^{-it/\varepsilon^2} \overline{v}_\infty(x,t))$. For the cubic NLKG (1.1), (u_∞, v_∞) satisfies



(A) (B)

FIGURE 1. The temporal errors at $T = 1$ of the first-order NPI method for the cubic NLKG (1.1) with the initial value (6.1) (left) and (6.2) (right).



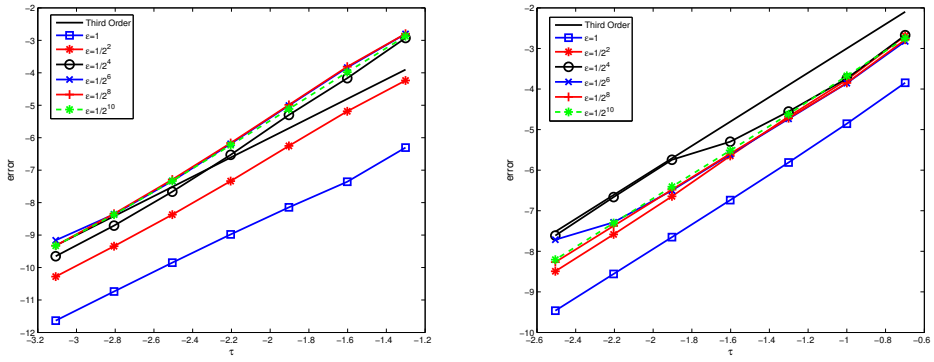
(A) (B)

FIGURE 2. The temporal errors at $T = 1$ of the second-order NPI method for the cubic NLKG (1.1) with the initial value (6.1) (left) and (6.2) (right).

the coupled cubic Schrödinger system

$$
\begin{aligned}
i\partial_t u_\infty &= \frac{1}{2}\Delta u_\infty + \frac{\lambda}{8}(|u_\infty|^2 + 2|v_\infty|^2)u_\infty,\ x \in \mathbb{R},\, t > 0,\\
i\partial_t v_\infty &= \frac{1}{2}\Delta v_\infty + \frac{\lambda}{8}(|v_\infty|^2 + 2|u_\infty|^2)v_\infty,\ x \in \mathbb{R},\, t > 0,
\end{aligned}
\tag{6.5}
$$

with initial data $u_\infty(t = 0) = \psi_0 - i\psi_1,\ v_\infty(t = 0) = \overline{\psi}_0 - i\overline{\psi}_1$. We take $\lambda = 1$ in the problem (1.1) with initial data (6.4).



(A) (B)

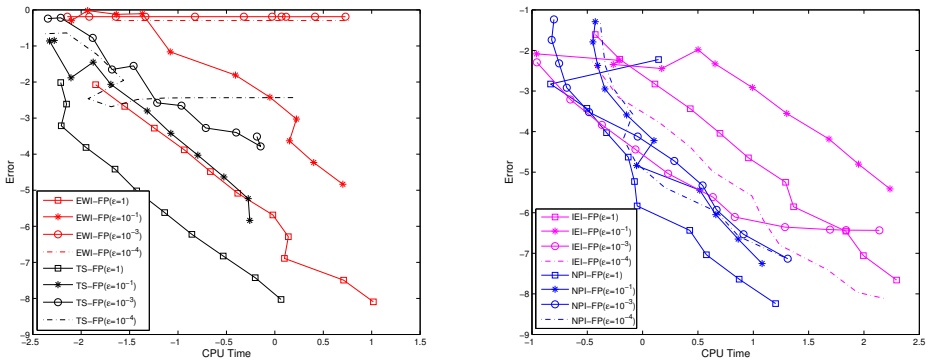
FIGURE 3. The temporal errors at $T = 1$ of the third-order NPI method for the cubic NLKG (1.1) with the initial value (6.1) (left) and (6.2) (right).

TABLE 6. Comparison of temporal errors and their corresponding CPU time(seconds) of different methods for the cubic NLKG (1.1) with (6.4) at $T = 1$ under $h = 1/16$.

$e_{h,\tau}(t_n = 1), \varepsilon = 1$	$\tau = 0.2$	$\tau/2^2$	$\tau/2^4$	$\tau/2^6$	$\tau/2^8$	$\tau/2^{10}$
EWI-FP	8.40E-3	5.26E-4	3.29E-5	2.01E-6	1.28E-7	8.05E-9
time(cpu)	5.83E-2	1.18E-1	3.43E-1	1.43	5.39	21.4
TS-FP	9.70E-3	6.12E-4	3.83E-5	2.39E-6	1.50E-7	9.35E-9
time(cpu)	2.57E-2	2.19E-2	5.06E-2	1.93E-1	6.98E-1	2.52
IEI-FP	2.47E-2	1.50E-3	9.07E-5	5.63E-6	3.51E-7	2.19E-8
time(cpu)	7.02E-1	2.23	9.02	36.2	144.9	549.7
NPI(second)	6.00E-3	3.74E-4	2.35E-5	1.47E-6	9.21E-8	5.76E-9
time(cpu)	1.53	1.43	2.07	4.14	12.8	48.7
$e_{h,\tau}(t_n = 1), \varepsilon = 10^{-4}$	$\tau = 0.2$	$\tau/2^2$	$\tau/2^4$	$\tau/2^6$	$\tau/2^8$	$\tau/2^{10}$
EWI-FP	5.06E-1	5.06E-1	5.06E-1	5.06E-1	5.06E-1	5.03E-1
time(cpu)	4.00E-2	1.57E-1	3.65E-1	2.56	5.73	23.0
TS-FP	2.18E-1	5.93E-2	3.40E-3	3.30E-3	3.30E-3	3.70E-3
time(cpu)	2.49E-2	7.57E-2	7.66E-2	2.74E-1	9.15E-1	3.68
IEI-FP	5.30E-3	1.68E-4	1.04E-5	6.49E-7	3.91E-8	7.63E-9
time(cpu)	5.91E-1	2.35	9.36	35.2	141.5	544.5
NPI(second)	4.65E-2	4.20E-3	2.67E-4	1.68E-5	1.05E-6	6.63E-8
time(cpu)	1.32	1.52	1.97	4.17	12.5	44.9

The problem (1.1) is solved numerically on an interval $\Omega = [-32, 32]$ with periodic boundary conditions. Figure 5(A) shows the error between $z(x,t)$ and $\psi(x,t)$, where $\psi(x,t)$ is numerically obtained by the third-order NPI method with $\tau = 10^{-4}, h = 1/16$ and $z(x,t)$ is computed by the time-splitting Fourier pseudospectral method [15] with $\tau = 10^{-5}, h = 1/16$. As shown in Figure 5(A), the solution of the cubic NLKG (1.1) converges to that of the limit system (6.5) quadratically in ε, i.e.

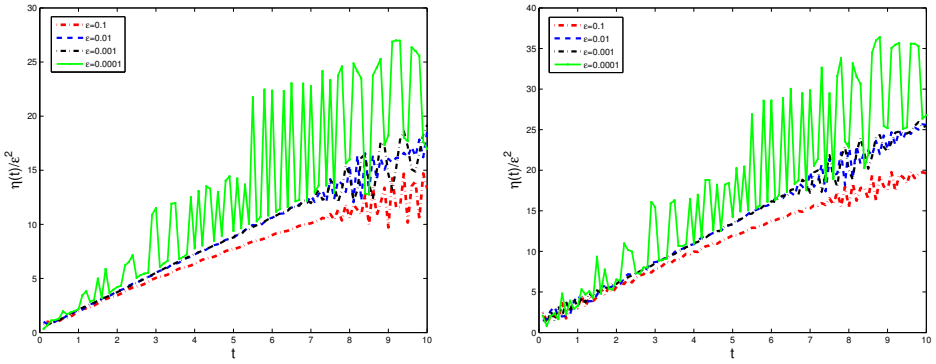
$$\eta(t) := \|\psi(\cdot,t) - z(\cdot,t)\|_{L^2} \le (C_1 + C_2 T)\varepsilon^2, \ 0 \le t \le T,$$



(A) (B)

FIGURE 4. Efficiency comparisons (accuracy v.s. computational time) of different second-order-in-time methods with varying ε (c.f. Table 6).

where C_1 and C_2 are two positive constants independent of ε and T.



(A) (B)

FIGURE 5. Time evolution of $\eta(t)$ for the initial value (6.4) of the cubic NLKG (1.1)(left) and the quadratic NLKG(5.1)(right) under different ε.

Lastly, we investigate the quadratic NLKG (5.1) with $f(\psi) = \psi^2$, where the limit model is the linear Schrödinger equations [27], e.g. the system for (u_∞, v_∞) is (6.5) without the cubic nonlinear terms. Figure 5(B) shows the error between $z(x,t)$ and $\psi(x,t)$, where $\psi(x,t)$ is computed by the third-order NPI method ($\tau = 10^{-4}, h = 1/16$, and computational domain $\Omega = [-32, 32]$) and $z(x,t)$ is obtained by the exponential wave integrator Fourier pseudospectral method with $h = 1/16$ (linear system can be integrated exactly in time). As shown in Figure 5(B), the

quadratic NLKG (5.1) converges to the linear Schrödinger system quadratically in ε.

7. Conclusions

We proposed uniformly accurate NPI methods for the NLKG in the nonrelativistic limit regime. The strategy allows to construct uniformly accurate arbitrary high order in time methods. Detailed constructions of NPI methods were shown for the cubic/quadratic NLKG up to the third order in time. The key idea is to separate the oscillatory factor $e^{\mp iw/\varepsilon^2}$ from the non-oscillatory differential operator part $e^{is\mathcal{D}}$, and integrate the former exactly. The uniform temporal accuracy of the NPI methods can be improved by the Picard iteration. The resulting coefficients in the NPI schemes can be easily computed by the symbolic integration in Matlab. The rigorous error analysis of the arbitrary k-th order NPI method was carried out and numerical results confirmed the uniform convergence rates in time for NPI methods wr.t. $0 < \varepsilon \leq 1$. The idea of NPI methods can be applied to the similar problems, such as the Klein-Gordon-Zakharov equation in the high plasma frequency limit regime. In addition, how to implement high oder (≥ 3) NPI methods in a more efficient way will be considered in our future work.

8. Data availability statement

The codes and datas during the current study are available at `https://github.com/xuanxuanzhou/NPI-method-matlab-code-for-KG`

Appendix A. Details of the third-order NPI method

Here, we shall give the details of programming by using Matlab R2012a. At first, let $\psi_{\pm}^{n+1} = \psi_{\pm}^{n,3} := e^{\mp i\mathcal{D}_\varepsilon \tau}\psi_{\pm}^n + \delta_{\pm}^{n,1}(\tau) + \delta_{\pm}^{n,2}(\tau) + \delta_{\pm}^{n,3}(\tau)$, can be stated as below by specifying $\delta_{\pm}^{n,3}$, i.e. evaluating (2.22) for $k = 3$,

$$
\begin{aligned}
&\delta_{\pm}^{n,3}(s) = \\
&s^2 p_{-2}(\pm s)\frac{1}{2}\mathcal{B}^2\mathcal{F}_{1,\pm}^n + s^2 p_0(\pm s)\frac{1}{2}\mathcal{B}^2\mathcal{F}_{2,\pm}^n + s^2 p_2(\pm s)\frac{1}{2}\mathcal{B}^2\mathcal{F}_{2,\mp}^n + s^2 p_4(\pm s)\frac{1}{2}\mathcal{B}^2\mathcal{F}_{1,\mp}^n \\
&+ \sum_{k=1}^{6}\sum_{\sigma=\pm}[(\mp s q_{k,\sigma}(\pm s) + q_{k,1,\sigma}(\pm s))\mathcal{B}\mathcal{F}_{2,k,\pm\sigma}^n \pm q_{k,1,\sigma}(\pm s)\mathcal{F}_{3,k,\pm\sigma}^n] \\
&+ p_{-2,2}(\pm s)(1/2\mathcal{B}^2\mathcal{F}_{1,\pm}^n \pm \mathcal{B}\mathcal{G}_{3,\pm}^n + \mathcal{G}_{1,3,\pm}^n + \mathcal{E}_{1,\pm}^n) \\
&+ p_{0,2}(\pm s)(1/2\mathcal{B}^2\mathcal{F}_{2,\pm}^n \pm \mathcal{B}\mathcal{G}_{4,\pm}^n + \mathcal{G}_{2,3,\pm}^n + \mathcal{E}_{2,\pm}^n) \\
&+ p_{2,2}(\pm s)(1/2\mathcal{B}^2\mathcal{F}_{2,\mp}^n \pm \mathcal{B}\mathcal{G}_{4,\mp}^n + \mathcal{G}_{2,3,\mp}^n + \mathcal{E}_{2,\mp}^n) \\
&+ p_{4,2}(\pm s)(1/2\mathcal{B}^2\mathcal{F}_{1,\mp}^n \pm \mathcal{B}\mathcal{G}_{3,\mp}^n + \mathcal{G}_{1,3,\mp}^n + \mathcal{E}_{1,\mp}^n) \\
&+ p_{-2,1}(\pm s)(\mp s\mathcal{B}^2\mathcal{F}_{1,\pm}^n - s\mathcal{B}\mathcal{G}_{3,\pm}^n) + p_{0,1}(\pm s)(\mp s\mathcal{B}^2\mathcal{F}_{2,\pm}^n - s\mathcal{B}\mathcal{G}_{4,\pm}^n) \\
&+ p_{2,1}(\pm s)(\mp s\mathcal{B}^2\mathcal{F}_{2,\mp}^n - s\mathcal{B}\mathcal{G}_{4,\mp}^n) + p_{4,1}(\pm s)(\mp s\mathcal{B}^2\mathcal{F}_{1,\mp}^n - s\mathcal{B}\mathcal{G}_{3,\mp}^n) \\
&+ \sum_{k=1}^{4}\sum_{\sigma_1=\pm}\sum_{\sigma_2=\pm}(r_{k,\sigma_1,\sigma_2}(\pm s)\mathcal{H}_{k,\pm,\pm\sigma_1,\pm\sigma_2}^n + r_{k+4,\sigma_1,\sigma_2}(\pm s)\mathcal{H}_{k,\mp,\pm\sigma_1,\pm\sigma_2}^n) \\
&+ \sum_{k=1}^{6}\sum_{\sigma=\pm}[q_{k,2,\sigma}(\pm s)\mathcal{F}_{4,k,\pm\sigma}^n \pm q_{k,4,\sigma}(\pm s)\mathcal{F}_{4,k+6,\pm\sigma}^n + q_{k,3,\sigma}(\pm s)\mathcal{F}_{5,k,\pm\sigma}^n]
\end{aligned}
$$

$$+\sum_{j=1}^{3}\sum_{k=1}^{6}\sum_{\sigma=\pm} m_{j,k,\sigma}(\pm s)\mathcal{F}^n_{6,j,k,\pm\sigma},$$

where for $m=1,2$ and $\sigma_1,\sigma_2=\pm$,

$$\begin{aligned}
\mathcal{G}^n_{1,3,\pm} &= \mathcal{A}\left(\frac{1}{2}(\psi^n_\pm)^2\overline{\mathcal{B}^2\psi^n_\mp} + (\mathcal{B}^2\psi^n_\pm)\psi^n_\pm\overline{\psi^n_\mp}\right),\\
\mathcal{G}^n_{2,3,\pm} &= \mathcal{A}\Bigg(\psi^n_\pm\overline{\psi^n_\mp}(\mathcal{B}^2\psi^n_\mp) + (|\psi^n_\pm|^2+|\psi^n_\mp|^2)(\mathcal{B}^2\psi^n_\pm)\\
&\qquad + \frac{1}{2}(\psi^n_\pm)^2\overline{\mathcal{B}^2\psi^n_\pm} + \psi^n_\pm\psi^n_\mp\overline{(\mathcal{B}^2\psi^n_\mp)}\Bigg),\\
\mathcal{F}^n_{3,m,\pm} &= \mathcal{A}\left(2(\mp\psi^n_\mp\overline{\mathcal{B}\psi^n_\pm} \pm \overline{\psi^n_\pm}\mathcal{B}\psi^n_\mp)\mathcal{F}^n_{m,\mp} - 2(\pm\psi^n_\mp\mathcal{B}\psi^n_\mp)\overline{\mathcal{F}^n_{m,\pm}}\right),\\
\mathcal{F}^n_{3,m+2,\pm} &= \mathcal{A}\Bigg(2(\psi^n_-\overline{\mathcal{B}\psi^n_-} - \psi^n_+\overline{\mathcal{B}\psi^n_+} - \overline{\psi}^n_+\mathcal{B}\psi^n_+ + \overline{\psi}^n_-\mathcal{B}\psi^n_-)\mathcal{F}^n_{m,\mp}\\
&\qquad - 2(\psi^n_+\mathcal{B}\psi^n_- - \psi^n_-\mathcal{B}\psi^n_+)\overline{\mathcal{F}^n_{m,\pm}}\Bigg),\\
\mathcal{F}^n_{3,m+4,\pm} &= \mathcal{A}\left(2(\pm\psi^n_\pm\overline{\mathcal{B}\psi^n_\mp} \mp \overline{\psi^n_\mp}\mathcal{B}\psi^n_\pm)\mathcal{F}^n_{m,\mp} - 2(\mp\psi^n_\pm\mathcal{B}\psi^n_\pm)\overline{\mathcal{F}^n_{m,\pm}}\right),\\
\mathcal{E}^n_{1,\pm} &= \mathcal{A}(-2\psi^n_\pm(\mathcal{B}\psi^n_\pm)\overline{\mathcal{B}\psi^n_\mp} + \overline{\psi^n_\mp}(\mathcal{B}\psi^n_\pm)^2),\\
\mathcal{E}^n_{2,\pm} &= \mathcal{A}\Bigg(2\psi^n_\pm|\mathcal{B}\psi^n_\mp|^2 + 2\psi^n_\pm|\mathcal{B}\psi^n_\pm|^2 - 2\psi^n_\mp(\mathcal{B}\psi^n_\pm)\overline{\mathcal{B}\psi^n_\mp}\\
&\qquad - 2\overline{\psi^n_\mp}(\mathcal{B}\psi^n_\pm)\mathcal{B}\psi^n_\mp + \overline{\psi^n_\pm}(\mathcal{B}\psi^n_\pm)^2\Bigg),\\
\mathcal{H}^n_{1,\pm,\sigma_1,\sigma_2} &= \mathcal{A}(-2\psi^n_\pm F^n_{1,\sigma_1}\overline{F^n_{1,-\sigma_2}} + \overline{\psi^n_\mp}F^n_{1,\sigma_1}F^n_{1,\sigma_2}),\\
\mathcal{H}^n_{2,\pm,\sigma_1,\sigma_2} &= \mathcal{A}(-2\psi^n_\pm F^n_{1,\sigma_1}\overline{F^n_{2,-\sigma_2}} + \overline{\psi^n_\mp}F^n_{1,\sigma_1}F^n_{2,\sigma_2}),\\
\mathcal{H}^n_{3,\pm,\sigma_1,\sigma_2} &= \mathcal{A}(-2\psi^n_\pm F^n_{2,\sigma_1}\overline{F^n_{1,-\sigma_2}} + \overline{\psi^n_\mp}F^n_{2,\sigma_1}F^n_{1,\sigma_2}),\\
\mathcal{H}^n_{4,\pm,\sigma_1,\sigma_2} &= \mathcal{A}(-2\psi^n_\pm F^n_{2,\sigma_1}\overline{F^n_{2,-\sigma_2}} + \overline{\psi^n_\mp}F^n_{2,\sigma_1}F^n_{2,\sigma_2}),
\end{aligned}$$

and the rest nonlinear terms are described below

$$\begin{aligned}
\mathcal{F}^n_{4,m,\pm} &= \mathcal{A}\left(2\psi^n_\mp\overline{\psi^n_\pm}\mathcal{G}^n_{m,\mp} + (\psi^n_\mp)^2\overline{\mathcal{G}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{4,m+2,\pm} &= \mathcal{A}\left(2(|\psi^n_+|^2+|\psi^n_-|^2)\mathcal{G}^n_{m,\mp} + 2\psi^n_+\psi^n_-\overline{\mathcal{G}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{4,m+4,\pm} &= \mathcal{A}\left(2\psi^n_\pm\overline{\psi^n_\mp}\mathcal{G}^n_{m,\mp} + (\psi^n_\pm)^2\overline{\mathcal{G}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{4,m+6,\pm} &= \mathcal{A}\left(2\psi^n_\mp\overline{\psi^n_\pm}\mathcal{G}^n_{m,\mp} - (\psi^n_\mp)^2\overline{\mathcal{G}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{4,m+8,\pm} &= \mathcal{A}\left(2(|\psi^n_+|^2+|\psi^n_-|^2)\mathcal{G}^n_{m,\mp} - 2\psi^n_+\psi^n_-\overline{\mathcal{G}^n_{m,\pm}}\right), m=1,2,\\
\mathcal{F}^n_{4,m+10,\pm} &= \mathcal{A}\left(2\psi^n_\pm\overline{\psi^n_\mp}\mathcal{G}^n_{m,\mp} - (\psi^n_\pm)^2\overline{\mathcal{G}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{5,m,\pm} &= \mathcal{A}\left(2\psi^n_\mp\overline{\psi^n_\pm}\mathcal{B}\mathcal{F}^n_{m,\mp} + (\psi^n_\mp)^2\overline{\mathcal{B}\mathcal{F}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{5,m+2,\pm} &= \mathcal{A}\left(2(|\psi^n_+|^2+|\psi^n_-|^2)\mathcal{B}\mathcal{F}^n_{m,\mp} + 2\psi^n_+\psi^n_-\overline{\mathcal{B}\mathcal{F}^n_{m,\pm}}\right), m=1,2,\\
\mathcal{F}^n_{5,m+4,\pm} &= \mathcal{A}\left(2\psi^n_\pm\overline{\psi^n_\mp}\mathcal{B}\mathcal{F}^n_{m,\mp} + (\psi^n_\pm)^2\overline{\mathcal{B}\mathcal{F}^n_{m,\pm}}\right), \quad m=1,2,\\
\mathcal{F}^n_{6,1,k,\pm} &= \mathcal{A}\left(2(|\psi^n_+|^2+|\psi^n_-|^2)\mathcal{F}^n_{2,k,\pm} + 2\psi^n_+\psi^n_-\overline{\mathcal{F}^n_{2,k,\mp}}\right), k=1,2,\ldots,6,\\
\mathcal{F}^n_{6,2,k,\pm} &= \mathcal{A}\left(2\psi^n_\mp\overline{\psi^n_\pm}\mathcal{F}^n_{2,k,\pm} + (\psi^n_\mp)^2\overline{\mathcal{F}^n_{2,k,\mp}}\right), \quad k=1,2,\ldots,6,
\end{aligned}$$

$$\mathcal{F}^n_{6,3,k,\pm} = \mathcal{A}\left(2\psi^n_\pm\overline{\psi^n_\mp}\mathcal{F}^n_{2,k,\pm} + (\psi^n_\pm)^2\overline{\mathcal{F}^n_{2,k,\mp}}\right), \quad k = 1, 2, \ldots, 6.$$

Finally, the coefficients are given by $p_{0,2}(s) = e^{\frac{-is}{\varepsilon^2}}\frac{s^3}{3}$, $p_{\pm 2,2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s w^2 e^{\frac{\pm 2iw}{\varepsilon^2}}\,dw$, $p_{4,2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s w^2 e^{\frac{4iw}{\varepsilon^2}}\,dw$ and

$$q_{1+k,1,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} w g_{1,1}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$q_{2+k,1,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} w g_{2,1}(\pm w)\,dw, k = 0, 2, 4,$$

$$g_{1,1}(\pm w) = p_{-2}(\mp w) + p_4(\pm w),\ g_{2,1}(\pm w) = p_2(\mp w) + p_0(\pm w),$$

$$q_{1+k,2,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} g_{1,2}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$q_{2+k,2,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} g_{2,2}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$g_{1,2}(\pm w) = p_{-2,1}(\mp w) + p_{4,1}(\pm w),\ g_{2,2}(\pm w) = p_{2,1}(\pm w) + p_{0,1}(\mp w),$$

$$q_{1+k,3,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} g_{1,3}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$q_{2+k,3,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} g_{2,3}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$g_{1,3}(\pm w) = w(\pm p_{-2}(\mp w) \mp p_4(\pm w)),\ g_{2,3}(\pm w) = w(\mp p_2(\pm w) \pm p_0(\mp w)),$$

$$q_{1+k,4,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} g_{1,4}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$q_{2+k,4,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm(2-k)iw}{\varepsilon^2}} g_{1,4}(\pm w)\,dw,\ k = 0, 2, 4,$$

$$g_{1,4}(\pm w) = \mp p_{-2,1}(\mp w) \pm p_{4,1}(\pm w),\ g_{2,4}(\pm w) = \pm p_{2,1}(\pm w) \mp p_{0,1}(\mp w),$$

$$r_{1+m,\sigma_1,\sigma_2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s g_{1+\frac{m}{2},1}(\sigma_1 w) g_{1,1}(\sigma_2 w)\,dw, \quad m = 0, 2$$

$$r_{2+m,\sigma_1,\sigma_2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s g_{1+\frac{m}{2},1}(\sigma_1 w) g_{2,1}(\sigma_2 w)\,dw, \quad m = 0, 2$$

$$r_{5+m,\sigma_1,\sigma_2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{2iw}{\varepsilon^2}} g_{1+\frac{m}{2},1}(\sigma_1 w) g_{1,1}(\sigma_2 w)\,dw, \quad m = 0, 2,$$

$$r_{6+m,\sigma_1,\sigma_2}(s) = e^{\frac{-is}{\varepsilon^2}}\int_0^s e^{\frac{2iw}{\varepsilon^2}} g_{1+\frac{m}{2},1}(\sigma_1 w) g_{2,1}(\sigma_2 w)\,dw, \quad m = 0, 2,$$

$$m_{1,k,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} g_{k,6}(w)\,dw,\ m_{2,k,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\pm 2iw}{\varepsilon^2}} g_{k,6}(w)\,dw,$$

$$m_{3,k,\pm}(s) = \int_0^s e^{\frac{-i(s-w)}{\varepsilon^2}} e^{\frac{\mp 2iw}{\varepsilon^2}} g_{k,6}(w)\,dw,\ g_{k,6}(w) = q_{k,\pm}(w) + q_{k,\mp}(-w),\ 1 \le k \le 6.$$

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